Study of $\Theta^+(udud\bar{s})$ in lattice QCD with exact chiral symmetry

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We investigate the mass spectrum of the pentaquark baryon $(udud\bar{s})$ in quenched lattice QCD with exact chiral symmetry. Using three different interpolating operators for Θ , we measure the 3 × 3 correlation matrix and obtain the eigenvalues $A^{\pm}(t)$ with \pm parity for 100 gauge configurations generated with Wilson gauge action at $\beta = 6.1$ on the $20^3 \times 40$ lattice. For the lowest-lying $J^P = 1/2^-$ state, its mass is almost identical to that of the KN s wave, while for the lowest-lying $J^P = 1/2^+$ state, its mass is smaller than that of the KN p wave, especially for the regime $m_u < m_s$. By chiral extrapolation (linear in m_{π}^2) to $m_{\pi} = 135$ MeV, we obtain the masses of the lowest-lying states: $m(1/2^-) = 1424(57)$ MeV and $m(1/2^+) = 1562(121)$ MeV, in agreement with the masses of $m_K + m_N \approx 1430$ MeV and $\Theta^+(1540)$, respectively.

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I. INTRODUCTION

The recent experimental observation of the exotic baryon $\Theta^+(1540)$ (with the quantum numbers of K^+n) by LEPS Collaboration[1] at Spring-8—and the subsequent confirmation [2–8] from some experimental groups—has become one of the most interesting topics in hadron physics. The remarkable features of $\Theta^+(1540)$ are its strangeness S = +1 and its exceptionally narrow decay width (< 15 MeV) even though it is ~100 MeV above the *KN* threshold. Its strangeness S = +1 immediately implies that it cannot be an ordinary baryon composed of three quarks. Its minimal quark content is *ududs*. Nevertheless, there are quite a number of experiments [9] which so far have *not* observed $\Theta^+(1540)$ or any pentaquarks. This casts some doubts about the existence of $\Theta^+(1540)$.

Historically, the experimental search for $\Theta^+(1540)$ was motivated by the predictions of the chiral-soliton model [10], an outgrowth of the Skyrme model [11]. Even though the chiral solition model seems to provide very close predictions for the mass and the width of $\Theta^+(1540)$, obviously, it cannot reproduce all aspects of QCD, the fundamental theory of strong interactions. Now the central theoretical question is whether the spectrum of QCD possesses Θ^+ with the correct quantum numbers, mass, and decay width.

At present, the most viable approach to solve QCD nonperturbatively from the first principles is lattice QCD. Explicitly, one needs to construct an interpolating operator which has a significant overlap with the pentaquark baryon states. Then one computes the time-correlation function of this interpolating operator, and from which to extract the masses of its even and odd parity states, respectively. However, any $(udud\bar{s})$ operator must couple to hadronic states with the same quantum numbers (e.g., *KN* scattering states). It is necessary to disentangle the lowest-lying pentaquark states from the *KN* scattering states, as well as the excited pentaquark states.

To this end, we adopt the so-called variational method [12,13]. We use three different interpolating operators for $\Theta(udud\bar{s})$ to compute their 3 × 3 correlation matrix and from its eigenvalues we extract the masses of the even and odd parity states. This is the first lattice QCD study of Θ^+ with 3 × 3 correlation matrix. These three interpolating operators (with I = 0) are

$$(O_1)_{x\alpha} = [\mathbf{u}^T C \gamma_5 \mathbf{d}]_{xc} \{ \bar{\mathbf{s}}_{x\beta e}(\gamma_5)_{\beta\eta} \mathbf{u}_{x\eta e}(\gamma_5 \mathbf{d})_{x\alpha c} - \bar{\mathbf{s}}_{x\beta e}(\gamma_5)_{\beta\eta} \mathbf{d}_{x\eta e}(\gamma_5 \mathbf{u})_{x\alpha c} \},$$
(1)

$$(O_2)_{x\alpha} = [\mathbf{u}^T C \gamma_5 \mathbf{d}]_{xc} \{ \bar{\mathbf{s}}_{x\beta e} (\gamma_5)_{\beta\eta} \mathbf{u}_{x\eta c} (\gamma_5 \mathbf{d})_{x\alpha e} \\ - \bar{\mathbf{s}}_{x\beta e} (\gamma_5)_{\beta\eta} \mathbf{d}_{x\eta c} (\gamma_5 \mathbf{u})_{x\alpha e} \},$$
(2)

$$(O_3)_{x\alpha} = \boldsymbol{\epsilon}_{cde} [\mathbf{u}^T C \boldsymbol{\gamma}_5 \mathbf{d}]_{xc} [\mathbf{u}^T C \mathbf{d}]_{xd} (C \bar{\mathbf{s}}^T)_{x\alpha e}, \quad (3)$$

where **u**, **d**, and **s** denote the quark fields; ϵ_{cde} is the completely antisymmetric tensor; *x*, {*c*, *d*, *e*} and { α, β, η } denote the lattice site, color, and Dirac indices, respectively; and *C* is the charge conjugation operator satisfying $C\gamma_{\mu}C^{-1} = -\gamma_{\mu}^{T}$ and $(C\gamma_{5})^{T} = -C\gamma_{5}$. Here the diquark operator is defined as

$$[\mathbf{u}^T \Gamma \mathbf{d}]_{xa} \equiv \boldsymbol{\epsilon}_{abc} (\mathbf{u}_{x\alpha b} \Gamma_{\alpha \beta} \mathbf{d}_{x\beta c} - \mathbf{d}_{x\alpha b} \Gamma_{\alpha \beta} \mathbf{u}_{x\beta c}), \quad (4)$$

where $\Gamma_{\alpha\beta} = -\Gamma_{\beta\alpha}$. Thus the diquark transforms like a spin singlet (1_s) , color antitriplet $(\bar{3}_c)$, and flavor antitriplet $(\bar{3}_f)$. For $\Gamma = C\gamma_5$, it transforms as a scalar, while for $\Gamma = C$, it transforms like a pseudoscalar. Here O_1 , O_2 , and O_3 all transform like an even operator under parity.

The operator O_1 is similar to the naïve kaon \otimes nucleon operator which was used by Mathur *et al.* [14]. The operator O_2 was first considered by Zhu [15] and was adopted by Csikor *et al.* [16] in their lattice study. The difference between O_1 and O_2 is that, in the latter case, the color index of the $\mathbf{u}(\mathbf{d})$ quark in the kaon is swapped with that of the $\mathbf{d}(\mathbf{u})$ quark in the nucleon such that the "kaon" and the "nucleon" do not appear as color singlets. The operator O_3 is motivatied by the Jaffe-Wilzcek (diquark-diquarkantiquark) model [17], which was considered by Sugiyama *et al.* [18] and Sasaki [19] and was adopted by Chiu and Hsieh [20] and Ishii *et al.* [21].

In the Jaffe-Wilzcek model, each pair of [ud] forms a diquark which transforms like a spin singlet (1_s) , color antitriplet $(\bar{3}_c)$, and flavor antitriplet $(\bar{3}_f)$. Then the pentaquark baryon $\Theta([ud][ud]\bar{s})$ emerges as the color singlet in $(\bar{3}_c \times \bar{3}_c) \times \bar{3}_c = 1_c + 8_c + 8_c + \overline{10_c}$ and a member (with S = +1 and I = 0) of the flavor antidecuplet in $\bar{3}_f \times \bar{3}_f \times$ $\bar{3}_f = 1_f + 8_f + 8_f + \overline{10}_f$. Now, if one attempts to construct a local interpolating operator for $[ud][ud]\bar{s}$, then these two identical diquarks must be chosen to transform differently (i.e., one scalar and one pseudoscalar), otherwise $\epsilon_{abc}[ud]_{xb}[ud]_{xc}\bar{s}_{x\alpha a}$ is identically zero since diquarks are bosons. Thus, when the orbital angular momentum of this scalar-pseudoscalar-antifermion system is zero (i.e., the lowest-lying state), its parity is even rather than odd. Alternatively, if these two diquarks are located at two different sites, then both diquark operators can be chosen to be scalar; however, they must be antisymmetric in space, i.e., with odd integer orbital angular momentum. Thus the parity of lowest-lying state of this scalar-scalarantifermion system is even, as suggested in the original Jaffe-Wilzcek model. [Note that all correlated quark models e.g., Karliner-Lipkin model [22] and flavor-spin model [23], advocate that the parity of $\Theta^+(1540)$ is positive.]

Evidently, the diquark operator plays an important role in constructing sources for pentaquark baryons as well as 3-quark baryons. The possibility of forming multiquark hadrons through diquark correlations was proposed by Jaffe in 1977 [24]. Although the idea is essentially based on the color-spin interaction between the quarks (through one gluon exchange), its salient features seem to persist even at the hadronic distance scale where QCD is strongly coupled. Thus, it is interesting to see whether such multiquark hadrons (e.g., pentaquark baryons) do exist in the spectrum of QCD.

In this paper, we use the optimal domain-wall fermion [25] to study the pentaquark baryons. The salient features of optimal lattice domain-wall fermion are (i) the quark propagator as well as the effective 4D lattice Dirac operator for internal fermion loops have optimal chiral symme-

try for any N_s (number of sites in the fifth dimension) and gauge background; (ii) the quark fields and hadron observables manifest the discrete symmetries of their counterparts in continuum; (iii) the quark action is ultralocal on the five-dimensional lattice, thus the dynamical quark can be simulated with the standard hybrid Monte Carlo algorithm; (iv) the quark propagator in gauge background can be computed efficiently through the effective 4D lattice Dirac operator.

Before we turn to our results, it is instructive to review the current status of quenched lattice QCD for Θ^+ , as summarized in Table I. At first sight, current lattice QCD results for Θ^+ seem to disagree with each other. Note that the different claims listed in the last column of Table I already cover all possible outcomes. Obviously, some of the claims in Table I cannot be sustained for a long time, no matter what is the experimental outcome. Now if one compares the essential features among these *exploratory* lattice studies, one might understand what could be the causes for these different claims. In the following, we pinpoint the crucial features which may have direct impacts to these claims.

So far, all lattice QCD simulations are performed at unphysically large m_u , thus it is necessary to chirally extrapolate to physical m_u (or equivalently $m_{\pi} =$ 135 MeV). Then a crucial question is how good are the data points used for chiral extrapolation, i.e., how many data points are obtained with $m_u < m_s$ (an obviously physical condition ought to be satisfied), and what is the smallest m_u (or equivalently m_{π}) in these data points. These two questions are answered in the columns with headings $N(m_u < m_s)$ and m_{π}^{\min} , respectively. Obviously, if m_{π}^{\min} is too large, and/or the number $N(m_u < m_s)$ is too small, then the chiral extrapolation would tend to overestimate the masses, especially for the excited states.

Another important question is whether the interpolating operator one uses has a significant overlap with the pentaquark state. If it has little overlap with the pentaquark state, then the signal might be too weak to be detected. As we will see below, O_1 , O_2 , and O_3 all have good overlap with the lowest-lying negative parity state for the entire range of m_u . However, the lowest-lying negative parity state turns

TABLE I. Summary of current lattice QCD results for Θ^+ . Here all masses are in units of MeV; the lattice spacing (a) and the box size (L) are in units of Fermi. The notations for the symbols are W: Wilson fermion or Wilson gauge action; Ov: overlap fermion; Iw: Iwasaki gauge action; m_{π}^{\min} : the smallest pion mass; $N(m_u < m_s)$: the number of data points satisfying the condition $m_u < m_s$; $m(1/2^{\pm})$: the mass of $1/2^{\pm}$ state via chiral extrapolation; S/R: Scattering state/Resonance. There are two lattice studies [26,27] which have not been listed here due to the lack of information for some of the entries.

Ref.	Operator	Quark	Gauge	а	L	$m_\pi^{ m min}$	$N(m_u < m_s)$	$m(1/2^{-}), S/R$	$m(1/2^+), S/R$	Signal/Parity
[16]	$O_1 + \alpha O_2$	W	W	0.09	1.8	420	3	1539(50), R	2710(79)	Yes/-
[19]	03	W	W	0.07	2.2	650	1	1840(80), R	2940(130)	Yes/-
This work	$\{O_{1,2,3}\}_{3\times 3}$	Odwf	W	0.09	1.8	440	10	1433(72), S	1562(121), R	Yes/+
[14]	O_1	Ov	Iw	0.20	2.4/3.2	180	13	~1450, S	~1650, S	No
[21]	<i>O</i> ₃	W	W	0.18	2.1	656	0	1750(40), S	2250(120)	No

out to be nothing but the KN s-wave scattering state. On the other hand, for the positive parity channel, only O_3 has a significant overlap with the lowest-lying positive parity state, in the regime $m_u \leq m_s/2$. As we will see below, this positive parity state is ruled out to be KN p wave, KN* s wave (where N* is the lowest negative parity state of nucleon), or KN η' s wave (where η' is the artifact due to the quenched approximation).

At the end of this paper, we will return to Table I to discuss what could be the causes for the different claims in these exploratory lattice studies.

The outline of the paper is as follows: In Sec. II, we outline our computation of quark propagators. In Sec. III, we outline our determination of the lattice spacing a and the strange quark bare mass m_s . In Sec. IV, we present our results of the masses of the even and odd parity states extracted from the 3×3 correlation matrix of O_1 , O_2 , and O_3 . These are the first lattice QCD results using 3 \times 3 correlators for Θ^+ . In Sec. V, we investigate the KN scattering states with "disconnected" KN (i.e., without quark exchanges between K and N) correlation function and use them to identify the KN scattering states in the spectrum of 3×3 correlation matrix. In Sec. VI, we discuss the current lattice QCD results for Θ^+ and conclude with some remarks. In the appendix, we include our results of the masses of the even and odd parity states extracted from the time-correlation functions of O_1 , O_2 , and O_3 , respectively.

II. COMPUTATION OF QUARK PROPAGATORS

Now it is straightforward to work out the baryon propagator $\langle \Theta_{x\alpha} \bar{\Theta}_{y\delta} \rangle$ in terms of quark propagators. In lattice QCD with exact chiral symmetry, quark propagator with bare mass m_q is of the form $(D_c + m_q)^{-1}$ [28], where D_c is exactly chirally symmetric at finite lattice spacing. In the continuum limit, $(D_c + m_q)^{-1}$ reproduces $[\gamma_{\mu}(\partial_{\mu} + iA_{\mu}) + m_q]^{-1}$. For optimal domain-wall fermion with $N_s + 2$ sites in the fifth dimension,

$$D_{c} = 2m_{0} \frac{1 + \gamma_{5}S(H_{w})}{1 - \gamma_{5}S(H_{w})}, \qquad S(H_{w}) = \frac{1 - \prod_{s=1}^{N_{s}} T_{s}}{1 + \prod_{s=1}^{N_{s}} T_{s}}$$
$$T_{s} = \frac{1 - \omega_{s}H_{w}}{1 + \omega_{s}H_{w}}, \qquad H_{w} = \gamma_{5}D_{w},$$

where D_w is the standard Wilson Dirac operator plus a negative parameter $-m_0$ ($0 < m_0 < 2$), and $\{\omega_s\}$ are a set of weights specified by an exact formula such that D_c possesses the optimal chiral symmetry [25]. Since

$$(D_c + m_q)^{-1} = (1 - rm_q)^{-1} [D^{-1}(m_q) - r],$$

 $r = \frac{1}{2m_0},$

where

$$D(m_q) = m_q + (m_0 - m_q/2)[1 + \gamma_5 S(H_w)],$$

thus the quark propagator can be obtained by solving the system $D(m_q)Y = 1$ with nested conjugate gradient [29], which turns out to be highly efficient (in terms of the precision of chirality versus CPU time and memory storage) if the inner conjugate gradient loop is iterated with Neuberger's double pass algorithm [30]. For more details of our scheme of computing quark propagators, see Ref. [31].

We generate 100 gauge configurations with Wilson gauge action at $\beta = 6.1$ on the $20^3 \times 40$ lattice. Then we compute two sets of (point-to-point) quark propagators, for periodic and antiperiodic boundary conditions in the time direction, respectively. Here the boundary condition in any spatial direction is always periodic. Now we use the averaged quark propagator to compute the time-correlation function for any hadronic observable such that the effects due to finite *T* can be largely reduced [32].

Fixing $m_0 = 1.3$, we project out 16 low-lying eigenmodes of $|H_w|$ and perform the nested conjugate gradient in the complement of the vector space spanned by these eigenmodes. For $N_s = 128$, the weights $\{\omega_s\}$ are fixed with $\lambda_{\min} = 0.18$ and $\lambda_{\max} = 6.3$, where $\lambda_{\min} \le \lambda(|H_w|) \le \lambda_{\max}$ for all gauge configurations.

For each configuration, (point-to-point) quark propagators are computed for 30 bare quark masses in the range $0.03 \le m_q a \le 0.8$, with stopping criteria 10^{-11} and 2×10^{-12} for the outer and inner conjugate gradient loops, respectively. Then the chiral symmetry breaking due to finite N_s (= 128) is less than 10^{-14} ,

$$\sigma = \left| \frac{Y^{\dagger} S^2 Y}{Y^{\dagger} Y} - 1 \right| < 10^{-14},$$

for every iteration of the nested conjugate gradient, and the norm of the residual vector for each column of the quark propagator is less than 2×10^{-11} ,

$$||(D_c + m_a)Y - \mathbf{1}|| < 2 \times 10^{-11}$$

III. DETERMINATION OF a^{-1} AND m_s

After the quark propagators have been computed, we first measure the pion propagator and its time-correlation function and extract the pion mass $(m_{\pi}a)$ and the pion decay constant $(f_{\pi}a)$. With the experimental input $f_{\pi} = 132$ MeV, we determine $a^{-1} = 2.237(76)$ GeV.

The bare mass of strange quark is determined by extracting the mass of vector meson from the timecorrelation function

$$C_V(t) = \frac{1}{3} \sum_{\mu=1}^{3} \sum_{\vec{x}} \operatorname{tr} \{ \gamma_{\mu} (D_c + m_q)_{x,0}^{-1} \gamma_{\mu} (D_c + m_q)_{0,x}^{-1} \}.$$

At $m_q a = 0.08$, $M_V a = 0.4601(44)$, which gives $M_V = 1029(10)$ MeV, in good agreement with the mass of

TING-WAI CHIU AND TUNG-HAN HSIEH

 $\phi(1020)$. Thus we take the strange quark bare mass to be $m_s a = 0.08$. Then we have 10 quark masses smaller than m_s , i.e., $m_u a = 0.03$, 0.035, 0.04, 0.045, 0.05, 0.055, 0.06, 0.065, 0.07, 0.075. In this paper, we work in the isospin limit $m_u = m_d$.

IV. THE 3 × 3 CORRELATION MATRIX FOR $\Theta(udud\bar{s})$

Next we compute the propagators $\langle (O_i)_{x\alpha}(O_j)_{y\delta} \rangle$ with fixed $y = (\vec{0}, 0)$, and their time-correlation functions $C_{ij}^{\pm}(t)$ with \pm parity

$$C_{ij}^{\pm}(t) = \left\langle \sum_{\vec{x}} \operatorname{tr} \left[\frac{1 \pm \gamma_4}{2} \langle O_i(\vec{x}, t) \bar{O}_j(\vec{0}, 0) \rangle_f \right] \right\rangle_U,$$

where the trace sums over the Dirac space, and the subscripts f and U denote fermionic average and gauge field ensemble average, respectively. Then the 3×3 correlation matrix $C^{\pm}(t) = \{C_{ii}^{\pm}(t)\}$ can be constructed. Now, with the variational parameter t_0 , we diagonalize the normalized correlation matrix $C^{\pm}(t_0)^{-1/2}C^{\pm}(t)C^{\pm}(t_0)^{-1/2}$ and obtain eigenvalues $\{A_i^{\pm}(t)\}$, and from which to extract the masses $\{m_i^{\pm}\}$ of the lowest-lying and two excited states for \pm parity, respectively. In general, by varying t_0 , one could minimize the errors of the masses extracted from the eigenvalues, as well as to disentangle (optimally) the lowest-lying states from the excited ones, as shown in Refs. [12,13]. However, in this case, the relevant quantities (e.g., the effective masses) extracted from unnormalized correlation matrix seem to be as good as those of the normalized ones. Thus we restrict to unnormalized $C^{\pm}(t)$ in the following. Then the mass m_i^{\pm} can be extracted by single exponential fit to $A_i^{\pm}(t)$, for the range of t in which the effective mass $M_{\rm eff}(t) = \ln[A(t)/A(t+1)]$ attains a plateau.

In Figs. 1–4, the eigenvalues $A^{\pm}(t)$ corresponding to the lowest-lying and first excited states with $J^P = 1/2^{\pm}$ are plotted versus the time slices, for $m_u a = 0.03$ (the smallest quark mass in this study), together with their effective mass plots. Here we have suppressed any data point which has error (jackknife with single elimination) larger than its mean value. In each case, the mass m^{\pm} can be extracted by single exponential fit to $A^{\pm}(t)$ for the range of t in which the effective mass $M_{\text{eff}}(t) = \ln[A(t)/A(t+1)]$ attains a plateau. The results are (in units of a^{-1}):

$$m(1/2^{+})_{\text{lowest-lying}} = 1.034(80),$$

$$m(1/2^{+})_{1\text{st excited}} = 1.505(137),$$

$$m(1/2^{-})_{\text{lowest-lying}} = 0.8045(23),$$

$$m(1/2^{-})_{1\text{st excited}} = 1.190(388),$$

where all fits have confidence level greater than 0.6 and $\chi^2/d.o.f. < 1$. Obviously, the lowest-lying and the first excited states are disentangled in both parity channels.



FIG. 1 (color online). (a) The eigenvalue $A^+(t)$ of the lowest positive parity state for $m_u a = 0.03$. The solid line is the single exponential fit for $9 \le t \le 13$. (b) The effective mass $M_{\text{eff}}(t) = \ln[A(t)/A(t+1)]$ of $A^+(t)$ in Fig. 1(a).



FIG. 2 (color online). (a) The eigenvalue $A^{-}(t)$ of the lowest negative parity state, for $m_u a = 0.03$. The solid line is the single exponential fit for $11 \le t \le 17$. (b) The effective mass of $A^{-}(t)$ in Fig. 2(a).



FIG. 3 (color online). (a) The eigenvalue $A^+(t)$ of the first excited state with $J^P = 1/2^+$ for $m_u a = 0.03$. The solid line is the single exponential fit for $7 \le t \le 11$. (b) The effective mass of $A^+(t)$ in Fig. 3(a).



FIG. 4 (color online). (a) The eigenvalue $A^{-}(t)$ of the first excited state with $J^{P} = 1/2^{-}$ for $m_{u}a = 0.03$. The solid line is the single exponential fit for $9 \le t \le 13$. Note that the error becomes very large for t > 13. (b) The effective mass of $A^{-}(t)$ in Fig. 4(a).

In Fig. 5, the masses of the lowest-lying states with $J^P = 1/2^{\pm}$ are plotted versus m_{π}^2 . An interesting feature emerges in the positive parity channel. Its mass starts to fall more rapidly around the regime $m_u a \approx 0.045$ (i.e., $m_u \approx 0.56m_s$) signaling the onset of certain attractive interactions which lower the energy of this pentaquark state. Even taking into account of the error bar, the signal is unambiguous, as shown in Fig. 1 for $m_u a = 0.03$ (the smallest quark mass in this study). We suspect that this is the manifestation of



FIG. 5 (color online). The masses of the lowest-lying states of $\Theta(udud\bar{s})$, extracted from the eigenvalues of the 3×3 correlation matrix of O_1 , O_2 , and O_3 . The solid lines are chiral extrapolation (linear in m_{π}^2) using the smallest four masses.

diquark correlations when $m_{u,d}$ becomes sufficiently small. To check, we compare it with the positive parity states extracted from the time-correlation functions of O_1 , O_2 , and O_3 , respectively, (see Figs. 9–11 in the appendix). Then we see that similar phenomenon also happens in the positive parity channel of O_3 (Fig. 11), but not in O_1 (Fig. 9) or O_2 (Fig. 10). Since O_3 is the diquark-diquarkantiquark operator, it is consistent with our interpretation that diquark correlations emerge when $m_{\mu}a \leq 0.045 \simeq$ $0.56m_s$. On the other hand, one may wonder whether it could be an artifact due to low statistics. Our argument is that if it were due to low statistics, it must also appear in the positive parity channel of O_1 and O_2 . However, it is not the case. So we rule out the possibility that this rapid decrease of the mass of the positive parity state in the regime $m_{\mu}a \leq$ $0.045 \simeq 0.56 m_s$ is due to low statistics. In other words, it suggests that O_3 has the largest overlap with the pentaquark state, and the diquark correlations may play an important role in forming Θ^+ .

The next question is how to perform the chiral extrapolation to the physical limit where $m_{\pi} = 135 \text{ MeV} (m_{u,d} \simeq$ $m_s/25$). From the viewpoint of chiral perturbation theory, one should use the set of data points with the smallest m_{μ} (m_{π}^2) . Moreover, since our m_{π}^{\min} is about 440 MeV, which may not be sufficiently small to capture the chiral log behavior in chiral perturbation theory, thus we only use the lowest order terms (i.e., linear in m_{π}^2) for chiral extrapolation. Observing the onset of diquark correlations around $m_{\mu}a \simeq 0.45$, we naturally pick the smallest four masses (i.e., with $m_{\mu}a = 0.03, 0.035, 0.04, 0.045 \simeq$ $(0.56m_s)$ for chiral extrapolation linear in m_{π}^2 . At $m_{\pi} = 135$ MeV, we obtain the masses of the lowestlying states: $m(1/2^{-}) = 1424(57)$ MeV, and $m(1/2^{+}) =$ 1562(121) MeV, which agree with the masses of m_K + $m_N \simeq 1430$ MeV and $\Theta(1540)$, respectively. For the positive parity state, we also have performed a fully correlated fit with the smallest four masses, employing the procedure adopted in Ref. [33]. Our result is 1554(150) MeV with $\chi^2_{\rm full}$ /d.o.f. = 1.17(24), in agreement with the result of uncorrelated fit. By varying the fitting range of t, and the number of mass points, we estimate the systematic error to be 180 MeV.

V. DISTINGUISHING THE KN SCATTERING STATES

Now the question is whether the lowest-lying $J^P = 1/2^{\pm}$ states extracted from the 3 × 3 correlation matrix are scattering states or resonances. In order to obtain the mass spectrum of *KN* scattering states (which excludes any pentaquark states), we consider the time-correlation function of *KN* operator without any exchange of quarks between *K* and *N* in its propagator, i.e., the interaction between *K* and *N* is only through the exchange of gluons. Explicitly,

$$C_{\bar{K}N}^{\pm}(t) = \left\langle \sum_{\vec{x}} \operatorname{tr} \left[\frac{1 \mp \gamma_4}{2} \langle N(\vec{x}, t) \bar{N}(\vec{0}, 0) \rangle_f \right. \\ \left. \times \left\langle K(\vec{x}, t) \bar{K}(\vec{0}, 0) \rangle_f \right] \right\rangle_U,$$
(5)

where $N = [\mathbf{u}^T C \gamma_5 \mathbf{d}] \mathbf{d}$, and $K = \bar{\mathbf{s}} \gamma_5 \mathbf{u}$. Note that the parity projector has taken into account of the intrinsic parity of kaon.

The masses of lowest-lying *KN* scattering states are plotted in Fig. 6, versus the naïve estimates. Here the naïve estimates are $m_K + m_N$ for the *s* wave, and $\sqrt{m_K^2 + (2\pi/L)^2} + \sqrt{m_N^2 + (2\pi/L)^2}$ for the *p* wave, where *L* is the lattice size in spatial directions, and m_K and m_N are masses extracted from kaon and nucleon time-correlation functions, respectively.

For the $J^P = 1/2^-$ state, using the smallest four masses for chiral extrapolation to $m_{\pi} = 135$ MeV, we obtain $m_{KN}(1/2^-) = 1433(72)$ MeV, in agreement with $m_K + m_N \simeq 1430$ MeV. Further, its mass spectrum is almost identical to that of the lowest $J^P = 1/2^-$ state of Θ in Fig. 5 for the entire range of m_u . Thus we identify the lowest $J^P = 1/2^-$ state of $\Theta(udud\bar{s})$ with the KN s-wave scattering state.

On the other hand, for the $J^P = 1/2^+$ state in Fig. 6, its mass is higher than the naïve estimate $\sqrt{m_K^2 + (2\pi/L)^2} + \sqrt{m_N^2 + (2\pi/L)^2}$. This suggests that the *KN p* wave (in the quenched approximation) in a finite torus is more complicated than just two free particles with momenta $\vec{p}_K =$ $-\vec{p}_N = 2\pi\hat{e}_i/L$, i.e., their interaction through gluon exchanges cannot be ignored. Further, the mass of *KN p*-wave scattering state in Fig. 6 is always higher than the mass of the lowest-lying $J^P = 1/2^+$ state in Fig. 5. In particular, for $m_u < m_s$, the former is significantly higher than the latter. This seems to suggest that the lowest $J^P = 1/2^+$ state of $\Theta(udud\bar{s})$ is different from the *KN p*-wave scattering state.

However, there are other two-hadron scattering states which also have quantum numbers $J^P = 1/2^+$ and S =+1, namely, the *s*-wave scattering state of $KN\eta'$ (where η' is an artifact due to quenched approximation) and the *s*-wave scattering state of KN^* (where N^* is the negative parity state of nucleon). In the following, we check whether the lowest-lying $J^P = 1/2^+$ state extracted from the 3 × 3 correlation matrix could possibly be any one of these two-hadron scattering states.

The *s* wave of $KN\eta'$ has $J^P = 1/2^+$, and its mass is estimated to be $m_K + m_N + m_\pi$ [14]. In Fig. 7, it is clear that the lowest-lying $J^P = 1/2^+$ state of Θ is *different* from the *s* wave of $KN\eta'$ ghost state. Otherwise, they should be almost identical for the entire range of m_u , as in the case of KN *s* wave and the lowest-lying state with $J^P = 1/2^-$ in Fig. 6. So we exclude the possibility that the lowest-lying $J^P = 1/2^+$ state extracted from the 3×3 correlation matrix is due to quenched artifacts. Note that Mathur *et al.* [14] has claimed that the quenched artifact $KN\eta'$ (with negative spectral weight) would be seen in the positive parity channel if $m_\pi < 300$ MeV for the O_1 ($K \otimes \gamma_5 N$) operator. If this claim holds for any cases (gauge actions, lattice fermions, operators, etc.), then we should





FIG. 6 (color online). The masses of the lowest-lying *KN* scattering states extracted from $C_{KN}(t)$ (5) versus the naïve estimates (with dotted lines). The solid lines (for $J^P = 1/2^-$) are chiral extrapolations using the smallest four masses.

FIG. 7 (color online). The mass of the lowest-lying $J^P = 1/2^+$ state extracted from the 3 × 3 correlation matrix versus the *s* wave of $KN\eta'$ ghost state (with dotted lines).

not see $KN\eta'$, since our smallest pion mass is larger than 400 MeV.

Next, we turn to the s wave of KN^* , which also has $J^P =$ $1/2^+$, and its mass is estimated to be $m_K + m_{N^*}$. In Fig. 8, it is clear that the mass of KN^* s wave is *different* from the mass of the lowest $J^P = 1/2^+$ state extracted from the 3 \times 3 correlation matrix for the entire range of m_{μ} (except at the crossover $m_{\mu}a \simeq 0.03$). In the physical pion limit, the mass of the lowest $J^P = 1/2^+$ state is 1562(121) MeV, while $m_K + m_{N^*}$ is 2137(142) MeV. This rules out the possibility that the lowest-lying $J^P = 1/2^+$ state extracted from the 3×3 correlation matrix is the KN^{*} s-wave scattering state. Note that this disagrees with the claim of Ref. [27], which was based on their result obtained with Wilson quarks at unphysical quark masses. However, there is no reason to expect that baryon masses computed with two different lattice (fermion and gauge) actions would agree with each other, except in the continuum (and infinite volume) limit with physical quark masses. Thus, it is not surprising to see that, at unphysically large quark masses, our result of the mass of the lowest-lying state with even parity, $m(1/2^+)$, is higher than $m_K + m_{N^*}$, while the result of Ref. [27] seems to suggest that $m(1/2^+) \simeq m_K + m_{N^*}$. Now the emerging problem for Wilson fermion is to check whether the relationship $m(1/2^+) \simeq m_K + m_{N^*}$ remains valid in the physical pion limit. We suspect that even for Wilson fermion, it also would exhibit the inequality $m(1/2^+) < m_K + m_{N*}$ at sufficiently small quark masses, though the location of the crossover might be different from that of Fig. 8. At this point, it is instructive to check the result of Mathur et al. [14] which was obtained with the



FIG. 8 (color online). The mass of the lowest-lying $J^P = 1/2^+$ state extracted from the 3 × 3 correlation matrix, versus the KN^* s wave scattering state with mass $m_K + m_{N^*}$.

overlap fermion. From Ref. [14], one can extract $m(1/2^+)$, m_K , and m_{N^*} , respectively, then one immediately sees that $m(1/2^+)$ is larger than $m_K + m_{N^*}$ for $m_{\pi}^2 > 0.27 \text{GeV}^2$, but becomes smaller than $m_K + m_{N^*}$ for $m_{\pi}^2 < 0.27 \text{GeV}^2$, and it tends to ~ 1650 MeV in the physical pion limit. Obviously, the result of Mathur et al. [14] also suggests that the lowest state with even parity is different from the KN^* s wave, in agreement with our conclusion. Now a (physically irrelevant) question is where the KN^* s-wave scattering state lies, say, at unphysically heavy quark masses. Our conjecture is that in a finite torus, the KN^* s wave might turn out to be much heavier than the naïve estimate $m_K + m_{N^*}$ (similar to the case of KN p wave which is much heavier than its naïve estimate, as shown in Fig. 6), thus it always lies above the lowest $J^P = 1/2^+$ state, as one of the excited states in the positive parity channel.

Now, after ruling out the possibilities of being KN pwave, $KN\eta' s$ wave, or $KN^* s$ wave, the lowest-lying $J^P = 1/2^+$ state extracted from the 3×3 correlation matrix seems to be nothing but a resonance. If it is identified with $\Theta^+(1540)$, then it predicts that the parity of $\Theta^+(1540)$ is positive.

VI. DISCUSSIONS AND CONCLUDING REMARKS

Now we return to Table I to discuss what causes the different claims in these exploratory lattice studies.

Now, back to Fig. 5. If we had not measured any data points with $m_{\mu} < m_s/2$, then we could not have seen the rapid decrease of mass of the positive parity state (in the regime $m_{\mu}a \leq 0.045$) of which we interpret as the manifestation of diquark correlations at sufficiently small $m_{\mu d}$. Consequently, chiral extrapolations using data points with $m_u > m_s/2$ must yield much higher masses, especially for the positive parity state. For example, if we use the data points with $m_{\mu}a = 0.05, 0.055, 0.06, 0.065 <$ $m_{s}a$, then we obtain $m(1/2^{-}) = 1666(47)$ MeV, and $m(1/2^+) = 2178(104)$ MeV, with chiral extrapolation linear in m_{π}^2 . Further, if we use the data points with $m_u a = 0.07, 0.075, 0.08, 0.085 (> m_s a)$, then we obtain $m(1/2^{-}) = 1725(52)$ MeV, and $m(1/2^{+}) =$ 2616(103) MeV. In either one of these two cases, it seemingly rules out the possibility that the positive parity channel could accommodate any state with mass 1540 MeV. However, it is only an artifact due to chiral extrapolation with data points too far away from the physical reality $(m_{ud} \simeq m_s/25)$. This explains why the masses of the positive parity state in Refs. [19,21] are so high comparing to our result. Note that, in Refs. [19,21], the total number of data points is four, in which the number of "physical" data points (i.e. with $m_u < m_s$) is only one and zero (see Table I). Even though they claimed that the positive parity channel could not accommodate $\Theta^+(1540)$, it is most likely just an artifact due to their chiral extrapolations with data points too far away from the physical reality.

Next, we turn to the claims of Refs. [14,16]. From our mass spectra of O_1 (Fig. 9) and O_2 (Fig. 10), one can explain why Csikor *et al.* [16] (with O_1 and O_2) obtained a rather high mass for the positive parity state, while Mathur *et al.* [14] (with O_1) did not see pentaquark resonance in the positive parity channel. Namely, the interpolating operators O_1 and O_2 have little overlap with the pentaquark state in the positive parity channel. In fact, our mass spectra of O_1 and O_2 are consistent with those of Refs. [14,16].

Finally we discuss the results of this paper. This is the first lattice QCD study on Θ with 3 \times 3 correlation matrix. Presumably, it should provide a more reliable answer to the questions of signal/parity of Θ^+ than other lattice studies with only one operator. However, this is a quenched lattice QCD calculation (like other lattice studies on Θ^+ so far), with only one volume, and one lattice spacing, thus it is difficult for us to estimate the systematic error. For the lowest $J^P = 1/2^-$ state, it is identified with the KN s wave, by comparing its mass with $m_N + m_K$. For the lowest $J^P = 1/2^+$ state, by comparing its mass (as a function of m_{π}^2) to those of two-hadron scattering states having the same quantum numbers, it seems unlikely to be identified with any one of the following two-hadron scattering states: KN p wave, $KN\eta'$ s wave, and KN^* s wave. However, before it can be confirmed to be a resonance, it is necessary to check whether its mass and spectral weight are volume independent. To this end, we are performing computations on the $24^3 \times 48$ lattice with the same lattice spacing (i.e., Wilson gauge action at $\beta = 6.1$). If the lowest-lying state with $J^P = 1/2^+$ turns out to be a scattering state, then there is no evidence of pentaquark resonance in our study. On the other hand, if it turns out to be a resonance, then it can be identified with $\Theta^+(1540)$ since its mass is close to 1540 MeV. Nevertheless, one still has to find out whether its decay width could be as small as 15 MeV (compatible to that of Θ^+), which is the most challenging problem pertaining to Θ^+ .

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APPENDIX

Here we present our results of the masses of the even and odd parity states extracted from the time-correlation functions of operators O_1 (1), O_2 (2), and O_3 (3), respectively.



FIG. 9 (color online). The masses of the even and odd parity states extracted from the time-correlation function of O_1 . The solid lines are chiral extrapolation (linear in m_{π}^2) using the smallest four masses.

In Figs. 9–11, the masses of the $J = 1/2^{\pm}$ states are plotted versus m_{π}^2 , for O_1 , O_2 , and O_3 , respectively. Here all mass fits have confidence level greater than 0.6 and $\chi^2/d.o.f. < 1$. For O_1 and O_2 , their masses vary smoothly with respect to m_{π}^2 in both parity channels. On the other



FIG. 10 (color online). The masses of the even and odd parity states extracted from the time-correlation function of O_2 . The solid lines are chiral extrapolation (linear in m_{π}^2) using the smallest four masses.



FIG. 11 (color online). The masses of $J^P = 1/2^{\pm}$ states extracted from the time-correlation function of O_3 , the diquark-diquark-antiquark operator. The solid lines are chiral extrapolation (linear in m_{π}^2) using the smallest four masses.

hand, the positive parity state of O_3 undergoes a rapid decrease for $m_u a \le 0.045$, similar to the behavior of the lowest-lying $J^P = 1/2^+$ state extracted from the 3×3 correlation matrix (see Fig. 5). This seems to signal an onset of certain attractive interactions when the quark mass $m_{u,d}$ becomes sufficiently small. We conjecture that this is the manifestation of diquark correlations when $m_{u,d}$ approaches the physical limit.

Following the same argument in Sec. IV, we pick the smallest four masses (i.e., with $m_u a = 0.03, 0.035, 0.04, 0.045$) for chiral extrapolation (linear in m_{π}^2). At physical pion mass $m_{\pi} = 135$ MeV, we obtain

$$O_1: m(1/2^-) = 1430(66) \text{ MeV},$$

 $m(1/2^+) = 2301(134) \text{ MeV};$
 $O_2: m(1/2^-) = 1430(67) \text{ MeV},$
 $m(1/2^+) = 2346(156) \text{ MeV};$
 $O_3: m(1/2^-) = 1446(71) \text{ MeV},$
 $m(1/2^+) = 1843(136) \text{ MeV}.$

Note that for the $J^P = 1/2^-$ state, all three operators give almost the same mass which coincides with that [1424(57) MeV] extracted from the 3 × 3 correlation matrix of O_1 , O_2 , and O_3 . However, for the $J^P = 1/2^+$ state, the operator O_3 (the diquark-diquark-antiquark operator motivated by the Jaffe-Wilczek model) gives the lowest mass, which is the closest to that [1562(121) MeV] extracted from the 3 × 3 correlation matrix of O_1 , O_2 , and O_3 . This seems to imply that among { O_i , i = 1, 2, 3}, O_3 has the largest overlap with the pentaquark state, and the diquark correlations may play an important role in forming $\Theta^+(1540)$.

Further, we observe also that the diagonalization of the 3×3 correlation matrix indeed disentangles the contributions of the excited states and gives a smaller mass for the lowest-lying $J^P = 1/2^+$ state.

- T. Nakano *et al.* (LEPS Collaboration), Phys. Rev. Lett. 91, 012 002 (2003).
- [2] V. V. Barmin *et al.* (DIANA Collaboration), Phys. At. Nucl. **66**, 1715 (2003) [Yad. Fiz. **66**, 1763 (2003)].
- [3] S. Stepanyan *et al.* (CLAS Collaboration), Phys. Rev. Lett. 91, 252 001 (2003).
- [4] J. Barth *et al.* (SAPHIR Collaboration), Phys. Lett. B 572, 127 (2003).
- [5] A. E. Asratyan, A. G. Dolgolenko, and M. A. Kubantsev, Yad. Fiz. 67, 704 (2004) [Phys. At. Nucl. 67, 682 (2004)].
- [6] V. Kubarovsky *et al.* (CLAS Collaboration), Phys. Rev. Lett. **92**, 032 001 (2004); **92**, 049902(E) (2004).
- [7] A. Airapetian *et al.* (HERMES Collaboration), Phys. Lett. B 585, 213 (2004).
- [8] A. Aleev et al. (SVD Collaboration), hep-ex/0401024.
- [9] For a recent review, see K. Hicks, J. Phys. Conf. Series 9, 183 (2005).
- [10] D. Diakonov, V. Petrov, and M. V. Polyakov, Z. Phys. A 359, 305 (1997).

- [11] A. V. Manohar, Nucl. Phys. B248, 19 (1984); M. Chemtob, Nucl. Phys. B256, 600 (1985); M. Praszalowicz, in *Skymions and Anomalies*, edited by M. Jezabeck and M. Praszalowicz, (World Scientific, Singapore, 1987), p. 112.
- [12] C. Michael, Nucl. Phys. **B259**, 58 (1985).
- [13] M. Luscher and U. Wolff, Nucl. Phys. B339, 222 (1990).
- [14] N. Mathur et al., Phys. Rev. D 70, 074508 (2004).
- [15] S. L. Zhu, Phys. Rev. Lett. 91, 232 002 (2003).
- [16] F. Csikor, Z. Fodor, S. D. Katz, and T. G. Kovacs, J. High Energy Phys. 11 (2003) 070.
- [17] R.L. Jaffe and F. Wilczek, Phys. Rev. Lett. 91, 232003 (2003).
- [18] J. Sugiyama, T. Doi, and M. Oka, Phys. Lett. B 581, 167 (2004).
- [19] S. Sasaki, Phys. Rev. Lett. 93, 152 001 (2004).
- [20] T. W. Chiu and T. H. Hsieh, hep-ph/0403020v1. Note that in the v1, the seemingly reversal of level-ordering of even and odd parity states was due to a bug in our measurement code, which was fixed in August 2004. The corrected version (hep-ph/0403020v2) was posted in September

- [21] N. Ishii, T. Doi, H. Iida, M. Oka, F. Okiharu, and H. Suganuma, Phys. Rev. D 71, 034001 (2005).
- [22] M. Karliner and H.J. Lipkin, Phys. Lett. B 575, 249 (2003).
- [23] F. Stancu and D. O. Riska, Phys. Lett. B 575, 242 (2003).
- [24] R. L. Jaffe, Phys. Rev. D 15, 267 (1977); Phys. Rev. D 15, 281 (1977).
- [25] T. W. Chiu, Phys. Rev. Lett. 90, 071601 (2003); Phys. Lett. B 552, 97 (2003); hep-lat/0303008; Nucl. Phys. B Proc. Suppl. 129, 135 (2004).
- [26] C. Alexandrou, G. Koutsou, and A. Tsapalis, Nucl. Phys. B Proc. Suppl. 140, 275 (2005).

- [27] T. T. Takahashi, T. Umeda, T. Onogi, and T. Kunihiro, heplat/0410025.
- [28] T. W. Chiu, Phys. Rev. D 60, 034503 (1999); T. W. Chiu and S. V. Zenkin, Phys. Rev. D 59, 074501 (1999).
- [29] H. Neuberger, Phys. Rev. Lett. 81, 4060 (1998); Phys. Lett. B 417, 141 (1998).
- [30] H. Neuberger, Int. J. Mod. Phys. C 10, 1051 (1999); T. W. Chiu and T. H. Hsieh, Phys. Rev. E 68, 066704 (2003).
- [31] T. W. Chiu and T. H. Hsieh, Nucl. Phys. B673, 217 (2003); Phys. Rev. D 66, 014506 (2002).
- [32] T.W. Chiu and T.H. Hsieh, hep-ph/0501227.
- [33] Y. Iwasaki *et al.* (QCDPAX Collaboration), Phys. Rev. D 53, 6443 (1996).