Hadron Spectroscopic Methods in Lattice Quantum Chromodynamics

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– Thesis –

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1 Introduction

The theory that most accurately describes the strong interaction is quantum chromodynamics (QCD). One of the most important properties of QCD is asymptotic freedom, according to which the coupling constant decreases when the energy scale is increased. As a consequence the processes involving high energy exchange and phenomena occurring at very high temperatures can be well understood using perturbative calculations. This way the high energy regime of QCD can be tested with high energy collisions.

On the other hand, at low energies quantum chromodynamics has the property of confinement. This is the consequence of the fact that when one tries to separate quarks from each other, the potential between them increases linearly. Therefore, free quarks and gluons cannot be produced, only their bound states, the hadrons can be observed. In this low energy region the coupling constant becomes so large which makes perturbative theory break down. Thus, hadrons such as nucleons and pions cannot be studied using perturbative calculations. Therefore, a reliable nonperturbative method for describing the low energy region of QCD is required.

This nonperturbative method is lattice QCD. Since its first appearance the lattice technique has evolved enormously, which together with the improvement in computer technology made lattice QCD the primary tool for examining the nonperturbative properties of hadrons.

After the appearance of the first experimental sign of the $\Theta^+$ pentaquark several lattice groups performed calculations in order to find its experimentally yet unknown quantum numbers. These results, however, seemed to be inconsistent with each other. Therefore, the need emerged for a comprehensive search, in which all the states having the same quantum numbers as the $\Theta^+$ can be identified up to above the expected mass of the $\Theta^+$. For this, however, due to the possibly complicated wave function of the pentaquark, operators with trivial spatial structure are not sufficient. The first aim of my thesis is to construct spatially nontrivial operators with definite spin, and to perform a comprehensive search in both parity channels for the $\Theta^+$ pentaquark.

The difficulty of the need to find the correct interpolating operators, which also emerged during the search for the $\Theta^+$, has led to the second aim of my thesis: to find a spectroscopic method that is able to give the masses of particles based solely on their quantum numbers.
2 Methods

All calculations were carried out using the Wilson plaquette gauge action. The quenched approximation is known to describe the stable hadron spectrum with reasonable accuracy, therefore, we used quenched gauge configurations in our search for the Θ⁺ pentaquark. For the calculation of quark propagators the Wilson fermion discretization was used.

The scale was determined using the static quark-antiquark potential. For finer lattices the value \( r_0 = 0.469(7) \) fm of the Sommer scale was used, while on coarser lattices we used the value \( \sqrt{\sigma} = 465 \) MeV of the string tension.

The spatial extensions of the lattices used in the search for the Θ⁺ pentaquark were \( L_s = 2.24 \) fm and \( L_s = 1.86 \) fm. At such box sizes the Θ⁺ pentaquark is the lowest state in the positive parity channel, and the second lowest state in the negative parity channel. For a reliable signal of the Θ⁺ pentaquark all the nucleon-kaon (N − K) scattering states up to above the expected mass of the Θ⁺ have to be identified and clearly distinguished from the pentaquark state. Therefore, at our volumes at least two interpolating operators having positive parity and at least three operators with negative parity are required.

Since some of the pentaquark wave functions suggested in the literature cannot be utilized with operators having trivial spatial structure, besides trivial ones we used operators with extended spatial structure for our calculations.

- Operators with negative parity:
  - \( O_1 \): Nucleon-kaon with trivial spatial structure.
  - \( O_2 \): Diquark-diquark-antiquark with trivial spatial structure.
  - \( O_3 \): Nucleon-kaon shifted by \( L_s/2 \) having a trivial relative angular momentum.

- Operators with positive parity:
  - \( O_4 \): Diquark-diquark-antiquark shifted by one lattice spacing with a relative angular momentum of \( l = 1 \).
  - \( O_5 \): Nucleon-kaon shifted by \( L_s/4 \) with a relative angular momentum of \( l = 1 \).

In order to find the linear combinations of the above operators that have the best overlap with the lowest lying states we used the cross-correlator technique already successfully applied in glueball spectroscopy.

Near the very low physical quark masses the calculation of the correlators of five-quark operators using Wilson fermions is very expensive, and the obtained propagators are rather noisy. Therefore, we used somewhat higher quark masses, which gave us pion masses in the range \( m_\pi = 400 − 630 \) MeV. Therefore, instead of the masses \( m \) of the states we investigated the less quarkmass-dependent values \( m/(m_N + m_K) \).
The method for obtaining the masses of states using thermodynamic considerations was based on the fact that the free energy of a given quark number sector follows a linear behaviour at very low temperatures. The slope of the linear gives information about the multiplicity of the ground state in the given channel, and the $T \to 0$ limit is equal to the mass of the lowest state.

The canonical partition functions are the Fourier coefficients of the grand canonical partition function when considered as a function of imaginary chemical potentials. Therefore, in order to obtain the free energy of a given quark number sector the corresponding Fourier coefficient of the grand canonical partition function has to be measured.

The grand canonical partition function at nonzero chemical potentials can be written as the expectation value taken on zero chemical potential configurations of the quotient of the fermion determinant at the chemical potentials in question and the fermion determinant at zero chemical potentials. The explicit chemical potential dependence of this determinant ratio can be expressed using the eigenvalues $\lambda$ of the reduced fermion matrix. These eigenvalues have the symmetry $\lambda \leftrightarrow 1/\lambda^*$, therefore, only the eigenvalues lying in the complex unit circle appear in the expression of the determinant ratio.

At low temperatures the eigenvalues lying in the complex unit circle are very small, therefore, the determinant ratio can be given as a Taylor series of these eigenvalues. Only the largest of these eigenvalues give significant contribution to the terms of the series. The reduced fermion matrix was produced using multiple precision calculations, then its relevant eigenvalues were obtained using the double precision version of the ARPACK library.

In order to test the spectroscopic method we performed numerical calculations with Kogut–Susskind (staggered) fermions. In order to test whether the staggered root taking modifies the results we performed calculations using 2, 4 and 8 staggered quark tastes.
3 Results

1. I have given a method to obtain interpolating operators with extended spatial structure that transform according to the spin $s = \frac{1}{2}$ representation of the cubic group, the symmetry group of a lattice with finite lattice spacing.

2. Using this method I constructed the operator basis used in the search for the pentaquark. Due to the possibilities of the nontrivial spatial structure I was able to obtain operators having spin $s = \frac{1}{2}$ corresponding to the nucleon-kaon scattering states as well as diquark-diquark-antiquark type states in both parity channels. Using this operator basis all the nucleon-kaon scattering states in both parity channels up to above the expected mass of the pentaquark were successfully identified.

3. I have shown that when using Wilson fermions with a Wilson parameter different from one a matrix analogous to the staggered reduced fermion matrix can be obtained. I have expressed the chemical potential dependence of the determinant ratio using the eigenvalues of this matrix.

4. I have expressed the Fourier coefficients of the determinant ratio as a power series of the eigenvalues of the reduced fermion matrix for both staggered and Wilson fermions. I have shown how the non-$Z_3$ invariant terms that have zero expectation value can be cancelled out from the series expansion. Taking advantage of the symmetry of the reduced fermion matrix I have given a robust numerical method for obtaining its relevant eigenvalues.

5. I have shown that although the applicability of the spectroscopic method based on thermodynamic considerations is rather limited, it can be used to give the masses of the ground states of the different isospin sectors. I have tested the method performing calculations with dynamical staggered fermions, and found that the obtained mass of the Goldstone pion, which is the ground state in the $I_3 = 1$ sector, is consistent with the mass obtained using the Euclidean correlator technique.
4 Conclusions

During the search for the $\Theta^+$ pentaquark the volume dependence of the lowest two states were consistent with the lowest two nucleon-kaon scattering states in both the negative and positive parity channels (Figure 1).

This statement is even more strengthened when one examines the wave functions of these states. In the positive parity channel, where one expects the $\Theta^+$ to be the ground state, the diquark-diquark-antiquark type operator gives negligible contribution into the ground state. In the negative parity channel the diquark-diquark-antiquark type operator also gives minor contribution into the lowest two states (Figure 2). Therefore, all the scattering states up to above the expected mass of the $\Theta^+$ pentaquark were found and identified. Assuming that the combination $m_{\Theta^+}/(m_N + m_K)$ does not depend significantly from the quark masses, we can state that no pentaquark signal was found.

The spectroscopic method based on the canonical partition functions can be used in principle to obtain the masses of baryons, or even for measuring the bonding energies of multi-baryon states. However, it turns out that such calculations are so demanding that practically they cannot be carried out. Nevertheless, the method can be used to measure the energies of the ground states of the different isospin sectors. The ground state in the $I_3 = \pm 1$ sector is the Goldstone pion, and by performing calculations in higher isospin sectors even pion-pion interactions can be examined. The numerical results show that irrespective of the staggered root taking the spectroscopic method based on thermodynamic considerations is consistent with the Euclidean correlator technique (Figure 3).

5 Publications


Figure 1: The volume dependence of the lowest two measured masses and the lowest two $N - K$ scattering states in the negative (left panel) and positive (right panel) parity channels. The dashed line indicates the expected mass of the $\Theta^{+}$ taken from the experiments.

Figure 2: The contribution of the different operators into the lowest two states in the negative (left panel) and positive (right panel) parity channels.
Figure 3: The difference of the free energies in case of 2 (top left panel), 4 (top right panel) and 8 (bottom panel) dynamical staggered fermions. The dashed lines show the linear fits. The $T \to 0$ extrapolated values are compared to the pion masses obtained using Euclidean correlators.