Wave Function of the Roper from Lattice QCD

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Abstract

We apply the eigenvectors from a variational analysis in lattice QCD to successfully extract the wave function of the Roper state, and a higher mass $P_{11}$ state of the nucleon. We use the $2+1$ flavour $32^3 \times 64$ PACS-CS configurations at a near physical pion mass of 156 MeV. We find that both states exhibit a structure consistent with a constituent quark model. The Roper $d$-quark wave function contains a single node consistent with a $2S$ state, and the third state wave function contains two, consistent with a $3S$ state. A detailed comparison with constituent quark model wave functions is carried out, obtained from a Coulomb plus ramp potential. These results validate the approach of accessing these states by constructing a variational basis composed of different levels of fermion source and sink smearing. Furthermore, significant finite volume effects are apparent for these excited states which mix with multi-particle states, driving their masses away from physical values and enabling the extraction of resonance parameters from lattice QCD simulations.

Keywords: Roper Resonance, Wave Functions, Lattice QCD

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1. Introduction

The wave function and associated probability distribution of a particle in a potential are fundamental to the very nature of quantum mechanics. In the non-relativistic case, the entire spectrum of the particle can be determined by solving the Schrödinger equation. In quantum field theory, a Schrödinger-like probability distribution can be constructed for bound states by analogy, by taking a simplified view of the full quantum field theory wave functional in the form of the Bethe-Salpeter wave function \cite{1}, herein referred to as simply the ‘wave function’.

Recent advances in the isolation of nucleon excited states through correlation-matrix based variational techniques in lattice QCD now enable the exploration of the structure of these states and how these properties emerge from the fundamentals of QCD. In this letter, we report the first results for the wave function of the first even-parity excitation of the nucleon, the Roper \cite{2}.

Early explorations of these states considered a non-relativistic constituent quark model. The probability distributions of quarks within hadrons were determined using a one-gluon-exchange potential augmented with a confining form \cite{3,4}. These models have been the cornerstone of intuition of hadronic probability distributions for many decades, and have been complemented with features such as meson-cloud dressing.

In this investigation, we will confront these early predictions for quark probability distributions in excited states directly via Lattice QCD. Visualizations of the probability distributions for ground states on the lattice \cite{5} have been used to observe interesting physical effects such as Lorentz contraction \cite{6,7}, quarks aligning with a magnetic field and diquark clustering \cite{8}. Furthermore, the probability distribution can be used as a diagnostic tool, allowing finite volume effects and other lattice artifacts to be easily visualized and understood \cite{9}.

The Bethe-Salpeter wave function underlying the probability distributions can be defined in the form of a gauge-invariant Bethe-Salpeter amplitude. For the wave function of the $d$ quark about two $u$ quarks in the proton, $|p\rangle$, the amplitude takes the form

$$
\psi^d_d(y) \propto \int d^4x \epsilon^{abc} u^a(x) C\gamma_5 \left[ P \exp \left( ig \int_x^{x+y} A(x') \cdot dx' \right) d(x+y) \right] u^b(x') |p\rangle , \tag{1}
$$

which exploits a string of flux to connect the quarks in a
gauge invariant manner. Here we have selected the standard form of the proton interpolating field $\chi_\uparrow$. $u$ and $d$ represent the up and down quark fields respectively with colour indices $a$, $b$ and $c$ and $C$ is the charge conjugation matrix.

In a relativistic gauge theory the concept of a hadronic wave function is not unique. For example, in the gauge invariant form there is an explicit path dependence. For large separations of the quarks an average over the paths is desirable. This leads us to consider other Bethe-Salpeter amplitudes in which the gauge degree of freedom is fixed to a specific gauge. In lattice field theory, Coulomb and Landau gauges are most common due to their local gauge fixing procedure.

Landau gauge is a smooth gauge that preserves the Lorentz invariance of the theory. It is a popular choice in the field and we select it here. While the size and shape of the wave function are gauge dependent, our selection of Landau gauge is vindicated in Sec. 3. There we illustrate how the ground state wave function of the proton and their detailed comparison with traditional non-relativistic quark model predictions.

### 2. Lattice Techniques

Hadron spectroscopy is a highly complex problem. Though it is relatively simple to see higher energy resonances of hadrons in colliders, apart from simple quantum numbers, properties more fundamental to the nature of these resonances remain elusive to experiment.

Robust methods have been developed that allow the isolation and study of states associated with these resonances in Lattice QCD [10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. In this study, we apply the variational method [20, 21] to extract the ground state and first two $P_{11}$ excited states of the proton associated with the Roper [2].

In order to construct the wave function, the quark fields in the annihilation operator are each given a spatial dependence,

$$ \chi_\uparrow(\vec{x}, 0, \vec{z}, 0; t) = e^{abc}(u^{Ta}(\vec{x} + \vec{y}) C \gamma_5 d^{b}(\vec{x} + \vec{z})) u^{c}(\vec{x} + \vec{w}), $$

while the creation operator remains local. This generalizes $G(\vec{p}, t)$ to a wave function proportional to $G(\vec{p}, t; \vec{y}, \vec{z}, \vec{w})$. In principle, we could allow each of these coordinates, $\vec{y}$, $\vec{z}$, $\vec{w}$, to vary across the entire lattice, however, we can reduce the complexity by taking advantage of the hyper-cubic rotational and translational symmetries of the lattice and considering the system centre of mass. A description of the probability distribution of a particular quark within the proton can be formed by holding the spatial location of two of the quarks fixed and calculating the third quark’s amplitude at every lattice site. We focus on the probability distribution of the $d$ quark from Eq. (5), with the $u$-quarks fixed at the origin, i.e.

$$ \chi_\uparrow(\vec{x}, 0, \vec{z}, 0; t) = e^{abc}(u^{Ta}(\vec{x}) C \gamma_5 d^{b}(\vec{x} + \vec{z}, t)) u^{c}(\vec{x}, t). $$

The coordinate $\vec{x}$ then represents the centre of the system, providing an origin analogous to a potential well in the non-relativistic case.

The variational method [20, 21] is a well-established method [22] for extracting the excited state spectra of hadrons. Noting that the only time dependence in the two-point function lies in the exponential, we are able to construct the following relation

$$ G_{ij}(t_0 + \Delta t) u_j^\alpha = e^{-m_\Delta \Delta t} G_{ij}(t_0) u_j^\alpha, $$

where $u^\alpha$ are the right eigenvectors of the eigenvalue equation,

$$ (G^{-1}(t_0) G(t_0 + \Delta t))_{ij} u_j^\alpha = e^{-m_\Delta \Delta t} u_i^\alpha. $$
Similarly, we can construct the left eigenvector equation

$$v_i^a (G(t_0 + \Delta t) G^{-1}(t_0))_{ij} = e^{-m_i \Delta t \beta} v_j^a. \quad (9)$$

To project a single state, one applies the eigenvectors to the parity-projected variational matrix

$$v_i^a G^t_j(t) \alpha \beta \equiv \delta_{\alpha \beta} e^{-m_i \Delta t \beta}. \quad (10)$$

The effective mass can then be calculated from the projected two-point functions as $m(t) = \log(G(t)/G(t + 1))$. While the effective mass is insensitive to a wide range of variational parameters [18], we follow Ref. [18] and select $t_0$ to be 2 time slices after the source with $\Delta t = 2$.

Different interpolators exhibit different couplings to the proton ground and excited states and hence can be used to construct a variational basis. The limited number of local interpolators restricts the size of the operator basis [10]. To remedy this, one can exploit the smearing dependence of the coupling of states to one or more standard interpolating operators in order to construct a larger variational basis where the $\chi_i$ and $\bar{\chi}_j$ from Eq. (2) contain a smearing dependence. This method has been shown to allow access to states associated with resonances such as the Roper, $N^*(1710)$ [18] and the $\Lambda(1405)$ [26].

The non-local sink operator used to construct the wave function is unable to be smeared, such that the standard technique of Eq. (10) cannot be applied. However, Eq. (7) illustrates it is sufficient to isolate the state at the source using the right eigenvector. Thus, the probability distributions are calculated with each smeared source operator and the right eigenvectors calculated from the standard variational analysis are then applied in order to extract the individual states. As demonstrated in Fig. 1, clean projection of two excited states is obtained. We note how the plateaus commence at $t = t_0 = 2$, where the correlation matrix analysis has been applied. As the fourth state may accommodate a superposition of all remaining spectral strength in the correlator, we do not consider it further.

Our focus on $\chi_1$ in this investigation follows from the results of Ref. [22], where the lowest-lying excitation of the nucleon was shown to be predominantly associated with the $\chi_1$ interpolating field. The results from their $8 \times 8$ correlation matrix of $\chi_1$ and $\chi_2 = e^{i m u}(u^\gamma_5(x) C \overline{d}^t(x)) \gamma_5 \overline{u}(x)$ revealed that $\chi_2$ plays a marginal role in exciting the Roper. The coefficients of the Roper source eigenvector multiplying $\bar{\chi}_i$ are near zero. Instead this interpolating field is key to obtaining good overlap with the $N(1710)$ excited state of the nucleon. Further comparison with Ref. [22], identifies the third state extracted herein as the fifth state of the $8 \times 8$ analysis, illustrated in Fig. 6 of Ref. [22] as the green star at the lightest quark mass.

In summary, the wave function for the $d$ quark in state $\alpha$ having momentum $\vec{p}$ observed at Euclidean time $t$ is

$$\phi_d^\alpha(\vec{p}, t; \bar{Z}) = \sum_{\bar{x}} e^{-i \vec{p} \cdot \bar{Z}}$$

$$\text{tr} (\gamma_0 \pm 1) \langle \Omega | T \chi_1(\vec{x}, 0, \bar{z}, 0; t) \bar{\chi}_j(0, 0) | \Omega \rangle u_j^t,$$

where $\chi_1(\vec{x}, 0, \bar{z}, 0; t)$ is given by Eq. (6).

As discussed above, $\chi_1$ has the spin-flavour construct that is most relevant to the excitation of the Roper from the QCD vacuum. As such, it is an ideal choice for revealing the spatial distribution of quarks within the Roper. However, the selection of $\chi_1$ in Eq. (11) is not unique and other choices are possible. For example, the selection of $\chi_2$ would reveal small contributions to the Roper wave function where vector diquark degrees of freedom are manifest. Similarly, $D$-wave contributions could be resolved through the consideration of a spin-3/2 isospin-1/2 interpolating field at the sink.

In carrying out our calculations, we average over the equally weighted $|U|$ and $|U^\dagger|$ link configurations as an improved unbiased estimator. The two-point function is then perfectly real and the probability density is proportional to the square of the wave function. In this analysis, we choose to look at the zero-momentum probability distributions three time slices after the source.

3. Simulation Results

We use the $2 + 1$ flavour $32^3 \times 64$ PACS-CS configurations [23], constructed with the Iwasaki gauge action [27] with $\beta = 1.90$, giving a lattice spacing of...
0.0907(13) fm, and the $O(a)$-improved Wilson action [28]. We use 198 gauge field configurations, and employ multiple sources per configuration, separated by at least one quarter of the temporal lattice extent. The hopping parameter for the light quarks is $\kappa_{ud} = 0.13781$, giving a pion mass of 156 MeV.

To cleanly access the first three states, a $4 \times 4$ variational basis is constructed using the $\chi_1$ operator with 16, 35, 100 and 200 sweeps of Gaussian smearing [29], corresponding to RMS smearing radii of 2.37, 3.50, 5.92 and 8.55 lattice units respectively. We fix to Landau gauge by maximizing the $O(a^2)$ improved fixing functional [30]

$$F_{\text{Imp}} = \sum_{x, \mu} \text{Re} \text{tr} \left( \frac{4}{3} U_\mu(x) - \frac{1}{12} u_0 \left( U_\mu(x) U(x + \hat{\mu}) + \text{h.c.} \right) \right)$$

using a Fourier transform accelerated algorithm [31].

The wave functions observed for all our states show an approximate symmetry over the eight octants surrounding the origin. To improve our statistics we average over these eight octants before presenting the results.

Our point of comparison with previous models of quark probability distributions comes from a non-relativistic constituent quark model with a one-gluon-exchange motivated Coulomb + ramp potential. The spin dependence of the model is given in Ref. [4] and the radial Schrodinger equation is solved with boundary conditions relevant to the lattice data; i.e. the derivative of the wave function is set to vanish at a distance $L_s/2$.

The ground state probability density for the $d$ quark about the two $u$ quarks at the origin obtained in our lattice calculations is illustrated in Fig. 2. We see that the well-known sharp-peaked shape associated with the Coulomb potential is reproduced.

The lattice data are compared with the constituent quark model in Fig. 3. Here, both the quark model probability distributions and the lattice results have been scaled such that the peak value is 1. The two quark model parameters adjusted in the fit are the string tension, $\sqrt{s} = 440 \pm 40$ MeV, and the constituent quark mass, $m_q \sim 370$ MeV (accommodating the fact our quark mass is above the physical value). Using a least-squares fit varying the parameters $m_q$ and $\sqrt{s}$, we find the ground state lattice results are described well with $\sqrt{s} = 400$ MeV and $m_q = 360$ MeV, which gives a ground state mass of 940 MeV and a first excited state mass of 1573 MeV. These parameters are held fixed in examinations of the excited states.

Lattice results for the $d$-quark probability distribution in the first excited state of the proton are presented in Fig. 4. The distribution exhibits a hydrogenic node structure consistent with a $2S$ state, indicating that the state includes a radial excitation of the $d$ quark. This structure also indicates that the ideal combination of operators to access this state on the lattice would be superposed Gaussians of different widths and opposite signs. This observation validates the approach of combining multiple smearing levels to construct the variational basis and indeed the alternating signs of superposed Gaussians are observed in Refs. [19, 22].

The isovolume of this probability distribution illustrated in Fig. 5 clearly shows the nodal structure, with an inner sphere surrounded by a near-spherical shell. The deviation from spherical symmetry in the outer shell directly displays the important interplay between the energy of the excited state observed in the lattice simulation and the finite volume of the lattice. At this very light quark mass the distortion of the probability den-
Figure 4: The probability distribution of the $d$ quark about the two $u$ quarks at the origin in the first excited state. The darkened ring around the peak indicates a node in the probability distribution, consistent with a $2S$ state.

Figure 5: The isovolume of the probability distribution of the $d$ quark in the first excited state (colour map as in Fig. 4). The outer edge can be seen to be affected by the boundary, indicating a necessary finite-volume effect associated with multi-particle components of the state.

Figure 6: Comparison of the first excited state $d$-quark probability distribution from our lattice QCD calculation (crosses) with the quark model (solid curve). The quark model predicts the node in approximately the correct location, but deviates at the boundary.

4. Summary

In this world-first study of the quark probability distribution within excited states of the nucleon, we have shown that both the Roper and the second excited state examined herein display the node structure associated with radial excitations of the quarks. On comparing these probability distributions to those predicted by a constituent quark model, we find good qualitative similarity with interesting differences. The discovery of a node structure provides a deep understanding of the success of the smeared-source/sink correlation matrix methods of Ref. [18].

Finite volume effects were shown to be particularly significant for the excited states explored herein at relatively light quark mass. As these excited states have a multi-particle component, the interplay between the lattice volume, the wave function and the associated energy are key to extracting the resonance parameters of the Roper.

Future calculations will explore the structure of the Roper in more detail, examining the mass dependence of the wave functions, more general spatial configurations of the quark positions, and the introduction of isospin-1/2 spin-3/2 interpolating fields to reveal the role of $D$-wave contributions to the Roper. While our use of improved actions suppresses lattice discretisation errors, ultimately simulations will be done at a variety of lattice spacings directly at the physical quark masses to connect the lattice QCD simulations to the continuum results of Nature.
Figure 7: The probability distribution of the $d$ quark in the second excited state of the nucleon. Two nodes are visible, consistent with a $3S$ state.

Figure 8: The isovolume of the probability distribution of the $d$ quark in the second excited state. The outermost node is compressed by the boundary into an almost square shape, indicating strong finite-volume effects.

Figure 9: Comparison of the second excited state $d$-quark probability distribution from the lattice (crosses) with the quark model (solid curve). The nodes in the lattice data fall in between those predicted by the quark model.

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