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## THE STATUS OF PENTAQUARK SPECTROSCOPY ON THE LATTICE\*

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The present work is a summary of the status of lattice pentaquark calculations. After a pedagogic introduction to the basics of lattice hadron spectroscopy we give a critical comparison of results presently available in the literature. Special emphasis is put on presenting some of the possible pitfalls of these calculations. In particular we discuss at length the choice of the hadronic operators and the separation of genuine five-quark states from meson-baryon scattering states.

### 1. Introduction

The recent experimental searches for and the discovery<sup>1,2</sup> of the previously theoretically predicted<sup>3</sup> exotic hadrons has sparked considerable activity and gave rise to diverse speculations regarding their structure, unexpectedly small width, parity, isospin and spin. The only presently available technique for computing low energy hadronic observables starting from first principles (i.e. QCD) within systematically controllable approach is lattice QCD.

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\*Based on talks the authors gave at various conferences.

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All this said, it might seem surprising that of the more than 200 papers devoted to the subject of exotic baryons in the past year, there were only four lattice papers. Besides critically reviewing the currently available lattice results, in the present work we also try to resolve this apparent paradox by discussing some of the difficulties and pitfalls of the lattice approach. The presentation is aimed for the general particle and nuclear physics community. For this reason, in Section 2 we start with an introduction to lattice hadron spectroscopy and also address two points that are usually not discussed in great detail in lattice papers, but are essential for the correct interpretation of lattice pentaquark results.

In our opinion the biggest challenge lattice pentaquark calculations face is how to choose the baryonic operators. Not only the errors, but also the very possibility to identify certain states depends crucially on the choice of operators. Unfortunately there is very little guidance here and many technical restrictions. Subsection 2.1 is devoted to this issue. Since the five-quark bound states we want to study can be close to threshold, it is essential in any lattice spectroscopy calculation to reliably distinguish between genuine five-quark bound states and meson-baryon scattering states. In Subsection 2.2 we discuss how this can be done.

Having set the stage, in Section 3 we give a critical review of the currently available lattice results and interpret them. In Section 4 we conclude by summarizing the status of lattice calculations and stressing what is needed to be done for a final consolidation of the lattice results.

## 2. Hadron spectroscopy on the lattice

### 2.1. *The choice of operators*

In the framework of lattice QCD the role of the regulator is played by a space-time lattice that replaces continuous space-time. As a result, in a finite spatial volume the infinite dimensional functional integral turns into a mathematically well defined finite dimensional integral. The lattice also opens the way to the explicit numerical computation of hadronic observables by Euclidean Monte Carlo techniques.

In hadron spectroscopy one would like to identify hadronic states with given quantum numbers. Practically this means the following. We compute the vacuum expectation value of the Euclidean correlation function  $\langle 0 | \mathcal{O}(t) \mathcal{O}^\dagger(0) | 0 \rangle$  of some composite hadronic operator  $\mathcal{O}$ . The operator  $\mathcal{O}$  is built out of quark creation and annihilation operators. In physical terms the correlator is the amplitude of the “process” of creating a complicated

hadronic state described by  $\mathcal{O}$  at time 0 and destroying it at time  $t$ .

After inserting a complete set of eigenstates  $|i\rangle$  of the full QCD Hamiltonian the correlation function can be written as

$$\langle 0|\mathcal{O}(t)\mathcal{O}^\dagger(0)|0\rangle = \sum_i |\langle i|\mathcal{O}^\dagger(0)|0\rangle|^2 e^{-(E_i-E_0)t}, \quad (1)$$

where

$$\mathcal{O}(t) = e^{-Ht} \mathcal{O}(0) e^{Ht} \quad (2)$$

and  $E_i$  are the energy eigenvalues of the Hamiltonian.

Note that since we work in Euclidean space-time (the real time coordinate  $t$  is replaced with  $-it$ ), the correlators do not oscillate, they rather die out exponentially in imaginary time. In particular, after long enough time only the lowest (few) state(s) created by  $\mathcal{O}$  give contribution to the correlator. The energy eigenvalues corresponding to those states can be extracted from exponential fits to the large  $t$  behaviour of the correlator.

In the simplest cases one is typically interested in hadron masses. A trivial but most important requirement in the choice of  $\mathcal{O}$  is that it should have the quantum numbers of the state we intend to study. Otherwise the overlap  $\langle i|\mathcal{O}^\dagger(0)|0\rangle$  would be zero and the corresponding exponent could not be extracted. In order to have optimal overlap with only one state  $|i\rangle$ ,  $\mathcal{O}^\dagger(0)|0\rangle$  should be as “close” to  $|i\rangle$  as possible.

A hadron mass is the ground state energy in a sector with given internal quantum numbers and zero momentum. Projection to the zero momentum sector is achieved by summing a local operator over all of three-space as

$$\mathcal{O}(\vec{p}=0) = \sum_{\vec{x}} e^{-i\vec{p}\vec{x}} \mathcal{O}(0, \vec{x})|_{\vec{p}=0} = \sum_{\vec{x}} \mathcal{O}(0, \vec{x}). \quad (3)$$

One of the most important experimentally still unknown quantum numbers of pentaquark states is their parity. Thus, we also briefly touch upon the parity assignment on the lattice. The simplest baryonic operators do not create parity eigenstates, rather they couple to both parity channels. Projection to the  $+/-$  parity eigenstates can be performed as

$$\mathcal{O}_\pm = \frac{1}{2}(\mathcal{O} \pm P\mathcal{O}P^{-1}). \quad (4)$$

For the simplest operators the parity operator  $P$  acts on  $\mathcal{O}$  as

$$P\mathcal{O}P^{-1} = \eta\gamma_0\mathcal{O}, \quad (5)$$

where  $\eta = \pm 1$  is the internal parity of the operator  $\mathcal{O}$ . For more complicated operators, in particular for non-pointlike ones, this might become

more involved. If the parity of a state is not known, it can be determined by computing the correlator in both parity channels and deciding which channel produces a mass closer to the experimentally observed one.

All quantum numbers fixed, there is still considerable freedom in the choice of  $\mathcal{O}$ . This freedom has to be exploited to ensure maximal overlap of  $\mathcal{O}^\dagger(0)|0\rangle$  with the desired state and minimal overlap with close-by competing, but unwanted states. This is essential not only for smaller errors. With the wrong choice of  $\mathcal{O}$  the desired state might be practically undetectably lost in the noise. Unfortunately, beyond the quantum numbers there is usually little if any guidance in the choice of  $\mathcal{O}$  and herein lies the biggest challenge of lattice pentaquark spectroscopy. It is almost impossible to *disprove* the existence of a given state. If one cannot detect it with a given operator  $\mathcal{O}$ , it might just mean that  $\mathcal{O}$  has too small overlap with the desired state and the signal is lost in the noise. Indeed, even in the case of the nucleon simple operators are known that have the correct quantum numbers, but too little overlap with the nucleon ground state and no nucleon signal can be extracted from their correlator<sup>4</sup>.

If the wave function of the quarks in the given hadronic state were known, that would dictate the form of the operator to be used. In the case of pentaquarks there are several suggestions in the literature and in principle it would be interesting to try operators corresponding to at least some of them. There are, however, two serious restrictions lattice calculations face in this respect. The first one concerns the spatial structure of the wave function, the second one its index structure. In the remainder of this section we discuss these.

Concerning the spatial structure of the wave function, we have to note that the correlation function in Eq. (1) is computed on the lattice by decomposing it in terms of single quark correlators  $\langle 0|q_\alpha(x)q_\beta^\dagger(y)|0\rangle$ . Those in turn are simply the matrix elements  $D^{-1}(x, \alpha; y, \beta)$  of the inverse of the lattice Dirac operator. If  $\mathcal{O}$  were to be based on an arbitrary five-quark wave function, the brute force computation of the correlator of  $\mathcal{O}$  would in general require quark propagators  $D^{-1}(x, \alpha; y, \beta)$  from any space-time point  $x$  to any other point  $y$ . On currently used lattice sizes this would require the computation and storage of order  $10^{13}$  matrix elements, taking up about 100 Terabytes and requiring hundreds of Teraflops of CPU power. This is clearly out of reach for presently available computers.

The only way around is to fix a quark wave function  $\psi_\beta(\vec{y})$  and store

only the matrix elements

$$d(x\alpha) = \sum_{\vec{y}\beta} D^{-1}(x, \alpha; y_0 = 0, \vec{y}, \beta) \psi_\beta(\vec{y}). \quad (6)$$

This choice drastically cuts down the computing requirements. Unfortunately, at the same time it also restricts  $\mathcal{O}$  to be built as a product of single quark wave functions with the single quarks being in some state  $\psi$ . One needs to perform as many Dirac operator inversions as the number of different quark wave functions contained in  $\mathcal{O}$ . Since Dirac operator inversion is usually the most expensive part of these computations, one typically settles with using only two different quark sources, one for the light quarks and one for the strange quark. In fact, all four lattice pentaquark studies have used this simplest choice.

Besides the spatial structure of  $\mathcal{O}$  the single quark spin, colour and flavour indices also have to be arranged properly for  $\mathcal{O}$  to have the desired quantum numbers. Even then the arrangement of indices is also not unique. An additional difficulty one faces here compared to conventional three quark hadron spectroscopy is that index summation becomes exponentially more expensive if we increase the number of quarks. While with three quarks this part of the calculation is usually negligible, even for the simplest five quark operators it takes up around 50% of the CPU time. This circumstance restricted the choice of pentaquark operators so far to the simplest ones.

To illustrate how these issues appear in practice we now discuss a few specific examples of  $\mathcal{O}$  that have already been used. In the first lattice study<sup>5</sup>  $\mathcal{O}$  had the same Dirac structure as that of nucleon plus kaon system, but colour indices were contracted differently, as<sup>6</sup>

$$\mathcal{O}_{I=0/1} = \epsilon_{abc} [u_a^T C \gamma_5 d_b] \{u_e \bar{s}_e i \gamma_5 d_c \mp (u \leftrightarrow d)\}, \quad (7)$$

where  $I = 0/1$  and the two alternative signs correspond to the isospin singlet and triplet channel respectively. One could also contract the colour indices as in the nucleon $\times$ kaon, a choice used by Mathur et al.<sup>13</sup>

Another possible way to contract the quark indices in  $\mathcal{O}$  is according to the diquark-diquark-antiquark picture of Jaffe and Wilczek<sup>7</sup>. They proposed to insert the two diquarks in

$$\mathcal{O}_{I=0} = \epsilon_{adg} [\epsilon_{abc} u_b^T C \gamma_5 d_c] [\epsilon_{def} u_e^T C \gamma_5 d_f] C \bar{s}_g^T. \quad (8)$$

in a relative P-wave.

In general, in a diquark-diquark-antiquark wave function of the form

(8) the two diquarks must be in different quantum states<sup>a</sup>. On the lattice, that would require the computation of several quark propagators. Instead, Sasaki avoided the diquark-diquark symmetry by omitting a  $\gamma_5$  from one of the diquarks<sup>8</sup>. The operator he, and following in his footsteps subsequently Chiu & Hsieh<sup>9</sup> considered, was

$$\mathcal{O}_{I=0} = \epsilon_{adg} [\epsilon_{abc} u_b^T C d_c] [\epsilon_{def} u_e^T C \gamma_5 d_f] C \bar{s}_g^T. \quad (9)$$

In summary, both in terms of spatial and index structure there are many more possibilities for  $\mathcal{O}$ , but on the lattice they all require considerably more CPU time than the ones explored so far. However, we expect that several other possibilities will be tried in the near future.

## 2.2. Separating two particle states

Pentaquark spectroscopy is further complicated by the presence of two-particle scattering states lying close to the pentaquark state. Lattice calculations are always performed in a finite spatial volume, therefore these scattering states do not form a continuum. They occur at discrete energy values dictated by the discrete momenta  $p_k = 2k\pi/L, k = 0, 1, \dots$ , allowed in a box of linear size  $L$ . In lattice pentaquark computations it is absolutely essential to be able to distinguish between these two-particle nucleon-meson scattering states and genuine five quark bound states.

In fact, the first experimentally found exotic baryon state, the  $\Theta^+(1540)$  lies just about 100 MeV *above* the nucleon-kaon threshold. This implies that for large enough time separation the correlation function is bound to be dominated by the nucleon-kaon state. However, the mass difference between the two states is quite small and the mass of the  $\Theta^+$  might still be reliably extracted in an intermediate time window, provided that

$$|\langle \Theta^+ | \mathcal{O} | 0 \rangle| \gg |\langle N + K | \mathcal{O} | 0 \rangle|. \quad (10)$$

Even then, identifying the  $\Theta^+$  is still a non-trivial matter since the  $\Theta^+$  ground state is embedded in an infinite tower of nucleon kaon scattering states with relative momenta allowed by the finite spatial box. Since the parity of the  $\Theta^+$  is unknown, we have to consider both parity channels. The situation is qualitatively different in the two channels.

If the  $\Theta^+$  had positive parity, its lattice identification would be somewhat simpler. This is because due to the negative internal parity of the kaon

<sup>a</sup>Otherwise the operator identically vanishes due to its symmetry with respect to the interchange of the diquarks.

it is only the scattering states with odd angular momentum that produce positive parity. The scattering state with zero relative linear momentum does not couple to these and consequently it does not appear in the positive parity channel. Therefore, the lowest scattering state here has relative momentum  $p = 2\pi/L$  and it is above the  $\Theta^+$ , provided the linear size of the spatial box is smaller than 4.5 fm. The box can thus be chosen small enough to ensure that the  $\Theta^+$  is the lowest state with positive parity and also to leave a large enough energy gap for its safe identification.

The situation is much less favourable in the negative parity channel. Using a similar argument one can show that here it is always the  $p_{\text{rel}} = 0$  scattering state that is the lowest. The best we can do is that with the proper choice of the spatial volume the  $\Theta^+$  ground state can be the second lowest state. Due care must be taken to ensure that  $\Theta^+$  is between the first two scattering states, well separated from both of them. This is essential because the reliable identification of higher lying states is much more difficult.

Finally, for a convincing confirmation of the pentaquark state in either parity channel, one also has to identify the competing scattering states observing the volume dependence dictated by the allowed smallest momentum. This would clearly require a finite volume analysis combined with a reliable method to extract *several* low lying states from the spectrum. Apart from the volume dependence of the masses, another powerful tool to distinguish between two-particle and one-particle states is to check the volume dependence of their spectral weights<sup>13</sup>.

There are essentially two possible ways of identifying more than one low lying state from correlators. Firstly, if there is a time interval where more than one state has an appreciable contribution to the correlator, a sum of exponentials can also be fitted as

$$\langle 0|\mathcal{O}(t)\mathcal{O}^\dagger(0)|0\rangle = C_1e^{-E_0t} + C_2e^{-E_1t} + \dots \quad (11)$$

For this method to yield reliable energy estimates for higher states, one usually needs extremely good quality data.

The other possibility is to make use of several different operators, compute all possible cross-correlators and diagonalize the Hamiltonian in the subspace spanned by the states created by those operators<sup>12,4,11</sup>. This is a very powerful method to identify excited states and it can also be combined with the first possibility.

### 2.3. Extrapolations, sources of errors and uncertainties

The lattice spectroscopy of hadrons built out of light quarks involves two extrapolations. Firstly, simulations at the physical  $u/d$  quark masses would presently be prohibitively expensive, therefore one has to do several calculations with heavier quarks and then extrapolate to the physical quark masses. A set of typical chiral extrapolations are shown in Fig. 1.

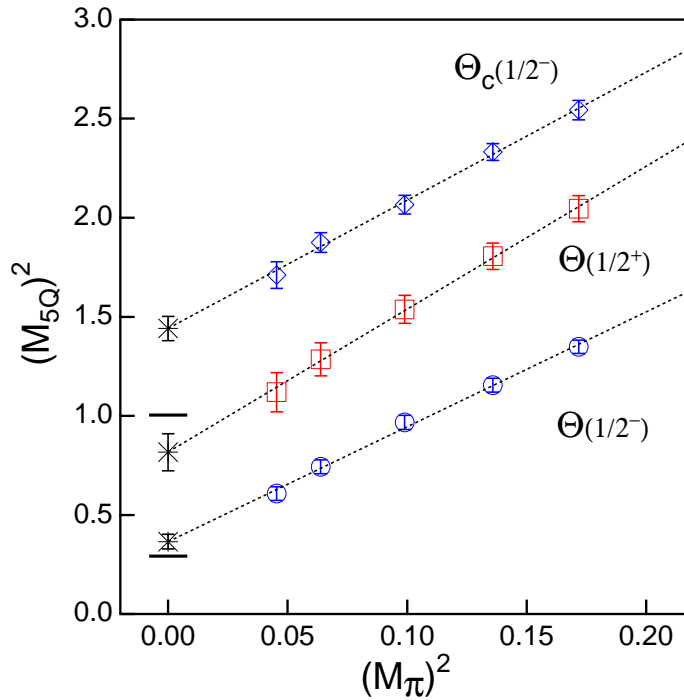


Figure 1. Chiral extrapolation of the masses different five quark states from Ref.<sup>7</sup>

The lightest quarks used in presently available pentaquark studies correspond to pion masses in the range 180-650 MeV (see Table 1).

Secondly, the space-time lattice is not a physical entity, it is just a regulator that has to be eventually removed to recover continuous space-time. This implies that physical quantities have to be computed on lattices of different mesh sizes and extrapolated to the zero lattice spacing (continuum) limit. Lattice simulations can differ from one another in many technical



Table 1. Lattice spacing and smallest pion mass of lattice pentaquark calculations.

	action	$a$ (fm)	smallest $m_\pi$ (MeV)
Csikor et al.	Wilson	0.17-0.09	420
Sasaki	Wilson	0.07	650
Liu et al.	chiral	0.20	180
Chiu & Hsieh	chiral	0.09	400

details and it is only the continuum limit of physical quantities that is meaningful to compare among different simulations.

In the remainder of this Subsection we briefly summarize the sources of errors and uncertainties in lattice simulations indicating also how to handle them.

- *Statistical errors* are well understood and can be kept at bay by increasing the statistics.
- *Extrapolations* in quark mass and lattice spacing are another source of uncertainty. Fortunately mass ratios of hadrons are usually quite insensitive in the present range of parameters.
- *Quenching*, i.e. neglecting the fermion determinant (omitting quark loops) is still a necessary compromise we have to live with in most of the lattice calculations. Fortunately experience tells us that stable hadron mass ratios have only a few per cent quenching error.
- *Finite volume* effects constitute another potential source of error. There are different sources of volume dependence that can be properly accounted for and even be used to distinguish between bound states and two particle scattering states.
- As we have already discussed the desired state can be *contaminated from other nearby states*, but this can be taken care of by a combination of the cross correlator technique and a careful finite volume analysis.
- Finally there is a theoretical uncertainty originating in the lack of any guidance in the *choice of operators* and the inability to choose  $\mathcal{O}$  optimally. This can result in larger statistical errors or even in a complete failure to identify an existing state. For this reason it is almost impossible to rule out the existence of a state with given energy and quantum numbers.

### 3. Results

Having set the stage we can now present the lattice results along with our interpretation. Four independent lattice pentaquark studies have been

presented. Their main results can be summarized as follows.

- *Csikor, Fodor, Katz and Kovacs*<sup>5</sup> identified a state in the  $I^P = 0^-$  channel with a mass consistent with the experimental  $\Theta^+$  and the lowest mass found in the opposite parity  $I^P = 0^+$  channel was significantly higher. Using  $2 \times 2$  cross correlators an attempt was also made to separate the  $\Theta^+$  and the lowest nucleon kaon state.
- *Sasaki*<sup>8</sup> using a different operator and double exponential fits, subsequently also found a state consistent with the  $\Theta^+$  also in the  $I^P = 0^-$  channel. He also managed to identify the charmed analogue of the  $\Theta^+$  640 MeV above the  $DN$  threshold. (The experimentally found anticharmed pentaquark lies only about 300 MeV above the threshold.)
- *Liu et al.*<sup>13</sup> reported that they could not see any state compatible with the  $\Theta^+$  in either parity isosinglet channel. Although their smallest pion mass was the closest to the physical one and the use an improved, chiral Dirac operator, they utilized the nucleon $\times$ kaon operator and their lattice is the coarsest of the four studies<sup>b</sup> On the other hand they made use of sophisticated multi-exponential fits with Bayesian priors.
- Finally *Chiu & Hsieh*<sup>10</sup>, in disagreement with the first two studies, saw a positive parity isosinglet state compatible to the  $\Theta^+$ , whereas the lowest state they found in the negative parity state was much higher. In a subsequent paper<sup>10</sup> they also identified states claimed to be charmed counterparts of the  $\Theta^+$ .

Our tentative interpretation of this somewhat controversial situation is as follows. Liu et al. used only one operator with exactly the same index structure as that of the nucleon kaon system. This might explain why they see only the expected scattering states.

The three remaining studies could be interpreted to have found genuine pentaquark states. All three agree that the lowest masses in the two parity channels differ by about 50%, but they do not agree on the parity of the  $\Theta^+$  state. While Csikor et al. and Sasaki suggest negative parity, Chiu & Hsieh claim positive parity. According to the interpretation of Chiu & Hsieh they found different parity because they used a quark action with better behaviour at small quark masses, albeit the same operator as Sasaki. The pion masses they use ( $\geq 400$  MeV) overlaps with those

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<sup>b</sup>.

of Sasaki ( $\geq 650$  MeV). In this region using the same hadron operator all other hadron masses in the literature obtained with these two quark actions agree (see e.g.<sup>9,14</sup>). Thus it is extremely unlikely that the same operator with different lattice actions produces such vastly different masses.

In our opinion a more likely resolution of this contradiction is that someone might have simply misidentified the parity. On the one hand, the results of Chiu & Hsieh and on the other hand, those of Sasaki (and Csikor et al.) would become compatible with each other if parities were flipped in one of them. A possible hint for a parity mismatch is provided by Chiu & Hsieh in their second paper<sup>10</sup>. They considered two operators with opposite internal parities, but otherwise having exactly the same quantum numbers. Contrary to physical expectations, their ordering of the lowest mass states in the two parity channels turned out to depend on the internal parity of the operator. This suggests that internal parity might not have been properly taken into account (see Eq. 5). Finally we would like to note that at this stage we can merely offer these speculations and the issue has to be resolved by an independent study.

#### 4. Conclusions

In summary, lattice QCD is the only known systematic approach to calculate the features of the pentaquarks from first principles (i.e. QCD). There have been four independent exploratory lattice pentaquark studies so far with somewhat different findings. One of them sees only the expected scattering state. Three analyses suggest mass states around the experimentally detected pentaquarks. In order to justify these signals as pentaquark states one should convincingly separate them from the existing nearby scattering states. None of the groups carried out this analysis. Furthermore, it should be realized that none of these analyses can be complete for the following reason. In such a complete analysis one should see the pentaquark in one parity channel and the lowest expected scattering state in the other. All of the three groups reported energy states coinciding with the pentaquark mass in one of the parity channels; however, in the other channel the energy state is much higher than the expected scattering state.

Since both parities have been suggested by lattice works, at least one of the results will coincide with the parity to be found experimentally. Nevertheless, no convincing final answer from lattice QCD can be claimed unless the above program has been completed. More specifically, it cannot be ruled out that pentaquark states observed so far on the lattice turn out

to be mixtures of nucleon-kaon scattering states.

As we already emphasized, for a full picture one needs to systematically map out the lowest few states in all interesting channels. This will most likely be possible only with the use of non-trivial spatial quark wave functions, the study of several operators and the cross-correlator technique combined with a careful finite volume analysis. This is currently under way and we hope to be able to report new results in the near future.

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