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A comprehensive search for the Θ^+ pentaquark on the lattice

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We study spin 1/2 isoscalar and isovector, even and odd parity candidates for the $\Theta^+(1540)$ pentaquark particle using large scale lattice QCD simulations. Previous lattice works led to inconclusive results because so far it has not been possible to unambiguously identify the known scattering spectrum and tell whether additionally a genuine pentaquark state also exists. Here we carry out this analysis using several possible wave functions (operators), including spatially non-trivial ones with unit orbital angular momentum. The cross correlator matrix we compute is 14×14 with 60 non-vanishing elements. We can clearly distinguish the lowest scattering state(s) in both parity channels up to above the expected location of the pentaquark, but we find no trace of the latter. We conclude that there are most probably no pentaquark bound states at our quark masses, corresponding to m_π=400–630 MeV. However, we cannot rule out the existence of a pentaquark state at the physical quark masses or pentaquarks with a more exotic wave function.

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In the present paper we report on our extended search for the exotic Θ^+ particle on the lattice [1]. The difficulty of the lattice approach lies in the fact that the $\Theta^+(1540)$ mass is very close to the nucleon-kaon (KN) scattering threshold. In a finite box the continuum of KN scattering states turn into a stack of discrete energy levels with the $\Theta^+(1540)$ embedded somewhere among them. One then has the task of reliably separating the $\Theta^+(1540)$ from these nearby scattering states appearing in the same channel. In our opinion the confirmation of the existence of the $\Theta^+(1540)$ from lattice studies is completed only if all the states up to above the expected location of the $\Theta^+(1540)$ have been identified and the $\Theta^+(1540)$ can be clearly separated from the neighbouring scattering states.

All the published lattice studies so far used rotationally symmetric quark source arrangements and none of them could identify the lowest expected nucleon-kaon scattering state in *both* parity channels [2]-[10]. In the present paper we extend our previous pentaquark search including spatially non-trivial operators. This enables us to use a diquark-diquark-antiquark type wave function with unit diquark-diquark relative angular momentum [11].

For extracting the lowest few states in the given sector we consider a linear combination of operators of the form

$$\mathscr{R}(t) = \sum_{i=1}^{n} v_i \mathscr{O}_i(t). \tag{1}$$

The correlator of $\mathscr{R}$ can be expressed in terms of the $n \times n$ correlation matrix

$$C_{ij}(t) = \langle \mathscr{O}_i(t) \bar{\mathscr{O}}_j(0) \rangle \tag{2}$$

as

$$R(t) \ = \ \langle \mathscr{R}(t) \bar{\mathscr{R}}(0) \rangle \ = \ \sum_{i,j=1}^{n} v_i \bar{v}_j C_{ij}(t). \tag{3}$$

Morningstar and Peardon used this cross correlator to compute glueball masses on the lattice [12]. Their procedure was based on the effective mass defined for a general correlator as

$$m_{eff} \ = \ -\frac{1}{\Delta t} \ln \left(\frac{C(t+\Delta t)}{C(t)} \right). \tag{4}$$

Let us now consider the effective mass obtained from $R(t)$,

$$\begin{aligned} m(t) \ &= \ -\frac{1}{\Delta t} \ln \left[\frac{R(t+\Delta t)}{R(t)} \right] \\ &= \ -\frac{1}{\Delta t} \ln \left[\frac{\sum_{i,j=1}^{n} v_i \bar{v}_j C_{ij}(t+\Delta t)}{\sum_{i,j=1}^{n} v_i \bar{v}_j C_{ij}(t)} \right]. \end{aligned} \tag{5}$$

If the correlator contained only n different states, the linear combination with the lowest effective mass would yield exactly the ground state. A simple computation shows that the stationary points of the effective mass with respect to the variables $\{v_i\}_{i=1}^{n}$ are given by the solutions of the generalized eigenvalue equation

$$\sum_{j=1}^{n} C_{ij}(t+\Delta t) v_j \ = \ \lambda \sum_{j=1}^{n} C_{ij}(t) v_j. \tag{6}$$

We only asked for the lowest effective mass, but this eigenvalue problem can have many solutions. They can be interpreted using the following geometric picture. $C_{ij}(t)$ and $C_{ij}(t+\Delta t)$, both being Hermitian, can be considered to be the components of two quadratic forms on the n-dimensional space spanned by the v_i's. $C_{ij}(t)$ can be taken as an inner product on this vector space. The effective mass does not depend on the normalization of the vector $\{v_i\}$, so we can restrict it to be of unit length (with respect to the inner product just defined). The stationary points of the effective mass correspond to the principal axes of the second quadratic form, $C_{ij}(t+\Delta t)$. In the language of the generalized eigenvalue problem this is equivalent to the statement that two quadratic forms can always be simultaneously diagonalized in a vector space: there is a basis orthonormal with respect to one quadratic form and pointing along the principal axes of the other one.

In the absence of degeneracies the stationary points will have 0,1,2... unstable directions determining the coefficients that yield the ground state and the higher excited states. This holds exactly if there are only n states in the correlator. The importance of corrections coming from higher states can be estimated by checking how stable the whole procedure is with respect to varying t and Δt.

Our lattice configurations were generated with the standard Wilson gauge action at $\beta = 6.0$. For the measurements we used the Wilson fermion action with four different $\kappa_{u,d}$ values for the light quarks: 0.1550, 0.1555, 0.1558 and 0.1563. This spans a pion mass range of 400-630 MeV. For the strange quark we used a constant $\kappa_s = 0.1544$, which gives the required kaon mass in the chiral limit. The lattice size was $24^3 \times 60$ and for the largest quark mass we also performed simulations on a $20^3 \times 60$ lattice to see the volume dependence of the observed states. The number of configurations we used was around 200 except for the smaller volume, where we had about three times more.

For obtaining excited states the proper choice of operators is especially important. In the present study we opted for using five different types of spin 1/2 isoscalar operators, including spatially non-trivial ones.

- $\mathcal{O}_1$ Rotationally symmetric nucleon $\otimes$ kaon.
- $\mathcal{O}_2$ Rotationally symmetric diquark-diquark-antiquark introduced by Zhu [13] and subsequently used by Sasaki [3].
- $\mathcal{O}_3$ Nucleon $\otimes$ kaon shifted by $L_s/2$.
- $\mathcal{O}_4$ Diquark-diquark-antiquark with $l = 1$ relative orbital angular momentum.
- $\mathcal{O}_5$ Nucleon $\otimes$ kaon shifted by $L_s/4$.

The symmetric operators ($\mathcal{O}_1 - \mathcal{O}_3$) gave a good signal only in the negative parity channel while the antisymmetric operators ($\mathcal{O}_4, \mathcal{O}_5$) had reasonable overlap only with positive parity states. This can be understood since the parity transformation includes a spatial reflection and the nucleon-kaon system has a negative inner parity. Therefore we used only the operators $\mathcal{O}_1 - \mathcal{O}_3$ to extract negative parity states and operators $\mathcal{O}_4 - \mathcal{O}_5$ for positive parity. For more details of the operators and projection see [1].

After performing the spin and parity projections, we used the above described diagonalization procedure to separate the possible states in both parity channels. We varied both t and Δt required for the diagonalization over a range of $2-5$ and included the systematic uncertainties coming from this variation in the final error bars. We had to extract the lowest masses from the correlator of each stationary linear combination of the operators. It turned out that for the excited states neither a correlated nor an uncorrelated fit with a single exponential (cosh) was satisfactory since in the asymptotic region where a one exponential fit could work the data were rather noisy. We used the following technique instead.

If one plots the effective mass $\log(C(t)/C(t+1))$ as a function of t, it should show a plateau at asymptotically large t values. It is easy to show that the effective mass approaches its plateau exponentially:

$$m_{eff}(t) = m + a \cdot \exp(-bt) \quad t \to \infty, \tag{7}$$

where m is the lowest mass in the given channel. One can fit the effective masses with the above formula and use it to extract the lowest masses. In this way one also uses the information stored in the points before the plateau even if the plateau itself is noisy. This technique turned out to be very stable and we could start to fit the effective masses at $t = 2,3$. Fig. 1 illustrates the method for the first two states in the negative parity channel at $\kappa = 0.1550$.

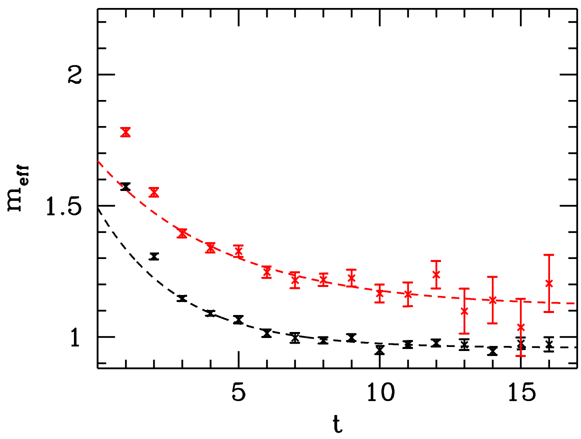

Figure 1: The effective masses for the first two states in the negative parity channel for $\kappa = 0.1550$ and the fitted exponentials.

In both parity channels we extracted the two lowest masses (which we denote by m_0 and m_1). It is straightforward to define the ratio $\alpha_i = m_i/(m_N + m_K)$ which compares the possible scattering and pentaquark states to the nucleon-kaon threshold. The experimental value of α for the Θ^+ particle is $\alpha_{\Theta^+} = 1.07$.

The summary of our results including also the pion, kaon and nucleon masses is given in Table 1. The zero momentum scattering state is just at the threshold. Above that scattering states are expected to appear at

$$E_k = \sqrt{m_K^2 + p_k^2} + \sqrt{m_N^2 + p_k^2}, \tag{8}$$

where

$$p_1 = \frac{2\pi}{aL_s}; \qquad p_k = p_1, \sqrt{2}p_1, \sqrt{3}p_1, \ldots \tag{9}$$

The ratio of E_1 to the threshold is 1.151, 1.166, 1.177, 1.202 for $\kappa = 0.1550, 0.1555, 0.1558$ and 0.1563, respectively for our larger volumes. For the smaller volume ($L_s = 20$) at $\kappa = 0.1550$ this ratio is 1.211. We can see that in all cases the measured mass ratios are consistent with the scattering states. The expected and measured volume dependences of the first excited state for negative parity and the ground state for positive parity is shown in Fig. 2.

For the highest quark mass, where we had the largest statistics we also performed the whole analysis for the isovector channel. The extracted masses and their volume dependence turned out to be qualitatively similar to those in the isoscalar channel.

The individual results in the odd and even parity channels can be summarized as follows (based on the statistically most significant, highest quark mass and assuming that $m_{\Theta^+}/(m_N + m_K)$ does not change significantly with the quark mass).

1. *Odd parity.* We extracted the two lowest lying states. The lower one is identified as the lowest scattering state with appropriate volume dependence (in this case the p=0 scattering means no volume dependence). This state is 6σ below the Θ^+ state. The volume dependence of the second lowest state is consistent with that of a scattering state with non-zero relative momentum. For our larger/smaller volumes this state is $1.8/2.1\sigma$ above the Θ^+ state. None of these two states could be interpreted as the Θ^+ pentaquark.

2. *Even parity.* The two lowest lying states are identified. The volumes are chosen such that even the lowest scattering state is above the expected Θ^+ pentaquark state. The volume dependence of the lowest state suggests that it is a scattering state. For both volumes this state is 6σ above the Θ^+ state. Since the energy of the second lowest state is even larger, none of them could be interpreted as the Θ^+ pentaquark.

To summarize in both parity channels we identified all the nearby states both below and above the expected Θ^+ state. Having done that no additional resonance state was found. This is an indication that in our wave function basis no Θ^+ pentaquark exists (though it might appear in an even larger, more exotic basis, with smaller dynamical quark masses or approaching the continuum limit).

The comparison of our results with those of others is not an easy task. Nevertheless, it is fair to say that existing lattice studies ([3, 4, 5, 6, 8, 9]) are not precise enough so that – contrary to first impression – really strong contradictions can not be claimed to exist.

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Table 1: The measured pion, kaon and nucleon masses and the ratio of the first two five-quark states in both parity channels to the KN threshold.

size	parity	$\kappa_{u,d}$	am_π	am_K	am_N	α_0	α_1
$24^3 \times 60$	–	0.1550	0.296(1)	0.317(1)	0.642(6)	1.01(1)	1.16(5)
$24^3 \times 60$	–	0.1555	0.259(1)	0.301(1)	0.613(5)	0.99(1)	1.16(5)
$24^3 \times 60$	–	0.1558	0.234(1)	0.290(1)	0.592(6)	0.99(1)	1.14(8)
$24^3 \times 60$	–	0.1563	0.185(1)	0.272(1)	0.545(7)	0.98(2)	1.28(13)
$20^3 \times 60$	–	0.1550	0.295(1)	0.316(1)	0.647(7)	1.00(1)	1.24(8)
$24^3 \times 60$	+	0.1550	0.295(1)	0.316(1)	0.636(6)	1.16(2)	1.45(16)
$24^3 \times 60$	+	0.1555	0.258(2)	0.299(2)	0.615(14)	1.13(3)	1.39(15)
$24^3 \times 60$	+	0.1558	0.233(2)	0.288(2)	0.595(12)	1.09(5)	1.39(17)
$24^3 \times 60$	+	0.1563	0.184(3)	0.270(2)	0.552(10)	1.14(8)	1.31(32)
$20^3 \times 60$	+	0.1550	0.295(1)	0.316(1)	0.647(6)	1.21(2)	1.48(12)

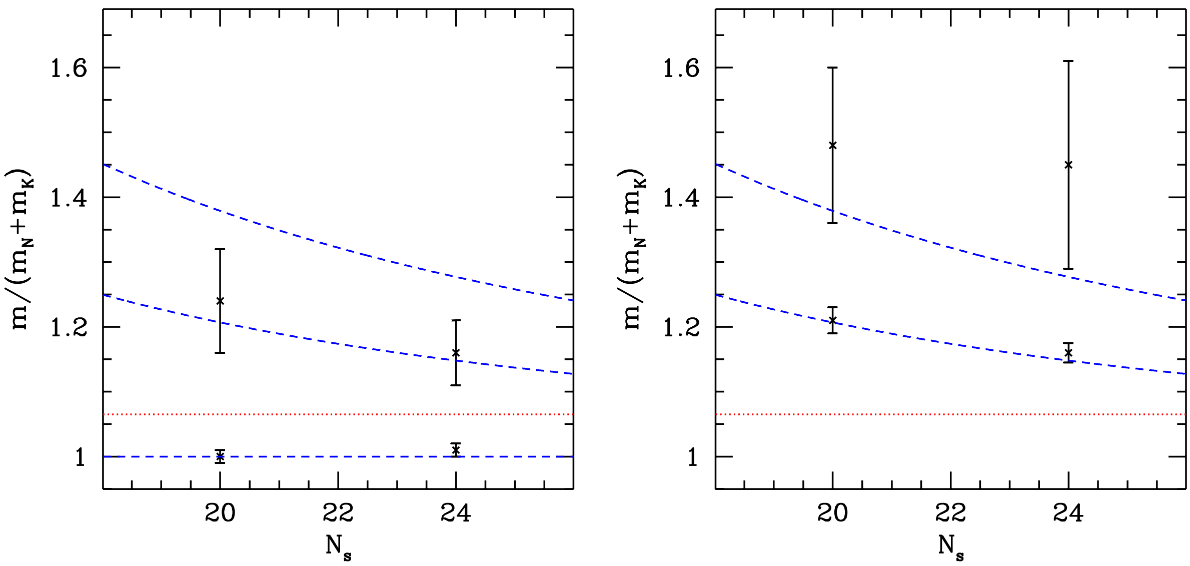

Figure 2: The volume dependence of the two lowest states in the two parity channels (left panel: negative parity; right panel: positive parity). The dashed lines indicate the expected scattering states with 0 momentum and the first two non-vanishing momenta. The dotted line shows the experimental value of the pentaquark state.

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