Baryon operators and spectroscopy in lattice QCD

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The construction of the operators and correlators required to determine the excited baryon spectrum is presented, with the aim of exploring the spatial and spin structure of the states while minimizing the number of propagator inversions. The method used to construct operators that transform irreducibly under the symmetries of the lattice is detailed, and the properties of example operators is studied using domain-wall fermion valence propagators computed on MILC asqtad dynamical lattices.

1. INTRODUCTION

The determination of the excited baryon spectrum is an important step on the road to understanding the dynamics of QCD, and it is, for example, a vital element of the Jefferson Laboratory experimental program. Lattice gauge theory has a pivotal role not only in providing \textit{ab initio} calculations of the masses of the lowest lying states, but also in establishing the quark and gluon content of the states. There has thus been increasing activity amongst the lattice community that has demonstrated that the masses of the lowest-lying baryon states of both parities for spin-1/2 and spin-3/2 are accessible to lattice calculation, and there have been calculations of the mass of the first positive-parity, spin-1/2 excitation of the nucleon, the so-called Roper resonance.

Most of these calculations have been made in the quenched approximation to QCD, and an important component of future lattice studies will be a careful analysis of the systematic uncertainties on these results. However, the confrontation of lattice calculations with experiment will require a more complete understanding of the spectrum, obtaining both the masses of the higher spins and of the radial excitations. Furthermore, the discovery of the quark and gluon structure of the excited states will require a more extensive basis of interpolating operators than used so far, allowing both for excited glue and for multi-quark operators. The aim of this talk is to describe the design of such operators, and in particular to construct operators that transform irreducibly under the symmetries of the lattice.

The remainder of this talk is laid out as follows. In the next section, the methodology of computing the spectrum is described, and the symmetries used to classify baryon states are detailed. Gauge-invariant “elemental” operators that have the correct flavor structure and that explore the spatial structure of the baryons are then introduced. The reduction of these operators to ones that transform irreducibly under the cubic symmetry of the lattice is then performed. Finally, the reduction is illustrated for the case of point-like elemental operators obtained using domain-wall fermion (DWF) valence propagators computed on a dynamical asqtad-fermion background.
2. THE SPECTRUM FROM LATTICE CALCULATIONS

The computation of the spectrum of states in lattice QCD is in principle straightforward.

1. Choose an interpolating operator $O$ that has a good overlap with $P$, the state of interest,

$$\langle 0 | O | P \rangle \neq 0,$$

and ideally a small overlap with other states having the same quantum numbers.

2. Form the time-sliced correlation function

$$C(t) = \sum_{x} \langle \bar{O}(\vec{x}, t) O^\dagger(\vec{0}, 0) \rangle.$$

3. Insert a complete set of states between $O$ and $O^\dagger$. The time-sliced sum puts the intermediate states at definite momentum, and we find

$$C(t) = \sum_{\vec{x}} \sum_{P} \int \frac{d^3k}{(2\pi)^3 2E(\vec{k})} \times \langle 0 | \bar{O}(\vec{x}, t) | P(\vec{k}) \rangle \langle P(\vec{k}) | O^\dagger(\vec{0}, 0) \rangle | 0 \rangle$$

$$= \sum_{P} \frac{\langle 0 | O | P \rangle |^2}{2E_P(0)} e^{iE_P(0)t},$$

where the sum over $P$ includes the contributions from two-particle and higher states.

4. Continue to Euclidean space $t \rightarrow it$, yielding

$$C(t) = \sum_{P} \frac{\langle 0 | O | P \rangle |^2}{2m_P} e^{-m_P t},$$

so that the correlator falls off exponentially with the mass of the lightest state at large times.

In order to obtain the mass of the higher resonances in Eqn. 1, the most appealing approach is to apply variational methods[1,2], beginning with the computation of a matrix of correlators

$$C_{ij}(t) = \sum_{x} \langle \bar{O}_i(\vec{x}, t) O_j^\dagger(\vec{0}) \rangle,$$

where the $\{O_i\}$ form a basis of operators of definite quantum numbers. In the usual application of the variational technique, we find a basis of eigenvectors $V(t_0)$ that diagonalizes the transfer matrix $C(t_0)^{-1}C(t)$ for $t = t_0 + 1$ for some $t_0$ close to the source, and determine the spectrum from the eigenvalues of

$$V(t_0 + 1)^{-1}C(t_0)^{-1}C(t)V(t_0 + 1)$$

at subsequent times. The method relies on constructing a basis of operators $\{O_i\}$ that provides a good description of the states of interest, and the remainder of this talk will focus on the construction of that basis.

We classify the states of the continuum by their flavor structure, $F$, and by their parity $P$, total spin $J$ and “helicity” $J_z$. Whilst the flavor structure can be faithfully preserved in a lattice calculation, the parity, spin and helicity labels arise from looking at the symmetry properties of states under rotations and reflections. In a lattice calculation, we have replaced continuum space time by a hypercubic lattice, and thus must classify states according to the irreducible representations $\Lambda$ of the cubic group (for particles at rest); the row $\lambda$ within the representation is then the analogue of helicity.

In the following section, we will construct a set of elemental baryon operators $\{B^{\Lambda F}_{i}(x)\}$ having the correct flavor properties $F$. We will then use group theory to generate a set of baryon operators $\{B^{F\Lambda\lambda}(x)\}$ that transform irreducibly under the rotation and reflection symmetries of the lattice, and from which we will construct our correlation matrix

$$C_{ij}^{\Lambda\Lambda F}(t) = \sum_{x} \langle B_{i}^{\Lambda\Lambda F}(x) B_{j}^{\Lambda\Lambda F}(0) \rangle,$$

and hence extract the spectrum of states corresponding to $\Lambda, \lambda$.

3. ELEMENTAL BARYON OPERATORS

The color and flavor structure of the operators is dictated by the requirements of gauge invariance and of isospin respectively; it is natural in a lattice calculation to assume exact isospin symmetry, and to classify states and operators by
their isospin and strangeness, rather than according to SU(3) flavor.

The use of “smearing” has proven essential to reduce the coupling of operators to the higher excited states, and thus to ensure that the correlators Eqn. 2 are dominated by only a few states even close to the source. In the example given here, we will adopt a gauge-covariant spatial Laplacian to smear the fields:

\[ \hat{\psi}(x) = (1 + \sigma^2 \Delta / 4N)^N \psi(x) \]  

with the three-dimensional Laplacian defined by

\[ \hat{\Delta} \psi(x) = \sum_{k=\pm 1, \pm 2, \pm 3} (\hat{U}(k) \psi(x+k) - \psi(x)), \]  

where \( \hat{U} \) denotes a link variable that can be smeared according to, say, the APE prescription[3]. Both \( N \) and \( \sigma \) are tunable parameters, and in the limit \( N \to \infty \), Eqn. 5 reduces to Gaussian smearing of width \( \sigma \). Note that the square of the smeared field vanishes, in the manner of a simple Grassmann field.

An important consideration is to construct operators that enable us to build up the radial and orbital structure of the states. This is accomplished by additional powers of the Laplacian, and by spatial derivatives, respectively, so that the quark building blocks become:

\[ \chi^a_{Aaa}(x) = (\hat{\Delta}^n \hat{\psi}(x))_{Aaa}, \]  

\[ \xi^{npj}_{Aaa}(x) = (\hat{D}^{(p)} \hat{\Delta}^n \hat{\psi}(x))_{Aaa}, \]  

where \( A \) is a flavor index, \( a \) is a color index, \( a \) a Dirac spin index, and \( n \) is an integer. The \( p \)-link gauge-covariant forward displacement operator is defined by

\[ \hat{D}^{(p)}_j O(x) = \hat{U}_j(x) \ldots \hat{U}_{j+(p-1)\hat{j}} O(x+p\hat{j}), \]  

where \( j = 1, 2, 3 \), and \( p \) is an integer specifying the length of the displacement.

From these quark building blocks, we construct our elemental three-quark operators:

\[ \phi^F_{ABC} \equiv \epsilon_{abc} \chi^a_{Aaa} \lambda^{\hat{n}}_{B\hat{b}\hat{\alpha}} \chi^{p\hat{p}j}_{C\gamma\gamma}, \]  

\[ \phi^F_{ABC} \equiv \epsilon_{abc} \chi^a_{Aaa} \lambda^{\hat{n}}_{B\hat{b}\hat{\alpha}} \xi^{p\hat{p}j}_{C\gamma\gamma}, \]  

\[ \phi^F_{ABC} \equiv \epsilon_{abc} \chi^a_{Aaa} \xi^{p\hat{p}j}_{B\hat{b}\hat{\alpha}} \xi^{p\hat{p}k}_{C\gamma\gamma}. \]  

The flavor structure is specified by \( \phi^F_{ABC} \), whilst the Levi-Civita symbol ensures that these are color singlets. The radial and orbital structures are explored by varying \( n_1, n_2, n_3 \), and through the choices of \( p_1, p_2, j, k \) respectively. A large number of baryons can then be studied using a somewhat small number of quark propagator sources.

4. SYMMETRIES OF THE LATTICE

Proper rotations restricted to an isotropic cubic lattice form the cubic group \( O \). It has 24 elements, and five conjugacy classes and thus five single-valued irreducible representations: \( A_1, A_2, E, T_1, T_2 \), of dimensions 1, 1, 2, 3 and 3 respectively. If we allow for spatial inversions, corresponding to \( P = \pm 1 \), we obtain the group \( O_h \), and the irreducible representations acquire a further label, \( g \) or \( u \), corresponding to positive and negative parity states, respectively. The construction of operators transforming irreducibly according to the single-valued representations is well known, and has been crucial to identifying the states in lattice calculations of the glueball spectrum.

There are four two-dimensional spinorial representations of \( O_h \): \( G_{1g}, G_{1u}, G_{2g} \) and \( G_{2u} \), and two four-dimensional representations, \( H_g \) and \( H_u \)[4,5]. The irreducible representations \( J \) of the continuum group \( SU(2) \) are reducible under the cubic group \( O \); the number of times \( n^l_J \) that each of these reducible representations occurs in the irreducible representation \( \Gamma \) of \( O \) is shown in Table 1; the extension to \( O_h \) is straightforward.

Whilst full rotational symmetry is restored in the continuum limit, the irreducible representations of \( O_h \) contain states of many representations of \( SU(2) \), and in general the degrees of freedom, corresponding to different helicities, lie in different irreducible representations. Thus, for example, a state of spin \( 5/2 \) has four degrees of freedom in the four-dimensional representation \( H \), and two degrees of freedom in the two-dimensional representation \( G_2 \); the identification of the spin of a state is accomplished by looking for the approach to a common mass across the different irreducible representations in the continuum limit.
Table 1

| $J$ | $n^J_{G_1}$ | $n^J_{G_2}$ | $n^J_H$ |
|-----|-------------|-------------|---------|
| 1/2 | 1           | 0           | 0       |
| 3/2 | 0           | 0           | 1       |
| 5/2 | 0           | 1           | 1       |
| 7/2 | 1           | 1           | 1       |
| 9/2 | 1           | 0           | 2       |

The number of times $n^J_i$ that the irreducible representation $\Gamma$ of $O$ occurs in the reduction of the irreducible representation $J$ of $SU(2)$.

Central to the task of finding the $B^{\Lambda\Lambda\mathbf{F}}(x)$ is the projection formula

$$B^{\Lambda\Lambda\mathbf{F}}(x) = \frac{d_A}{g_{O_h\in O_n}} \sum \left[ \frac{D^\Lambda(\xi R)}{D^\Lambda(R)} U_R B^\mathbf{F}(\bar{x}) U_R^\dagger \right]$$

where $\Lambda$ refers to an $O_h$ irrep, $\lambda$ is the irrep row, $g_{O_h}$ is the number of elements in $O_h$, $d_A$ is the dimension of the $\Lambda$ irrep, $D^\Lambda(R)$ is a $\Lambda$ representation matrix corresponding to group element $R$, and $U_R$ is the quantum operator which implements the symmetry operations; the temporal argument is suppressed.

Application of this formula requires explicit representation matrices for every group element. Representation matrices for all allowed proper rotations can be generated from the matrices for $C_{4y}$ and $C_{4z}$, the rotations by $\pi/2$ about the $y$- and $z$-axes, respectively. The explicit matrices we use for these generators are given by

$$D^{(G_1)}(C_{4y}) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} = -D^{(G_2)}(C_{4y}),$$

$$D^{(G_1)}(C_{4z}) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 0 & 1+i \end{bmatrix} = -D^{(G_2)}(C_{4z}),$$

$$D^{(H)}(C_{4y}) = \frac{1}{2\sqrt{2}} \begin{bmatrix} 1 & -\sqrt{3} & \sqrt{3} & -1 \\ \sqrt{3} & -1 & -1 & \sqrt{3} \\ \sqrt{3} & 1 & 1 & -\sqrt{3} \\ 1 & \sqrt{3} & \sqrt{3} & 1 \end{bmatrix},$$

$$D^{(H)}(C_{4z}) = \frac{1}{\sqrt{2}} \begin{bmatrix} -1-i & 0 & 0 & 0 \\ 0 & 1+i & 0 & 0 \\ 0 & 0 & 1+i & 0 \\ 0 & 0 & 0 & -1+i \end{bmatrix}.$$
Table 2
Combinations of the operators $\Phi_{\alpha\beta\gamma}$ in Eqn. 13 which transform irreducibly under $O_h$ for the DeGrand-Rossi representation of the $\gamma$-matrices, employed by LHPC and MILC.

| Irrep | Row | Operators |
|-------|-----|-----------|
| $G_1g$ | 1 | $\Phi_{112} + \Phi_{334}$ |
| $G_1g$ | 2 | $-\Phi_{221} - \Phi_{443}$ |
| $G_1g$ | 1 | $\Phi_{123} - \Phi_{213} + \Phi_{314}$ |
| $G_1g$ | 2 | $\Phi_{124} - \Phi_{214} + \Phi_{324}$ |
| $G_1g$ | 1 | $2\Phi_{114} + 2\Phi_{332} - \Phi_{123} - \Phi_{213} + 2\Phi_{134} - \Phi_{314}$ |
| $G_1g$ | 2 | $-2\Phi_{223} - 2\Phi_{441} + \Phi_{124} - \Phi_{214} - 2\Phi_{234} + \Phi_{324}$ |
| $G_1u$ | 1 | $\Phi_{112} - \Phi_{334}$ |
| $G_1u$ | 2 | $-\Phi_{221} + \Phi_{443}$ |
| $G_1u$ | 1 | $\Phi_{123} - \Phi_{213} - \Phi_{314}$ |
| $G_1u$ | 2 | $\Phi_{124} - \Phi_{214} - \Phi_{324}$ |
| $G_1u$ | 1 | $2\Phi_{114} - 2\Phi_{332} - \Phi_{123} - \Phi_{213} - 2\Phi_{134} + \Phi_{314}$ |
| $G_1u$ | 2 | $-2\Phi_{223} - 2\Phi_{441} + \Phi_{124} + \Phi_{214} + 2\Phi_{234} - \Phi_{324}$ |
| $H_g$ | 1 | $\sqrt{3}(\Phi_{113} + \Phi_{331})$ |
| $H_g$ | 2 | $\Phi_{114} + \Phi_{332} + \Phi_{123} + \Phi_{213} - 2\Phi_{134} + \Phi_{314}$ |
| $H_g$ | 3 | $\Phi_{223} - \Phi_{441} + \Phi_{124} + \Phi_{214} - 2\Phi_{234} + \Phi_{324}$ |
| $H_g$ | 4 | $\sqrt{3}(\Phi_{224} + \Phi_{442})$ |
| $H_u$ | 1 | $\sqrt{3}(\Phi_{113} - \Phi_{331})$ |
| $H_u$ | 2 | $\Phi_{114} - \Phi_{332} + \Phi_{123} + \Phi_{213} + 2\Phi_{134} - \Phi_{314}$ |
| $H_u$ | 3 | $\Phi_{223} - \Phi_{441} + \Phi_{124} + \Phi_{214} + 2\Phi_{234} - \Phi_{324}$ |
| $H_u$ | 4 | $\sqrt{3}(\Phi_{224} - \Phi_{442})$ |

Eqn. 14. Finally, we form the correlators

$$C_{ij}(t) = \sum \Gamma_i \bar{\Gamma}_j \langle \Phi_{\alpha\beta\gamma}(x, t) \bar{\Phi}_{\alpha\beta\gamma}(0) \rangle,$$  \hspace{1cm} (17)

where the $\Gamma_i, \bar{\Gamma}_j$ are given in Table 2. While the computation of the generalized baryon correlators is computationally quite demanding, the subsequent calculation of the 20 $\times$ 20 matrix of correlators of Eqn. 17 can be performed in a matter of minutes on a workstation, even for several hundred configurations.

It is instructive to list some of the properties of the correlation matrix Eqn. 17:

- Cross-correlations between operators within different irreducible representations vanish.
- Cross-correlations between the operators of different rows within the same representation vanish.
- The different rows within a representation can be chosen to have the same normalisation, so that correlators thus constructed have the same expectation values.
- Cross-correlations between the same row of different embeddings of the same irreducible representation do not vanish; they can be constructed to vanish only on a particular time slice.

Thus the strategy for extracting the mass spectrum from the data is now clear. Firstly, choose a particular irreducible representation, possibly averaging over the rows within that representation. Then form the matrix of correlators between all the averaged operators within that representation, and extract the spectrum using, say, the method of Eqn. 3.

The talk concludes with an examination of the correlators on an ensemble of lattice data, and in particular a verification of the properties above.
To perform this study, we employ an ensemble of around 300 configurations computed on a $20^3 \times 64$ lattice with $N_f = 2+1$ flavors of asqtad staggered quarks having $am_u/am_s = 0.01/0.05[8]$. The lattice spacing $a = 0.124$ fm is obtained from the $1\text{P}-1\text{S}$ splitting in the Upsilon spectrum[9].

We employ domain-wall fermions at a single mass $m = 0.01$ for the valence quarks, which are computed on “chopped” $20^3 \times 32$ lattices, with $N_5 = 16$; to reduce the residual mass, the configurations are first blocked using a non-perturbative HYP blocking scheme[10]. Smeared sources are used, using $\sigma = 4.35$ and $N = 30$ in Eqn. 5, but local sinks, and thus the correlators are not positive definite; full details of the calculation will appear in a subsequent paper [11].

The effective masses obtained from the diagonal correlators using the three embeddings of $G_{1g}$ and $G_{1u}$ are shown in figure 1. The plot reveals a clear signal for both positive- and negative parity states from each of the three embeddings. Note that the three usual baryon interpolating operators, for example in ref. [7], correspond to linear combinations of the operators used here; the identification of a “good” baryon operator corresponding to the nucleon, and a baryon operator having a good overlap onto the Roper resonance, should appear through the variational analysis. The effective masses for $H_g$ and $H_u$ are shown as the lower plot in figure 1; there is a clear separation from the mass of the ground-state nucleon, with the negative-parity state being lower in mass, as observed experimentally.

We illustrate the orthogonality properties in two ways in figure 2: firstly, by confirming that the cross-correlators between different irreducible representations are indeed zero, and secondly by verifying that those between different rows of the same irreducible representation vanish. The orthogonality properties are clearly well satisfied in these representative examples, indicating that the numerical implementation is under control.

6. CONCLUSIONS

We have detailed the design of operators needed to determine the excited baryon spectrum. The method used to construct operators transforming irreducibly under the symmetries of the lattice has been outlined, and the efficacy of the method illustrated. The calculation of “generalised” baryon correlators followed by group-theory projections is computationally efficient, and allows straightforward identification of the quantum numbers of the correlators. Furthermore, the methodology is readily extendible to more complicated operators, such as those for pentaquarks and those having excited glue.

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Figure 1. The upper figure shows the effective masses for the three different embeddings of $G_{1g}$ (smaller) and $G_{1u}$ (larger) as the three different plotting symbols, and valence quark mass $m = 0.01$. The points corresponding to the different embeddings are offset for clarity. The lower figure shows the effective masses for $H_u$ (diamond) and $H_g$ (square).

Figure 2. The upper figure shows the ratio $\langle G_{1g} G_{1u} \rangle / \langle G_{1g} G_{1g} \rangle$, whilst the lower figures shows $\langle G_{1g} G_{1g}^2 \rangle / \langle G_{1g} G_{1g} G_{1g} \rangle$. 