Excited Meson and Baryon States using Anisotropic Clover Lattices

Saul Cohen, Jozef Dudek, Robert Edwards, Balint Joo, Huey-Wen Lin,
David Richards[*], Christopher Thomas, Anthony Thomas
Jefferson Lab
Jimmy Juge
University of the Pacific
John Bulava, Justin Foley, Colin Morningstar
Carnegie Mellon University
Stephen Wallace, Eric Engelson
University of Maryland
Nilmani Mathur
Tata Institute
Mike Peardon, Sinead Ryan
Trinity College, Dublin

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Abstract

We propose to employ the anisotropic $N_f = 2+1$ dynamical clover configurations for a study of the meson and baryon resonance spectrum, and for the radiative transitions between mesons. We will perform the computations at values of the light-quark masses down to pion masses of 383 MeV, using a new method for computing the necessary hadron correlation functions. **We request the equivalent of 11.0M 6n-node hours, and archival storage of 75 TByte, equivalent to 101K 6n node-hour, and 15TByte of disk storage, equivalent to 203K 6n node-hour.**

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[*] email: dgr@jlab.org

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; the experimental investigation of the meson resonance spectrum, and in particular the search for mesons with exotic quantum numbers, is the aim of the GlueX Collaboration at JLab@12GeV.

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 a comprehensive study of the meson and baryon spectrum, employing the anisotropic clover gauge configurations generated under the proposal of *Edwards et al.*.; in addition we will perform the first investigation of the radiative transitions between mesons comprised of light quarks, providing vital input to the expectations for the GlueX experiment. Given the strategic goal of USQCD to address the key questions in hadronic physics, we believe this proposal satisfies the criteria for a Class-A proposal.

1.1 Meson spectrum and radiative transitions

A major goal of the JLab 12GeV upgrade involves the study of meson states produced in photoproduction reactions in the GlueX detector. Photoproduction has been proposed (within QCD-motivated models) to be a favourable method for the production of exotic hybrid mesons, those mesons having J^{PC} outside the set allowed to a fermion-antifermion pair. The hybrid hypothesis is that an excited gluonic field in addition to a quark-antiquark pair can give rise to these quantum numbers.

In this proposal we aim to continue our project to compute the excited meson spectrum, including exotics, and the photocouplings of these states in advance of the switch on of GlueX.

Over the past few years the JLab lattice group has made progress in developing a methodology for the extraction of photocouplings including those involving excited states and exotics. These initial trials have been done using charm mass quarks allowing for a comparison to the experimental radiative transition data in charmonium. This work is presented in a series of papers, starting with [5] in which ground-state transitions were successfully extracted. In [7] an excited state spectrum of charmonium was extracted, including even the difficult case of near-degenerate states, using a broad operator basis and variational solution methods (see an example in figure 1). The optimum excited state operators from this study were used in [6] to extract photocouplings involving excited and exotic mesons (examples are presented in figure 2). In summary we appear to have a reliable computational technique with which to extract the spectrum and photocouplings.

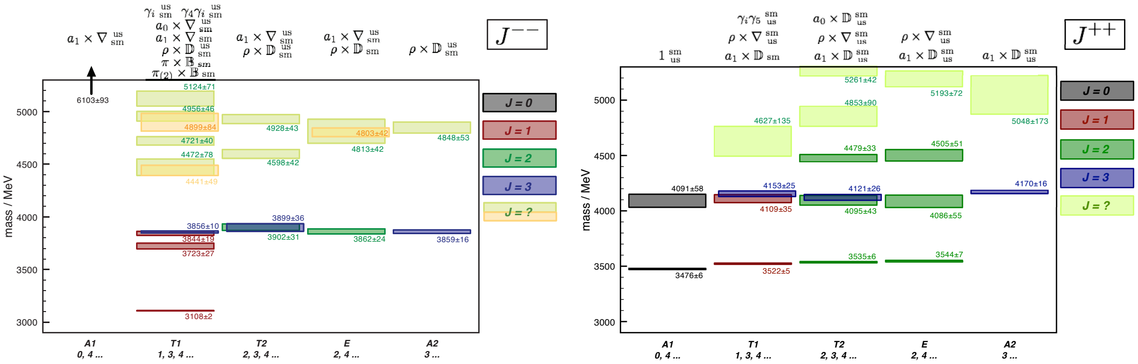

Figure 1: Extracted quenched charmonium mass spectrum for $PC = --, ++$ listed by lattice irreducible representation. Operator labels listed in [7]

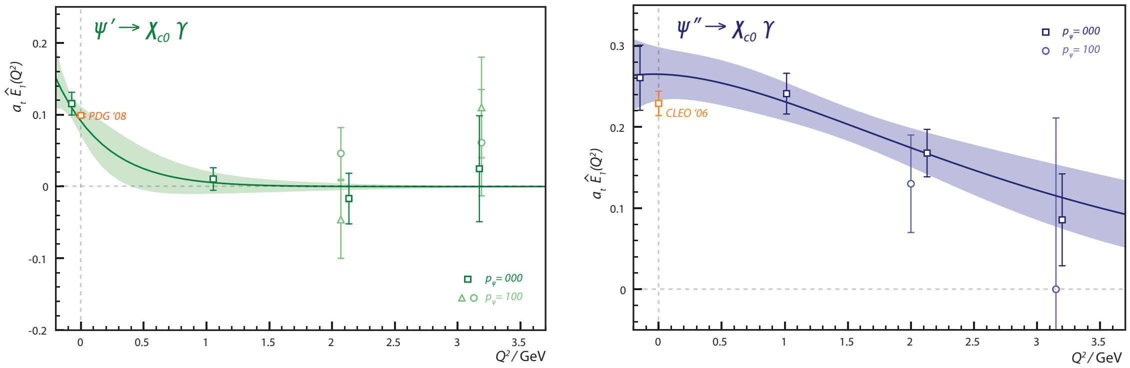

Figure 2: First and second excited vector state electric dipole transition form-factors to the ground state scalar in charmonium. Experimental results for real photons from PDG and CLEO-c.

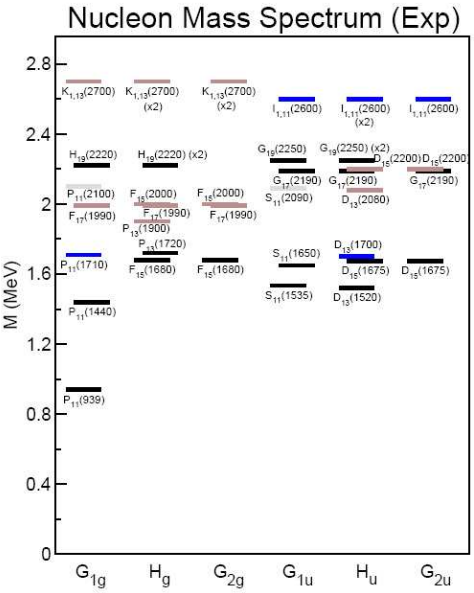

Figure 3: The figure shows the experimental masses assigned according to the irreps. of the cubic group[10]. The spins can be identified by seeking degeneracies between energy levels in the different irreps. in the approach to the continuum limit.

1.2 Baryon spectroscopy

The determination of the spectrum of baryon resonances is a major goal of the experimental program at Jefferson Laboratory, and in particular of the CLAS experiment. The *Excited Baryon Analysis Center* at Jefferson Laboratory is dedicated to the partial-wave analysis of worldwide pion photoproduction data with the aim of extracting the baryon spectrum. It is thus important to have high-quality lattice calculations to relate these analyses to QCD. As in the case of the meson calculation above, the application of the variational method, and the construction of a basis of interpolating operators satisfying the symmetries of the lattice are essential to this task. The need to extract as many energy eigenvalues as possible in each lattice irreducible representation is clear from Figure 3, 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.

The LHP Collaboration developed techniques to enable the construction of baryon interpolating operators in two papers[3, 4]. Following a previous study in the quenched approximation to QCD[11], we now have the first glimpses of the $I = 1/2$ nucleon spectrum using two flavors of dynamical quarks[12], using Wilson lattices generated under the USQCD INCITE award at ORNL. Results were obtained for two pion masses, 416(36) MeV and 578(20) MeV. The lowest four energies were reported in each of the six irreducible representations of the octahedral group, at each pion mass, as illustrated in Figure 4. Most

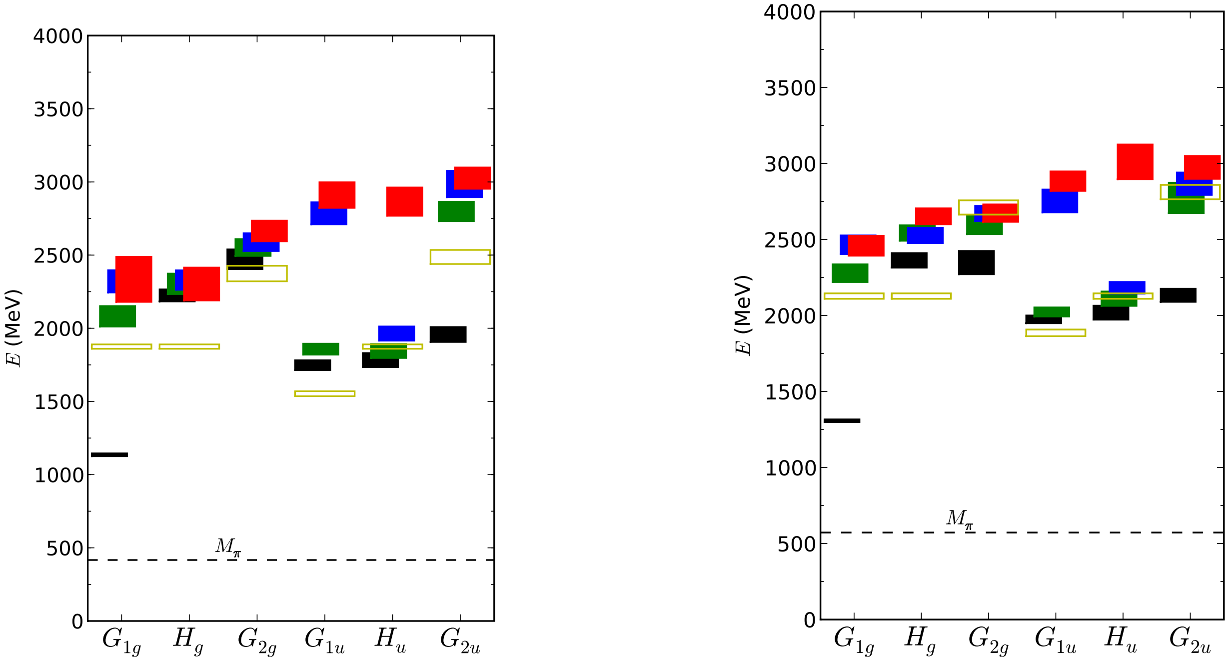

Figure 4: The left- and right-hand panels show the spectrum of $I = 1/2$ baryon resonance, indicated by the solid boxes, obtained on $N_f = 2$ Wilson fermion lattices at $m_\pi = 416$ and 578 MeV respectively[12]; the errors are indicated by the vertical width of the box. The open boxes show the expected thresholds for multiparticle states.

notably, clear evidence was found for a $5/2^-$ state in the pattern of negative-parity excited states, agreeing with the pattern seen in experiment, and the first time a spin-5/2 state has been realized in a lattice QCD calculation.

1.3 Research Plans

The aim of this proposal is to capitalize on the results outlined above by studies of the meson spectrum and radiative transions, and of the baryon spectrum, on the $N_f = 2 + 1$ anisotropic clover lattices generated under the USQCD proposal of *Edwards et al.*.[8, 9], using a new computational technique for the valence quark calculations that we will introduce below. More specifically, we aim to extend the investigation of the meson spectrum and radiative transitions from states composed of the heavier charm quarks in the quenched approximation to QCD to states composed of the quarks at the strange quark mass and below, and to a region where states become unstable under the strong interactions. We aim to investigate the baryon spectrum with three flavours of propagating quarks, and likewise extend the calculations to a regime where some of the baryon resonances become unstable.

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 four values of the light-quark pseudoscalar mass down to $m_\pi = 383$ MeV, on the lattice volumes shown in Table 1; note that the first of these ensembles corresponds to three degenerate quark flavors.

2.2 Computation of valence-quark propagators

The most computationally demanding part of the second step of the correlation function computations is the evaluation of the needed quark propagators. It is not computationally possible to compute all of the individual elements of M^{-1}, nor even the individual elements from all spatial sites on one time slice to all spatial sites on another time slice. In the usual point-to-all method, this problem is circumvented by exploiting translational invariance to remove the summation over spatial sites at the source time-slice (but not the sink time-slice). In this way, we only need to obtain the solutions x of the linear system of equations $Mx = y$ for a reasonably small number of source vectors y. However, the need for good multi-hadron operators in our operator sets disallows the point-to-all technique, requiring instead so-called "all-to-all" propagators.

Historically, all-to-all propagators have been computed using a stochastic method, generally with some variance-reduction technique. However, we realized in the summer of 2008 that a slight redefinition of smearing enabled us to exploit a clever choice of source vectors y so that we need only obtain solutions x of $Mx = y$ for a reasonably small number of y vectors, while still being able to carry out summations over all spatial sites at both the source and sink time slices. The trick is to observe that we can write the three-dimensional Jacobi-smearing matrix as

$$L^{(J)} \equiv (1 - \frac{\kappa}{n}\Delta)^n = \sum_{i=1} f(\lambda_i) v^{(i)} \otimes v^{*(i)}, \tag{1}$$

where $v^{(i)}$ is the i^{th} eigenvector of Δ with eigenvalue λ_i, and $f(\lambda_i) = (1 - \frac{\kappa\lambda}{n})^n$. We then truncate the sum in eqn. 1 at some value m. Providing m is taken sufficiently large, which we have found to be 64 or less for the lattices of interest, this will remove the high frequency modes and hence accomplish the aim of smearing; we christen this new method "distillation" or "Laplacian Heaviside (LAPH) smearing".[15].

Focusing now on the construction of meson two-point functions,

$$C_M(t,t') = \langle 0 \mid \bar{d}(t')\Gamma^B(t')u(t')\bar{u}(t)\Gamma^A(t)d(t)|0\rangle \tag{2}$$

we see that this can be written

$$C_M(t,t') = \mathrm{Tr}\langle \phi^A(t')\tau(t',t)\Phi^B(t)\tau^\dagger(t',t), \rangle \tag{3}$$

where

$$\begin{aligned} \Phi^{A,ij}_{\alpha\beta} &= v^{*(i)}(t)[\Gamma^A(t)\gamma_5]_{\alpha\beta} v^{(j)}(t') && (4)\\ \tau^{ij}_{\alpha\beta}(t,t') &= v^{*(i)}(t') M^{-1}_{\alpha\beta}(t',t) v^{(j)}(t). && (5) \end{aligned}$$

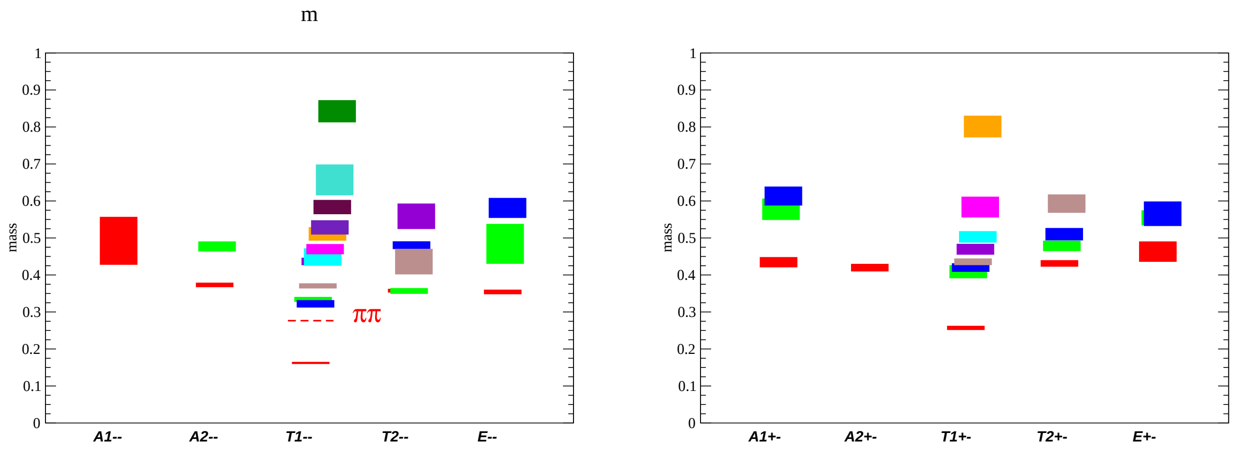

Figure 5: The left- and right-hand figures show preliminary fits to the meson spectrum for $PC = --$ and $PC = +-$ obtained on $16^3 \times 128$ lattices at $m_\pi = 448$ MeV using the distillation method described in the text.

with $i, j = 1, \ldots, m$, α and β are spinor indices, and t, t' the source and sink timeslices respectively; the trace in eqn. 3 is over the (truncated) eigenvector space. The Φ's of eqn. 4 depend only on the choice of operators and the underlying gauge fields; the propagation of the quarks is contained in the "perambulators" of eqn. 5, and these are independent of the operators. These same perambulators can also be used for multiparticle correlators,and analogous expressions exist for baryon correlation functions. Furthermore, the method can be extended both to deal with "multi-hadron" operators with annihilation diagrams at source or sink, and for three-point functions; we will exploit all of these extensions in this proposal. As an illustration of the efficacy of the method, we shown in Figure 5 a preliminary analysis of the excited meson spectrum for $PC = --$ and $PC = +-$[15].

The computational cost is dominated by the calculation of the perambulators of eqn. 5; in this proposal we typically compute these for 64 eigenvectors $v^i(t)$ from four different timeslices t. This relatively large number of matrix inversions allows us to efficiently exploit eigenvector deflation methods; with sufficient number of eigenvectors we essentially eliminate critical slowing down of the solver with decreasing quark mass.

For each of these ensembles, we will compute valence quark propagators at quark masses corresponding to the light and strange quarks, except of course at the $N_f = 3$ ($m_\pi = 833$ MeV) point. The use of two volumes is to facilitate the delineation of the single- and multi-particle states. For the $m_\pi = 833$ and 560 lattices, we will perform a comprehensive study of two-particle states through the use of multiparticle interpolating fields, calculated through a variant of the distillation method.

3 Software

The generation of the *perambulators* and *generalized perambulators* will use the USQCD-supported *Chroma* software suite. The construction of the hadronic correlators employs *adat*, typically running on a single multi-core node under OpenMP.

Size	m_π(MeV)	L (fm)	$m_\pi L$
$16^3 \times 128$	833	1.9	8.5
$20^3 \times 128$	833	2.4	10.5
$16^3 \times 128$	560	1.9	5.6
$20^3 \times 128$	560	2.4	7.0
$16^3 \times 128$	448	1.9	4.3
$16^3 \times 128$	383	2.4	3.5
$24^3 \times 128$	383	2.9	5.3

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

Size	m_π(MeV)	N_{eigen}	N_{t0}	N_{dil}	N_{cfg}	**6n node-hours**	Storage(TByte)
$16^3 \times 128$	833	64	4	16	600	1.06M	1.5
$20^3 \times 128$	833	64	4	16	200	0.69M	0.5
$16^3 \times 128$	560	64	4	16	550	0.97M	1.4
$20^3 \times 128$	560	64	4	16	160	0.55M	0.4
$16^3 \times 128$	448	64	4	0	650	0.23M	0.33
$16^3 \times 128$	383	64	4	0	550	0.19M	0.28
$24^3 \times 128$	383	64	4	0	600	0.71M	0.3
					Total:	**4.40M**	**4.3**

Table 2: The table provides the cost of generating light (u/d) quark perambulators, as described in the text. For the lattices at $m_\pi = 833$ and 560 MeV we also include the cost of the propagators required to compute the disconnected contributions to hadron correlators.

4 Required Resources

4.1 Node-hours

We will compute valence quark propagators, the perambulators, at both the light (u/d) and strange quark masses, the computational costs for which are shown in Tables 2 and 3, respectively. 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 $m_\pi = 833$ MeV on the $16^3 \times 128$ lattices, and using the observation that, with deflation, the total number of iterations is independent of the quark mass, and indeed of the volume.

The computational cost of computing the meson and baryon correlation functions on each of our ensembles is shown in Tables 4 and 5, respectively. Note that this time is independent of the spatial extent of the lattice, depending only on the temporal extent, the number of source time slices, and the number of eigenvectors vectors. In the case of the meson spectrum, we will employ all 64 source vectors, whilst for the baryons, where computational cost of constructing the correlators is substantial, we will employ an optimal choice of 32 source vectors, and 8 operators at both source and sink for all isospin channels.

Size	m_π(MeV)	N_{eigen}	N_{t0}	N_{dil}	N_{cfg}	6n **node-hours**	Storage (Tbyte)
$16^3 \times 128$	560	64	4	16	550	0.97M	1.4
$20^3 \times 128$	560	64	4	16	160	0.55M	0.4
$16^3 \times 128$	448	64	4	0	650	0.23M	0.33
$16^3 \times 128$	383	64	4	0	550	0.19M	0.28
$24^3 \times 128$	383	64	4	0	600	0.71M	0.3
					Total:	**2.65M**	**2.28**

Table 3: The table provides the cost of generating strange (s) quark perambulators, as described in the text. For the lattices at $m_\pi = 560$ MeV, we also include the cost of the propagators required to compute the disconnected contributions to hadron correlators.

Size	m_π(MeV)	N_{cfg}	6n **node-hours**	Storage (Tbyte)
$16^3 \times 128$	833	600	8K	
$20^3 \times 128$	833	200	2.7K	
$16^3 \times 128$	560	550	22K	
$20^3 \times 128$	560	160	6.4K	
$16^3 \times 128$	448	650	26K	
$16^3 \times 128$	383	550	22K	
$24^3 \times 128$	383	600	24K	
		Total:	**111K**	**10**

Table 4: The cost and storage for calculating the meson spectrum for states that can be constructed from the light (u/d) and strange quarks, using 64 source smearing vectors and four time slices for the source, as described in the text.

The investigation of radiative transitions involves the calculation and of *Generalized Perambulators*, that play the role of sequential sources in the usual method, for both the light-light and strange-strange transitions. The cost of these are given in Table 6. The cost of computing the radiative-transition three-point functions is provided in Table 7.

SUMMARY OF REQUEST

- The cost of computing the u/d **and** s **QUARK PERAMBULATORS** is **7.05M 6n node-hours**.
- The cost of the **MESON SPECTRUM** is **111K 6n node-hours**
- The cost of the **BARYON SPECTRUM FOR** $N, \Delta, \Lambda, \Sigma, \Xi, \Omega$ is **2.7M 6n node-hours**.
- The cost of computing the **Generalized Perambulators** is **939K 6n node-hours**.

Size	m_π(MeV)	$N_{\rm cfg}$	6n **node-hours**	Storage (Tbyte)
$16^3 \times 128$	833	600	360K	
$20^3 \times 128$	833	200	120K	
$16^3 \times 128$	560	550	495K	
$20^3 \times 128$	560	160	144K	
$16^3 \times 128$	448	650	585K	
$16^3 \times 128$	383	550	495K	
$24^3 \times 128$	383	600	540K	
		Total:	**2.74M**	**13**

Table 5: The cost of computing the baryon spectrum for all possible flavor combinations of the baryons, using 32 source smearing vectors and four time slices for the source, as described in the text.

Size	m_π(MeV)	$N_{\rm eigen}$	$N_{t_{\rm src},t_{\rm snk}0}$	$N_{\rm moml}$	$N_{\rm cfg}$	**6n node-hours**	Storage(TByte)
$16^3 \times 128$	833	64	4	6	600	61K	3.6
$20^3 \times 128$	833	64	4	6	200	40K	1.2
$16^3 \times 128$	560	64	4	6	550	113K	6.6
$20^3 \times 128$	560	64	4	6	160	64K	1.9
$16^3 \times 128$	448	64	4	6	650	113K	7.8
$16^3 \times 128$	383	64	4	6	550	112K	6.6
$24^3 \times 128$	383	64	4	6	600	415K	7.2
					Total:	**939K**	**35**

Table 6: The table provides the cost of computing so-called *generalized perambulators*, for both the u/d and s quarks, as described in the text. Also shown is the storage cost.

Size	m_π(MeV)	$N_{\rm cfg}$	6n **node-hours**	Storage (TByte)
$16^3 \times 128$	833	600	8K	
$20^3 \times 128$	833	200	2.7K	
$16^3 \times 128$	560	550	22K	
$20^3 \times 128$	560	160	6.4K	
$16^3 \times 128$	448	650	26K	
$16^3 \times 128$	383	550	22K	
$24^3 \times 128$	383	600	92K	
		Total:	179K	10

Table 7: The cost of computing the radiative transtions between mesons that can be constructed from the light (u/d) and strange quarks, using 64 source smearing vectors.

- The cost of computing the **RADIATIVE TRANSITIONS** is **179K 6n node-hours**.

Thus the total is **11.0M 6n node hours**.

Finally, we request archival storage equivalent of **75 Terabyte** archival storage for the perambulators and generalized perambulators, which are of general use, and for the elemental meson and baryon operators, equivalent to **101,000 6n node-hours**. We also request **15 Terabyte** of disk storage, corresponding to the total diskspace for the largest ensemble, equivalent to **203,000 6n node-hours.**

Additional resources

We are ready to devote additional resources, should they become available, to extend the program to the large-volume ($32^3 \times 256$) lattice at $m_\pi = 383$, and to the lattices at $m_\pi = 230$ being generated under the proposal of *Edwards et al.*; the analysis could be performed both on the clusters, and on leadership-class facilities. This would enable us to advance our long term program to have control over the spectrum in the approach to the chiral limit.

5 Data Sharing

The perambulators and generalized perambulators are of use for other projects, a major advantage of the methodology.

6 Exclusivity

The computation of the meson resonance spectrum and radiative transitions, and of the baryon resonance spectrum 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 "perambulators" 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 2011.

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