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Search for a New Kind of Particles: The $\Theta^+(1540)$ in Lattice QCD

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In the last years several independent experiments have claimed the observation of a new kind of particles called pentaquarks. The most prominent of these is the $\Theta^+(1540)$. Lattice QCD should be able to decide whether such states exist or not. We report on a study of the pentaquark $\Theta^+(1540)$, using a variety of different interpolating fields. We do not find any evidence for the existence of a Θ^+ with positive parity. We do observe, however, a signal compatible with normal nucleon-kaon scattering states. For negative parity the results are inconclusive, due to the potential mixture with nucleon-kaon and N^*-kaon scattering states.

1 Introduction

The possible discovery of the pentaquark-candidate $\Theta^+(1540)$ by the LEPS Collaboration at SPring-8[1] has initiated great interest in exotic baryons. While normal hadrons consist of either three valence quarks (baryons like the proton) or a valence quark-antiquark pair (mesons like the pion) these new states are supposed to have four valence quarks and one valence-antiquark. Their possible existence has been predicted since many years, but the great question was always how stable they would be. If the experimental data were correct they would have to live about a factor 100 longer than normal hadron resonances, which would be truely spectacular. Since then, there has been a large number of experiments that have confirmed this result[2–11] but also about the same number that could not confirm it[12–19]. Presently the experimental situation is highly unsettled[20,21], but the tendency goes clearly into the direction that the experimental signals for the $\Theta^+(1540)$ were artefacts.
Lattice QCD should be able to come up with a clear prediction, implying that it should come before the experimental situation is settled, but so far no conclusive answer was reached[22–30].
The difficulties are not only lying on the theoretical side, lattice QCD calculations also require a large amount of computer resources. In our calculations we performed a qualitative study using different types of spin-$\frac{1}{2}$ operators (called sources) with the quantum numbers of the Θ^+. We compute all cross-correlators and use the variational method[31,32] to extract the lowest lying eigenvalues. The construction of the so-called cross-correlation matrix is especially complicated for a particle which is as complex as the pentaquark. Thus, high performance code and a large parallel machine with access to many CPUs are needed. This is why we could perform this project only at Jülich.

2 Theoretical Basics

Let us describe first some fundamental facts about lattice QCD and explain how the search for new hadrons is done.

All of QCD is contained in the generating functional:

$$Z[J^a_\mu, \bar{\eta}^i, \eta^i] = \int \mathcal{D}[A^{a\mu}, \bar{\psi}^i, \psi^i] \exp\left(\mathrm{i} \int d^4x \left[\mathcal{L}_{\mathrm{QCD}} - J^a_\mu A^a_\mu - \bar{\psi}^i \eta^i - \bar{\eta}^i \psi^i \right] \right) \quad (1)$$

There exists a fundamental relationship between quantum theory and statistical physics, which is exploited by lattice QCD.

$$\begin{gathered} t \leftrightarrow -\mathrm{i}\tau \\ \text{Schrödinger-Equ.} \leftrightarrow \text{Diffusion-Equ.} \\ -\mathrm{i}\frac{\partial}{\partial t}\psi(\vec{x},t) = \frac{1}{2m}\ \Delta\psi(\vec{x},t) \leftrightarrow \frac{\partial}{\partial t}P(\vec{x},t;\vec{x}_0,t_0) = D\ \Delta P(\vec{x},t;\vec{x}_0,t_0) \\ S = \int d^4x (T-V) \leftrightarrow \mathrm{i}\int d^4x_E (T+V) = \mathrm{i}S_E \\ e^{\mathrm{i}S} \leftrightarrow e^{-S_E} \end{gathered}$$

This relationship is exact in the same way as analytic continuation is an exact operation in mathematics and it implies that many classes of QCD problems can be solved by statistical means, i.e. Monte Carlo techniques, just like e.g. diffusion problems. The typical plane wave solutions of quantum mechanics translate into exponentially decaying correlations proportional to $\exp(-Ex_4)$. So, one puts combinations of quark-fields with the correct total quantum numbers onto some sites on a lattice of space-time points (typically smeared to about the physical size of the hadron under study) and evaluates their correlation as a function of separation in the Euclidean time direction. This correlation is dominated by the lowest energy state, which is the lowest mass state for the given set of quantum numbers. So for the nucleon one can use e.g. the source ($C = i\gamma^2\gamma^4 = C^{-1}$):

$$\hat{B}_\alpha(t,\vec{p}) = \sum_{\vec{x}} e^{\mathrm{i}\vec{p}\cdot\vec{x}} \epsilon_{ijk} \hat{u}^i_\alpha(x)\ \hat{u}^j_\beta(x) (C^{-1}\gamma_5)_{\beta\gamma} \hat{d}^k_\gamma(x) \quad (2)$$

and study the correlation

$$\begin{aligned} \langle 0|T\left\{\hat{B}(y_4)\hat{A}(x_4)\right\}|0\rangle \Rightarrow\ & e^{-(T-y_4+x_4)E_B} \langle B|\hat{B}(0)|0\rangle\langle 0|\hat{A}(0)|B\rangle \\ +\ & e^{-(y_4-x_4)E_A} \langle 0|\hat{B}(0)|A\rangle\langle A|\hat{A}(0)|0\rangle \end{aligned} \quad (3)$$

Where $\hat{A}$ generates a particles for which all quantum numbers are the negative of those of the nucleon but which has also negative parity, while the nucleon has positive parity (this is a consequence of the fact that the nucleon is a fermion). One can read off from equation (3) that if the correlation is plotted against $\tau = x_4$ one will find the positive parity states on the left side and the negative parity ones on the right. In the following we plot both regions seperately. As our lattice has an extent of 24 sites in the temporal direction this leaves us with a bit less than 12 sites per parity, see Fig.1.

While the ground state spectroscopy is thus very well understood, the spectroscopy of excited states is still in its infancy, especially in full QCD. Therefore, one uses very often the quenched approximation, in which the quark-antiquark fluctuations of the vaccuum are neglected. This approximation should be a reasonably good one for the pentaquark which is supposed to be stabilized by very specific properties of the gluon fluctuations, namely gluon field configurations with non-trivial topology. (The gluons are treated exactly in the

quenched approximation.) On the practical side, dynamical calculations for this problem are presently computationally simply out of reach.
For excited states, instead of calculating a single correlator, which would be sufficient to extract the ground state, one calculates a whole matrix of correlators using different operators for creating and annihilating the considered particle. Of course, these operators must have the right quantum numbers and internal structure (e.g. s- versus p-wave function) to have sufficent overlap with the physical states in question.
The operators for the pentaquark are especially complicated, for they contain five quarks, whereas mesons and baryons only contain two or three quarks, respectively. Thus, the construction of operators with the right quantum numbers is a more difficult task. Furthermore the computational effort is growing exponentialy with the number of constituent quarks of the considered particle. In our calculation we considered a large number of operators. The simplest ones which have been suggested by Csikor/Fodor[22] are the following:

$$I_{0/1} = \epsilon_{abc}[u_a^T C\gamma_5 d_b]\{u_e \bar{s}_e i\gamma_5 d_c \mp (u \leftrightarrow d)\}, \tag{4}$$

where we used vector notation for the Dirac spinors and explicitly denoted the color indices. There are also other more complicated ones which have been suggested by Sasaki[23] or L. Ya. Glozman[33]. We then use all possible combinations of these operators to compute a matrix of correlators.

Before we were able to start our calculations for the Pentaquark Θ^+, we first have performed calculations for Nucleon and Kaon on the same lattice. We needed the results from these calculations for a comparison with the results from the analysis of our Θ^+ data.

Before we discuss the analysis of the results of our calculations in Section 4 and draw a conclusion in Section 6 we would like to give some details of how these calculations have been performed on the JUMP cluster at NIC in Jülich.

3 Details of the Calculation

To get the chiral limit we use 10 different quark masses on a $12^3 \times 24$ lattice. We organize our code that every CPU is computing the correlator for quark mass and one timeslice. So, after one run we have a complete 5×5 cross correlation matrix for the whole lattice and one s-quark mass (see 4). So we need also a second s-quark mass to interpolate to the physical s-quark mass. Without a parallel computer like the JUMP cluster at NIC, we would not be able to perform this calculation. Every single parallel job takes about 3 hours of computing time. To run such a task with a serial code would last more than 800 hours because of the IO handling which is not necessary on the JUMP cluster due to the large memory on the CPUs.

4 Analysis of the Results

We use the five interpolators to calculate a cross correlation matrix $C_{ij}(t)$ on the JUMP cluster which is then inserted into the generalized eigenvalue problem

$$C_{ij}(t)\vec{v}_i^{(k)} = \lambda^{(k)}(t)C_{ij}(t_0)\vec{v}_i^{(k)}. \tag{5}$$

size $L^3 \times T$	$12^3 \times 24$
β	7.90
a [fm]	0.148
a^{-1} [MeV]	1333
L [fm]	≈ 1.8
#conf N	100
quark masses am_q	0.02, 0.03, 0.04, 0.05, 0.06, 0.08, 0.10, 0.12, 0.16, 0.20
smearing parameters:	$n = 18$, $\kappa = 0.210$
s-quark mass am_s	0.0888(17)

Table 1. Parameters of our calculations.

The solutions of this equation behave like

$$\lambda^{(k)}(t) \propto \exp\left(-m^{(k)}(t-t_0)\right). \tag{6}$$

These eigenvalues are used to compute effective masses according to

$$m_{eff}(t) = \ln\left(\frac{\lambda(t)}{\lambda(t+1)}\right). \tag{7}$$

Ordering the five eigenvalues according to their absolute value the largest eigenvalue in the positive parity channel should give the Θ^+ mass, if Θ^+ is a positive parity particle. Else the second largest eigenvalue in the negative parity channel should give the Θ^+ mass, where the largest eigenvalue corresponds to the a N-K scattering state at rest.
In our quenched calculation, we use the Chirally Improved Dirac operator[35–39]. The gauge fields are generated with the Lüscher-Weisz gauge action[40,41] at $\beta = 7.90$. The strange quark mass is fitted using the pseudoscalar K meson. The parameters of our calculation are collected in Table 1.

5 Results

The results of our calculations are shown in Fig. 1, where we plot the effective masses of the two lowest lying states of both parity channels obtained with the cross-correlation technique. These states are approaching a possible plateau very slowly as we expected, since states consisting of five quarks are very complicated and therefore should contain a large number of excited states which have to die out before the effective mass reaches a plateau. We use in addition to the cross-correlation technique Jacobi smeared Gaussian quark sources for all our quarks to improve the signal for the lowest lying states.
The lower horizontal line in the negative parity channel is the sum of the nucleon and kaon mass at rest in the ground state obtained from a separate calculation on the same lattice. Since we project the final state to zero momentum a scattering state can also be a two particle state where the two particles have the same but antiparallel momentum, i.e.

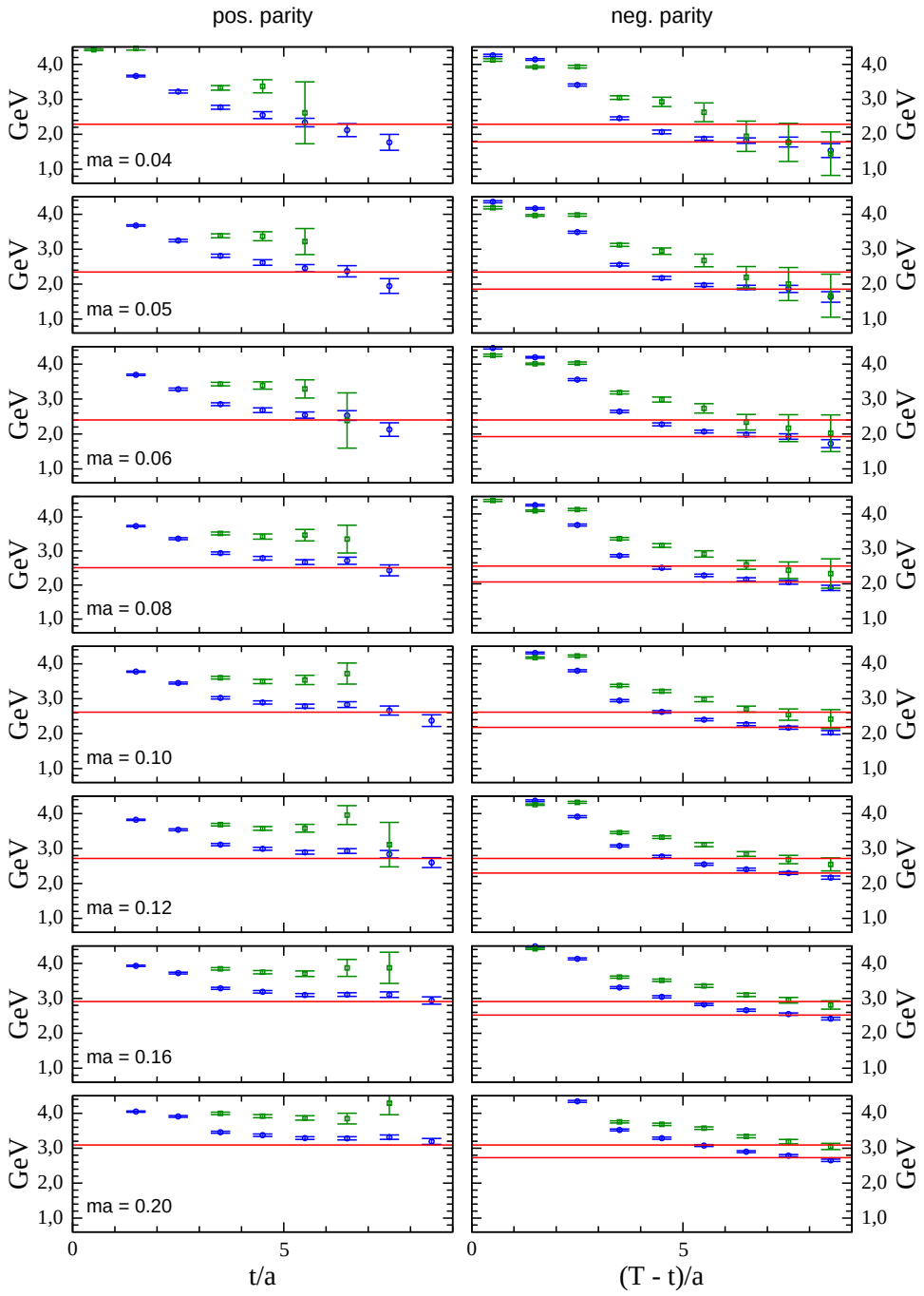


Figure 1. Results from cross-correlation of five interpolators. We use Jacobi smeared Gaussian quark sources for all our quarks. Only the effective masses of the two largest eigenvalues are plotted.

$\vec{p_N} = -\vec{p_K}$. We use the relativistic E-p-relation to calculate the energy of such states,

$$E = \sqrt{p^2 + m_N^2} + \sqrt{p^2 + m_K^2}, \tag{8}$$

where the smallest momentum is $2\pi/L \approx 700\,\mathrm{MeV}$ on our lattice. In Fig. 1 this energy is represented by the upper horizontal line.
We find effective mass plateaus which are consistent with N-K scattering states in the negative parity channel as we expect. We find that the second state is noisy but within errors consistent with the energy in (8). Therefore, it is most likely that we do not observe a Θ^+ state in the negative parity channel. However, this conclusion is not completely certain, if the Θ^+ is broad, because such a Θ^+ state would mix strongly with the continuum states. In the positive parity channel one expects to find either a bound Θ^+ or an excited N-K scattering state. For such an excited state there are several possibilities, e.g., N^*-K, or N-K with a relative angular momentum, and so on.
On the positive parity side, we also show the two lowest lying states obtained from our calculation. Both of them can be identified with continuum states in the sense of Eq. (8) Especially the second one is far too heavy to describe a Θ^+ state. It probably corresponds to an excited N-K scattering state. If there were a signal belonging to the Θ^+ it is supposed to lie below the red line assuming that the chiral extrapolation (e.g. the extrapolation to the nearly vanishing physical up- and down-quark masses) of the Θ^+ does not lead to dramatic effects below our smallest quark mass.

6 Conclusion

In this article we present the results of a pilot study of the Θ^+ using different types of operators. We find that for negative parity our results are in good agreement with a N-K scattering state in the ground state and a quite noisy signal for the first excited state.
For positive parity we find a second state typically more than $500\,\mathrm{MeV}$ heavier than the Θ^+ and which is thus not compatible with a Θ^+ mass of $1540\,\mathrm{MeV}$. This state is probably a higher scattering state.
Thus our calculation do not show any hints for a Θ^+ in the quenched approximation with chiral fermions for the positive parity channel. In the negative parity channel we would need smaller errors to be able to make a really firm statement in favour of or against the existence of a Θ^+ state, but it is clear that there is no indication for such a state in our data. One should also be aware that lattice data cannot rule out the existence of a state with near to zero overlap with the chosen sources. Therefore, it is crucial that many different attempts are made with many different sources to search for the pentaquark states. This is what happens presently.

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