Baryon Spectroscopy using Anisotropic Clover Lattices

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Abstract

We propose to employ the anisotropic $N_f = 2+1$ dynamical clover configurations for a study of the baryon resonance spectrum for the baryons that can be constructed from u/d and s quarks. We will perform the computation at three values of the pion mass: $m_\pi = 875, 560$ and 315 MeV, and employ two lattice volumes at the lightest mass with the aim of delineating single- from two-body energies. **We request the equivalent of 2.1M 6n-node hours.**

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1 Physics Goals

In order to really understand QCD and hence test whether it is the complete theory of the strong interaction, we must determine the spectrum of mesons and baryons that it implies and test those spectra against high quality experimental measurements. The complete combined analysis of available experimental data on the photoproduction of nucleon resonances is the 2009 milestone in Hadronic Physics (HP), and the measurement of the electromagnetic properties of the low-lying baryons is an HP 2012 milestone.

Given the current intense experimental efforts in hadron spectroscopy, the need to predict and understand the hadron spectrum from first principles calculations in QCD is clear. Hence, our goal in this proposal is to embark on a comprehensive study of the baryon spectrum, employing the anisotropic clover gauge configuration currently being generated. Given that an important strategic goal of USQCD is to employ lattice QCD calculations to address the key questions in hadronic physics, we believe this proposal satisfies one of the criteria for a Class-A proposal.

1.1 Resonances and Lattice QCD

A comprehensive picture of resonances requires that we go beyond a knowledge of the ground state mass in each channel, and obtain the masses of the lowest few states of a given quantum number. This we can accomplish through the use of the variational method[1, 2]. Rather than measuring a single correlator $C(t)$, we determine a matrix of correlators

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

where $\{O_i; i = 1, \ldots, N\}$ are a basis of interpolating operators having given quantum numbers. We then solve the generalized eigenvalue equation

$$C(t)u = \lambda(t, t_0)C(t_0)u$$

to obtain a set of real (ordered) eigenvalues $\lambda_n(t, t_0)$, where $\lambda_0 \geq \lambda_1 \geq \cdots \geq \lambda_{N-1}$. At large Euclidean times, these eigenvalues then correspond to the different energies E_n as follows

$$\lambda_n(t, t_0) \longrightarrow e^{-E_n(t-t_0)} \left[1 + O(e^{-\Delta E_n(t-t_0)})\right]. \tag{1}$$

where $\Delta E_n = \min\{\mid E_n - E_i \mid : i \neq n\}$. The eigenvectors u are orthogonal with metric $C(t_0)$, and a knowledge of the eigenvectors can yield information about the structure of the states. A variation of this method, which we explore below, is to fix the basis at some reference time slice t^*, and then examine the spectrum in this preconditioned basis of operators.

Crucial to the application of variational techniques is the construction of a basis of operators that have a good overlap with the lowest-lying states of interest. These operators should have the property that they respect the symmetries of the lattice, rather than being a mere discretization of continuum interpolating operators. The LHP Collaboration has developed techniques to enable the construction of baryon interpolating operators[3, 4]. An important theme in our analysis is the need to extract as many energy levels as feasible

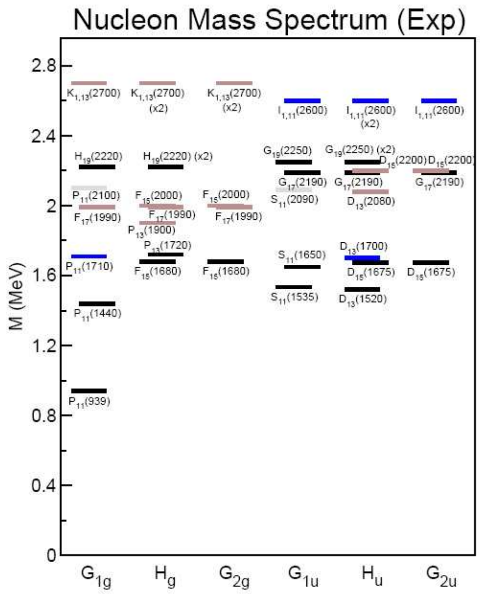

Figure 1: The figure shows the experimental masses assigned according to the irreps. of the cubic group.[5]. The spins can be identified by seeking degeneracies between energy levels in the different irreps. in the approach to the continuum limit.

in each irreducible representation (irrep.) admitted by the lattice. The reason for this is clear from Figure 1, where we show the masses of the observed isospin-1/2 states, but assigned not according to their continuum spin irreducible representations, but rather assigned according to the irreps. of the cubic group; there is a dense spectrum of states in each lattice irrep., and the spins of the states can be identified by seeking degeneracies between energies in different irreps. in the approach to the continuum limit.

All of our hadronic operators are constructed using gauge-covariantly displaced smeared quark fields as the building blocks; the use of smeared quark fields is essential both to reduce the statistical noise, and to ensure the dominance of low-lying states as close to the source as possible[5]. The displacements are along the six directions allowed by the spatial cubic lattice. A displaced quark and a displaced antiquark field can be joined together to form a gauge-invariant meson operator, while three displaced quark fields can be connected to form a gauge-invariant baryon operator. The specific orientations we employ are shown in Figure 2. The group-theoretical projection method is used to combine the different orientations of these elemental operators to form operators transforming irreducibly under the cubic group.

1.2 Recent Progress and Current Analysis

We had previously completed exploratory studies on small $12^3 \times 48$ quenched anisotropic Wilson lattices, with $a_s \simeq 0.1$ fm, $\xi \simeq 3$ and $m_\pi = 675$ MeV, focusing on the nucleon $I = 1/2$ sector[5]. This has now been extended to larger $24^3 \times 64$ lattices at a lighter pion mass $m_\pi = 490$ MeV, though using a more restricted basis of operators[6]. The pattern of

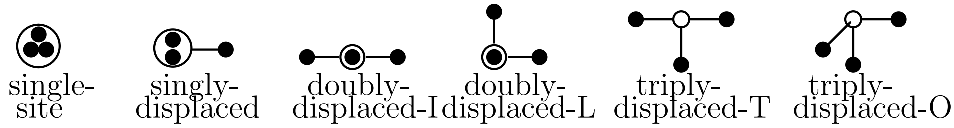

Figure 2: The spatial arrangements of the extended three-quark baryon operators. Smeared quark-fields are shown by solid circles, line segments indicate gauge-covariant displacements, and each hollow circle indicates the location of a Levi-Civita color coupling. For simplicity, all displacements have the same length in an operator.

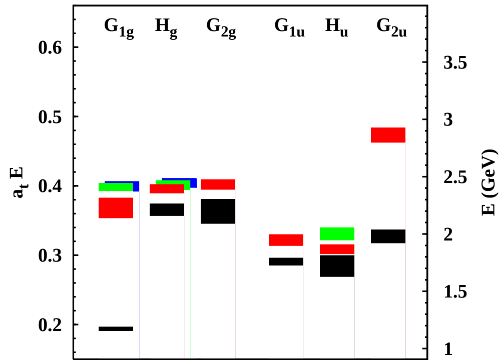

Figure 3: The energies obtained for each symmetry channel of $I = \frac{1}{2}$ baryons are shown based on the $24^3 \times 64$ lattice data. The scale on the left side shows energies in lattice units and the scale on the right side shows energies in GeV. The scale was set using the string tension. Errors are indicated by the vertical size of the box.

states in the $I = 1/2$ sector is shown in Figure 3, and confirms the tantalizing suggestion, noted earlier[5], of the existence of a band of negative-parity states well separated from the higher positive-parity band, as observed experimentally.

These studies have important implications. Firstly, they demonstrate the ability to extract many energy eigenvalues in an anisotropic lattice calculation. Secondly, in order to perform this analysis, a sufficiently large basis of operators, and in particular displaced operators, is required, and that basis should encompass a range of possible quark geometries. Thus we will include operators of the single-site, doubly-displaced-I, doubly-displaced-L and triply-displaced-T configurations of Figure 2.

We are now extending this study, using our current USQCD allocation, to full QCD, using the $N_f = 2$ anisotropic Wilson gauge configurations at $a_s \simeq 0.1$ fm and $a_s/a_t = 3$. The preliminary results we present here are obtained from an ensemble of 860 configurations on a $24^3 \times 64$ lattice, with $m_q = -0.4125$ corresponding to a pion mass $m_\pi = 400$ MeV, close to but somewhat lower than that used in the quenched study above. The configurations are separated by 20 trajectories, but we bin successive configurations to account for possible autocorrelations, yielding an ensemble of size 430. The spectrum of the lowest-lying positive-parity baryon states, using conventional single-correlator methods, is shown in Figure 4, together with the effective mass in the nucleon channel; reliable extraction of any negative-parity channels is problematic.

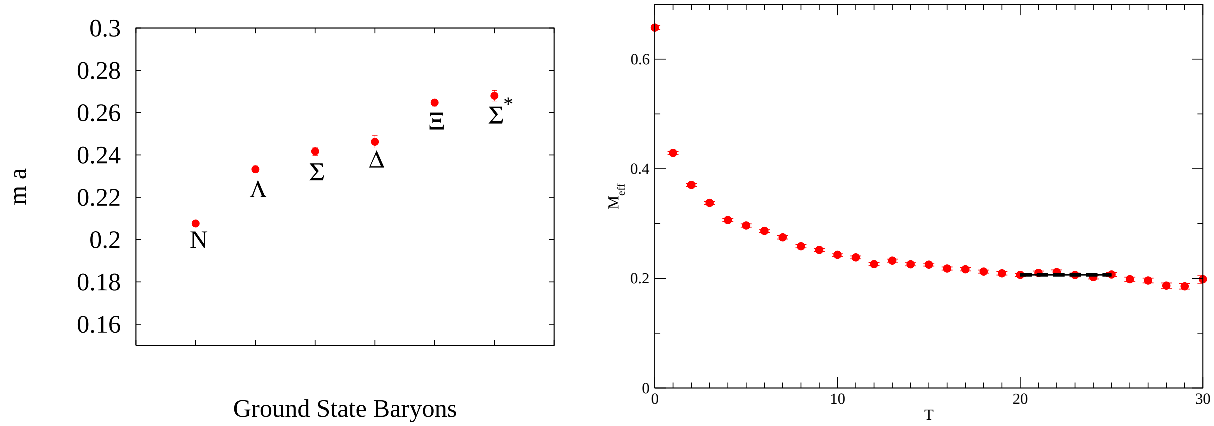

Figure 4: The left-hand panel shows the low-lying baryon spectrum obtained on the $N_f = 2$ lattices with $m_\pi = 400$ MeV; the right-hand panel shows the nucleon effective mass for smeared-source and smeared-sink, together with a single-exponential fit to the data.

In order to perform our analysis, we use the simplification of the variational method alluded to earlier: we solve the generalized eigenvalue equation at some reference time $t* > t_0$, to obtain variational coefficient v_{ak}:

$$C(t^*)v_k = \lambda_k C(t_0)v_k. \tag{2}$$

We then use the $\{v_k\}$ to transform our operators to a new preconditioned basis at all t, wherein the correlation matrix is diagonal at $t = t^*$. We employ the dominant operators in this new basis, that is those with the largest eigenvalues at $t = t^*$, in the subsequent analysis. This variation has particular advantages for baryons, where a straightforward application of the variational method is delicate due to the states, of opposite parity, propagating in the backward direction on the lattice. For the preliminary results discussed here, we start with a 16×16 correlation matrix constructed from the operators of our quenched analysis, and employ only the five dominant operators in the preconditioned basis.

Figure 5 shows the effective masses corresponding to the five dominant diagonal operators in our preconditioned correlation matrix; the efficacy of our diagonalization procedure, even for the ground state nucleon, is revealed by comparing the left-hand panel with the effective-mass plot in Figure 4. The result of single-exponential fits to the diagonal elements of the correlator corresponding to the lowest four energies in the G_{1g} channel is shown in Figure 6; the corresponding fits in the G_{1u} channel require that we include a single (lighter) state of opposite parity propagating backwards on our lattice.

1.3 Research Plans

This proposal seeks to exploit the methodology outlined above to perform the first comprehensive study of the baryon resonance spectrum in full QCD. We will focus on all of the baryons that can be constructed from u/d and s quarks, namely the nucleon, Δ, Λ, Σ,

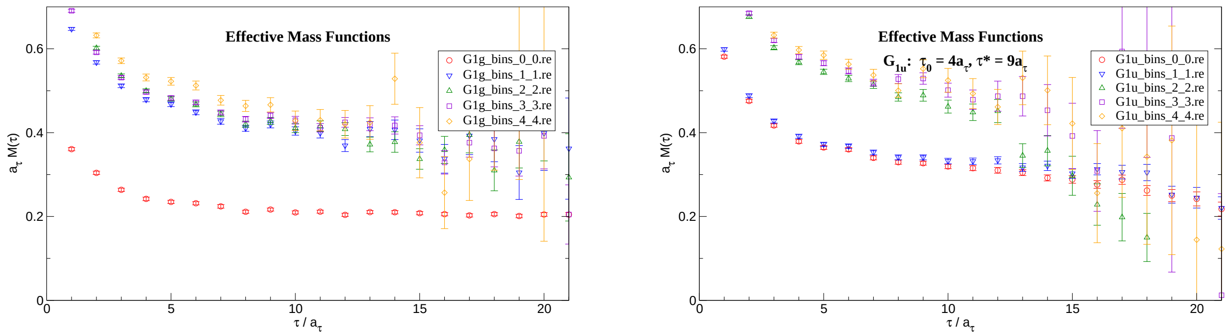

Figure 5: The left- and right-hand panels show the effective masses in the $I = \frac{1}{2} G_{1g}$ and G_{1u} irreps. constructed from the dominant diagonal elements of the correlation matrix diagonalized at $t^* = 9$.

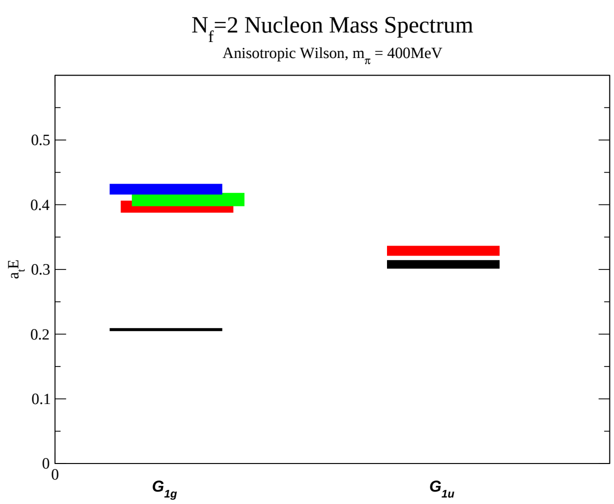

Figure 6: The figure shows the lowest energy eigenvalues from fits to the diagonal elements of the preconditioned G_{1g} and G_{1u} correlators, as described in the text.

Size	m_π(MeV)	L (fm)	$m_\pi L$
$16^3 \times 128$	875	1.92	8.5
$16^3 \times 128$	580	1.92	5.6
$20^3 \times 128$	315	2.4	3.8
$24^3 \times 128$	315	2.9	4.5

Table 1: The parameters of the lattices being used for this proposal.

Ξ and Ω. Cascades in particular are exciting both theoretically and experimentally, since they are expected to be narrow. Furthermore, there is a paucity of information about the quantum numbers of some of the states, presenting lattice QCD with an opportunity for "discovery".

2 Computational Strategy

2.1 Actions and Parameters

We will use the $N_f = 2+1$ anisotropic clover gauge configurations that are being generated as part of the proposal of *Edwards et al.*, at three values of the light-quark pseudoscalar mass, 875, 560 and 315 MeV, on the lattice volumes shown in Table 1; note that the first of these ensembles corresponds to three degenerate quark flavors. For each of these ensembles, we will compute valence quark propagators at quark masses corresponding to the light and strange quarks, and form the baryon correlators as described below. The calculation at $m_\pi = 875$ MeV is in a regime where we expect the states under study to be stable, and to provide a reference point for the other ensembles. At the lightest of the quark masses in this proposal, we expect open channels to emerge in the energy spectrum for some of the higher energies, and therefore the choice of two volumes at this mass is to provide a means of delineating single- and two-particle states.

2.2 Correlator construction

The "measurement" element of the calculation is substantial, employing the construction of *generalized baryon correlators*:

$$B_{\alpha\beta\gamma,\bar\alpha\bar\beta\bar\gamma}(t;0) = \sum_{\vec{x}} \epsilon^{abc}\epsilon^{\bar a\bar b\bar c} P^{a\bar a}_{\alpha\bar\alpha}(x;0) Q^{b\bar b}_{\beta\bar\beta}(x;0) R^{c\bar c}_{\gamma\bar\gamma}(x;0), \tag{3}$$

where P, Q, R are each quark propagators that may contain displacements and smearings at both source and sink; Greek letters denote spinor indices at source and sink. The group-theory projections, involving the appropriate linear combinations of Dirac indices, are then performed subsequently on workstations.

The computation of the generalized baryon correlators is purely local, apart from a global sum, but involves a very large number of operations per site, around 2 million. Our exploratory studies aimed at delineating sufficiently many eigenvalues indicate the need for a very large basis of interpolating operators, and in particular the *generalized baryon correlators* of Eq. 3, of the order of 670 for the nucleon. In particular, the identification of the optimal basis of operators does not involve the reduction in the number of generalized baryon correlators required.

The construction of the generalized baryon correlators, whilst purely involving local operations together with a global sum, involves many floating-point operations. To ensure that these are performed as efficiently as possible, we implement a number of computational optimizations, such as saving diquark temporaries in the evaluation of Eq. 3 and only computing the generalized correlators for those Dirac indices contributing to our final baryon correlation functions. The evaluation of these correlators is independent of the quark masses, and whilst representing a substantial fraction of the cost of the calculation at the heaviest pion masses, that cost should become an increasingly small component with decreasing pion mass, as we note later.

3 Software

The valence work is rather I/O intensive, and therefore we propose continuing the valence spectroscopy calculations on the clusters at JLab or at FNAL. All the code running in this proposal is written using USQCD software, and in particular *Chroma*.

4 Required Resources

4.1 Node-hours

We will compute valence quark propagators at both the light (u/d) and strange quark masses. Two quark masses on each ensemble will enable us to study all the standard baryons (N, Δ, Λ, Σ, Ξ and Ω). Our estimate for the time, and in particular the number of iterations required to compute the clover fermion propagators, is obtained from those needed to compute propagators at 875 and 580 MeV, assuming

$$N_{\text{iter}} = A + \frac{B}{m_\pi^2}, \tag{4}$$

with the number of iterations independent of the volume.

For each quark mass, we will compute propagators from four sources, using the optimal smearing determined in our earlier quenched study. All required displacements can be obtained by rotation from a minimal set of three displaced sources; in addition we also need the undisplaced sources. The cost of the propagator inversions is listed in Table 2. The ability to extract excited-state masses relies on the measurement of comprehensive basis of operators we have constructed, and the construction of the correlators is a major component of the analysis; the cost is listed in Table 3.

Thus the total request is for **2.1M 6n-node-hours, or its equivalent on other clusters.**

Size	m_π(MeV)	$N_{\rm cfg}$	6n node-hours
$16^3 \times 128$	875	1000	18557
$16^3 \times 128$	580	1000	37114
$20^3 \times 128$	315	2000	454034
$24^3 \times 128$	315	2000	659255
		Total:	1168960

Size	m_π(MeV)	$N_{\rm cfg}$	6n node-hours
$16^3 \times 128$	580	1000	22463
$20^3 \times 128$	315	2000	91570
$24^3 \times 128$	315	2000	151629
		Total:	265662

Table 2: The upper table provides the cost of generating light (u/d) quark propagators from four sources, as described in the text. The lower table gives the cost of generating the s-quark propagators from four sources for all but the $N_f = 3$ lattices.

Size	m_π(MeV)	$N_{\rm cfg}$	N_{qqq}	6n node-hours
$16^3 \times 128$	875	1000	671	17450
$16^3 \times 128$	580	1000	2000	52012
$20^3 \times 128$	315	2000	2000	203175
$24^3 \times 128$	315	2000	2000	351086
			Total:	623723

Table 3: The cost of generating generalized baryon propagators on each of the ensembles, for a given valence $m_{u/d}$ and m_s; note that for the SU(3)-symmetric point, corresponding to $m_\pi = 875$ MeV, a smaller number of correlators is required.

Size	m_π(MeV)	$N_{\rm cfg}$	N_{qqq}	TByte (tape)	6n-equiv. node-hours
$16^3 \times 128$	875	1000	671	1.8	7200
$16^3 \times 128$	580	1000	2000	5.3	20920
$20^3 \times 128$	315	2000	2000	5.3	20920
$24^3 \times 128$	315	2000	2000	5.3	20920
			Total:	17.7	70800

Table 4: The tape storage requirements for the generalized baryon correlators, stored in *sparse* format.

Size	m_π(MeV)	$N_{\rm cfg}$	TByte (tape)	6n-equiv. node-hours
$16^3 \times 128$	875	1000	1.1	4400
$16^3 \times 128$	580	1000	2.2	8800
$20^3 \times 128$	315	2000	8.6	34400
$24^3 \times 128$	315	2000	14.8	59600
		Total:	26.7	106800

Table 5: The tape storage requirements for the the single-site propagators, at both the light- and strange-quark masses.

Criteria for Future Computations

The program articulated in the proposal of *Edwards et al.,* envisages the continuation to larger volumes, notably at $m_\pi = 315$ MeV, and a lighter mass at 250 MeV, as well as at 400 MeV; computational resources would be required for analysis of each of these lattices, for this project typically of the order of 30% of the cost of lattice generation. An important criterion in constructing our future baryon spectroscopy plans is the extent to which we will be able to delineate single- and scattering states on our two volumes at 315 MeV, and the efficacy of employing the stochastic methods being investigated in the proposal of *Juge et al.*.

4.2 Disk Space

We propose to archive on tape all the generalized-baryon correlator files, in a *sparse* format containing only the useful Dirac components.

In addition, we require sufficient disk space to store the largest of the ensembles of *generalized baryon correlators* in Table 4, together with sufficient space to store the correlation matrices projected into the irreduncible representations: a total of 8 Tbyte, or 160,000 6n-node-hours equivalent.

The single-site propagators at both the light- and strange-quark masses could be of potential use for other USQCD projects; it should be noted, however, that our choice of smearing parameters is very much signed to extract the resonance spectrum of baryons. The tape storage requirements for these propagators are listed in Table 5.

5 Data Sharing

The quark propagators computed from a "single-site" or local source are potentially of use in other projects, and we would be prepared to store them to tape as discussed above.

6 Exclusivity

The computation of the excited resonance spectrum using our lattice group-theory methods for baryons with various isospin and strangeness quantum numbers in the light-quark sector are exclusive elements of this proposal. We will in addition perform a conventional computation of the hadron spectrum and two-point matrix elements. We will make the saved propagators available as they are generated to members of the USQCD Collaboration, providing they are not used for the exclusive analyses above; we will release them without restriction July 2010.

References

[1] C. Michael, Nucl. Phys. B **259**, 58 (1985).

[2] M. Luscher and U. Wolff, Nucl. Phys. B **339**, 222 (1990).

[3] S. Basak *et al.* [Lattice Hadron Physics Collaboration (LHPC)], Phys. Rev. D **72**, 074501 (2005) [arXiv:hep-lat/0508018].

[4] S. Basak *et al.*, Phys. Rev. D **72**, 094506 (2005) [arXiv:hep-lat/0506029].

[5] A. C. Lichtl, arXiv:hep-lat/0609019.

[6] S. Basak *et al.*, Phys. Rev. D **76**, 074504 (2007) [arXiv:0709.0008 [hep-lat]].

[7] D. C. Moore and G. T. Fleming, Phys. Rev. D **74**, 054504 (2006) [arXiv:hep-lat/0607004].

[8] R. G. Edwards, U. M. Heller and T. R. Klassen, Phys. Rev. Lett. **80**, 3448 (1998) [arXiv:hep-lat/9711052].