Excited Meson and Baryon States using Anisotropic Clover Lattices

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Abstract

We propose to investigate the low-lying meson and baryon resonance spectrum at quark masses corresponding to pion masses of 380 and 230 MeV, using the anisotropic clover lattices generated under the program of *Edwards et al.*. A major goal is the inclusion of multi-hadron operators to enable the extraction of the momentum-dependent phase shifts. In addition, we will perform a study of the expected lightest "hybrid" meson, the 1^{-+}, on the ensemble of $48^3 \times 512$ lattices being generated under the *Blue Waters Early Science Program*, with the aim of exploring whether this state persists to the physical light-quark masses. We will exploit a stochastic variant of the "distillation" method to enable the efficient computation of the hadron correlation functions. We will employ GPUs for the solution of the Dirac equation, and clusters for the construction of the hadron correlation functions. **We request 2.67M GPU-hours on GPUs, and 39.6M Jpsi-equivalent core-hours on the clusters. We request tape storage of 667 TBytes, 2M J/Psi-equivalent core-hours, and disk storage of of 120 TBytes, 3.6M J/Psi-equivalent core-hours.**

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Physics Goals

A key goal of the nuclear physics program is a first principles description of strong-interaction physics from Quantum Chromodynamics. An important measure of that description is whether we can compute the spectrum of the theory, and then confront high quality experimental data. The complete combined analysis of available experimental data on the photoproduction of nucleon resonances, and the measurement of the electromagnetic properties of the low-lying baryons are the HP3 and HP7 DOE milestones in hadronic physics[1], with theory support integral to the current and future experimental program[2]; the experimental investigation of the meson spectrum, and in particular the search for mesons with exotic quantum numbers, is the aim of the GlueX Collaboration at JLab@12GeV, and the target of a new milestone HP15 (2018).

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, we have a multi-year program aimed at a comprehensive study of the meson and baryon resonance spectrum. A strategic goal of USQCD is to address the key questions in hadronic physics, and thus we believe our proposal satisfies the criteria for a *Class-A* proposal

Beyond determining the excited-state spectrum, we aim to gain an understanding of the effective degrees of freedom that emerge from QCD, and to explore the properties of some of these states. Thus our plans include the calculation of the electromagnetic form factors and transition matrix elements, providing vital input to experimental studies for both baryons and mesons, and the calculation of the quark distribution amplitudes that provide a description of hadronic structure probed in transition form factors at high momentum transfers. Our program exploits the anisotropic clover gauge configurations, designed for spectroscopy, generated under the proposal of *Edwards et al.*. The rest of this section describes progress towards these goals that has been made during the current allocation period, and our physics aims in 2012-2013.

Advances in 2011/2012

Key to our program has been the exploitation of the "distillation" quark source construction[3] to expand the range of spectroscopic quantities accessible to lattice QCD calculations, and to advance towards our goal of understanding meson and baryon resonances from first principles. Major advances over the past year include the calculation of the excited baryon spectrum, including the strong suggestion of the existence of "hybrid" baryons, the investigation of $I = 2\,\pi\pi$ scattering in a moving frame, enabling a far finer resolution of the $l = 0$ and $l = 2$ phase shifts in the elastic regime than that admitted by studies at rest, and the application of distillation to discern the spin-identified charmonium spectrum.

Excited Baryon Spectrum

A major achievement was the calculation of the excited baryon spectrum, with the continuum quantum numbers of the (single-particle) states reliably determined, on $16^3 \times 128$ lattices at pion masses down to 396 MeV. The method followed that of the meson spectroscopy: a basis of continuum interpolating operators was constructed including up to two derivatives, and which respected classical symmetries, which was then subduced to the appropriate lattice irreps.. As for the meson spectrum, the overlaps of the interpolating operators with the extracted states was key to determining the spin of the states, and the method exploited the remarkable degree of rotational symmetry observed at the hadronic scale[4]. The data at the lightest of our pion masses is shown in Figure 1, and exhibited a counting of levels consistent with the non-relativistic qqq constitutent quark model.

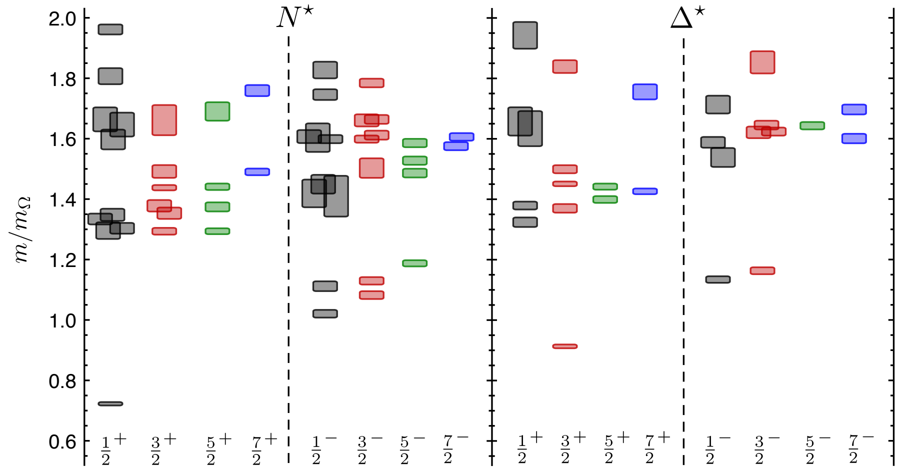

Figure 1: Spin-identified spectrum of Nucleons and Deltas from the lattices at $m_\pi = 396$ MeV, in units of the calculated Ω mass.

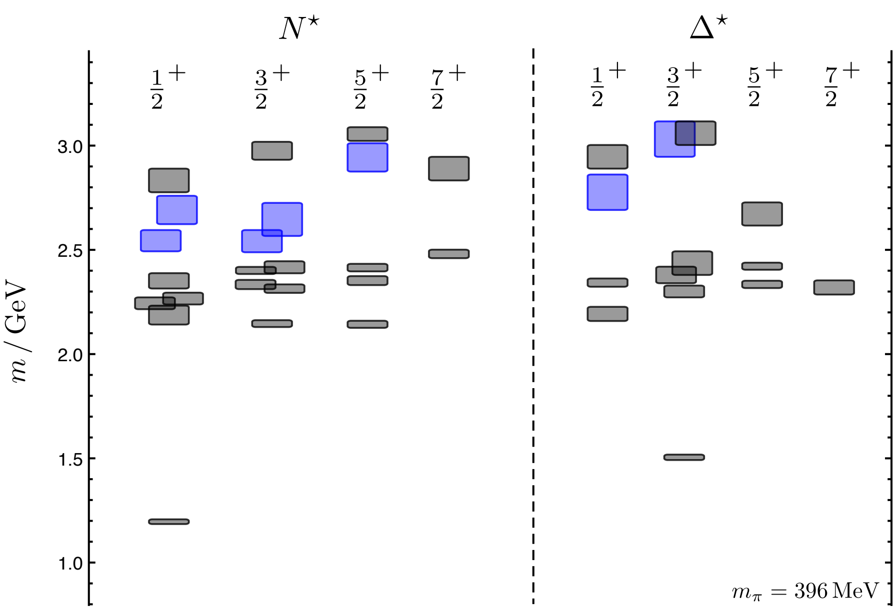

Figure 2: N and Δ spectrum at $m_\pi = 396$ MeV with the "hybrid" operators included in the basis; blue boxes denote states dominated by such operators and thereby identified as "hybrids".

In contrast to mesons, there are no "exotic" quantum numbers for baryons that *demand* a richer structure than that of three quarks with relative orbital angular momentum. As noted in reference [4], the operators associated with an excited gluon field, and which would vanish for a trivial gauge configuration, were not included in the basis. These operators were included in a subsequent reanalysis for the postive-parity N and Δ spectrum[5], shown in Figure 2, and revealed the presence of "hybrid" baryons dominated by operators with an excited gluon field. Remarkably, the mechanism giving rise to such gluonic excitations appears common to both mesons and baryons, as shown in Figure 3, where we show the excitation energy of both "hybrid" mesons and "hybrid" baryons.

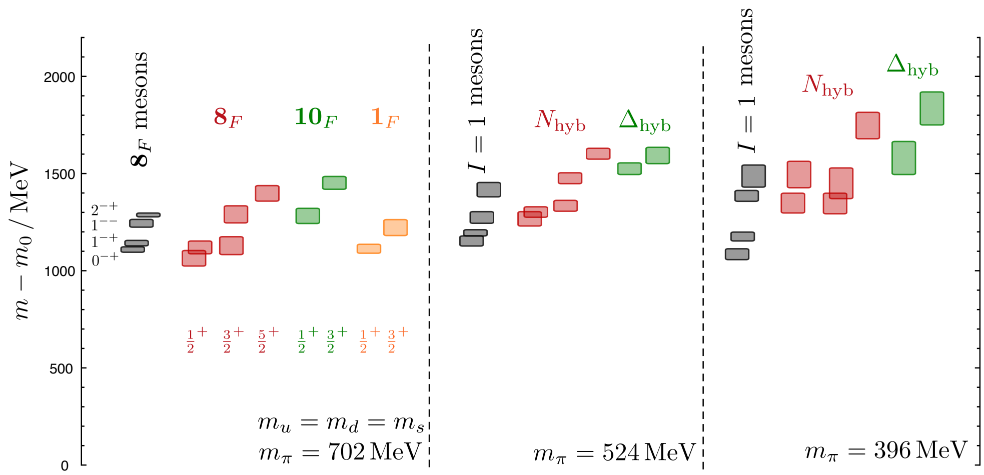

Figure 3: The excitation spectrum of hybrid mesons and baryons at three values of the light-quark mass; for mesons we show $m - m_\rho$, while for baryons we show $m - m_N$.

Helicity Operators for Hadrons in Flight

A prerequisite for the investigation of hadron resonances, and indeed for precise calculations of scattering phase shifts at sufficiently fine momentum resolutions, is a set of hadronic operators at non-zero momentum that respect the symmetries of a cubic lattice and of the cubic volume of the lattice. This has been accomplished, and is detailed for mesons in reference [6].

Even in the continuum in infinite volume, the z component of spin, M, is not a good quantum number unless the momentum is in the direction z. More convenient is a *helicity basis* $\{\mathbb{O}^{J,\lambda}(\vec{p})\}$, labelled by total angular momentum J and helicity λ, the projection of spin in the direction of $\vec{p}$, defined by

$$\mathbb{O}^{J,\lambda}(\vec{p}) = \sum_M \mathcal{D}^{(J)*}_{M\lambda}(R)\ \mathcal{O}^{J,M}(\vec{p}) \ , \tag{1}$$

where $\mathcal{D}^{(J)}_{M\lambda}(R)$ is a Wigner-$\mathcal{D}$ matrix for the rotation R of $(0, 0, |\vec{p}|)$ to $\vec{p}$, and $\mathcal{O}^{J,M}(\vec{p})$ are boosted operators of the form introduced in ref. [7]. Using only the constraints arising from 3-rotation symmetry, the overlap of a state of definite J^P (P, P' are the parities at rest) and helicity onto a helicity operator is given by

$$\left\langle 0 \middle| \mathbb{O}^{J,P,\lambda}(\vec{p}) \middle| \vec{p}; J'^{P'}, \lambda' \right\rangle = Z^{[J,J',P,P',\lambda]} \delta_{\lambda,\lambda'} \ . \tag{2}$$

We now follow the procedure adopted for the construction of operators for states at rest by subducing the continuum operators into the appropriate little-group irrep. Λ, with row $\mu = 1, \ldots, \dim[\Lambda]$.

$$\mathbb{O}^{[J,P,|\lambda|]}_{\Lambda,\mu}(\vec{p}) = \sum_{\hat{\lambda}=\pm|\lambda|} \mathcal{S}^{\tilde{\eta},\hat{\lambda}}_{\Lambda,\mu} \mathbb{O}^{J,P,\hat{\lambda}}(\vec{p}) \ , \tag{3}$$

where $\tilde{\eta} \equiv P(-1)^J$ with J and P the spin and parity of the operator $\mathbb{O}^{J,P,\lambda}(\vec{p} = \vec{0})$; note that parity is not a good quantum number at non-zero momentum. The subduced helicity operators are different orthogonal combinations of the two signs of helicity, $+|\lambda|$ and $-|\lambda|$. As in the case of particles at rest, we find that observing the subduced overlaps of our operators with states to identify is key to identifying the quantum numbers of the extracted energy levels at non-zero momentum. The efficacy of this approach is illustrated in Figure 4, where we show the spectrum of low-lying isovector mesons

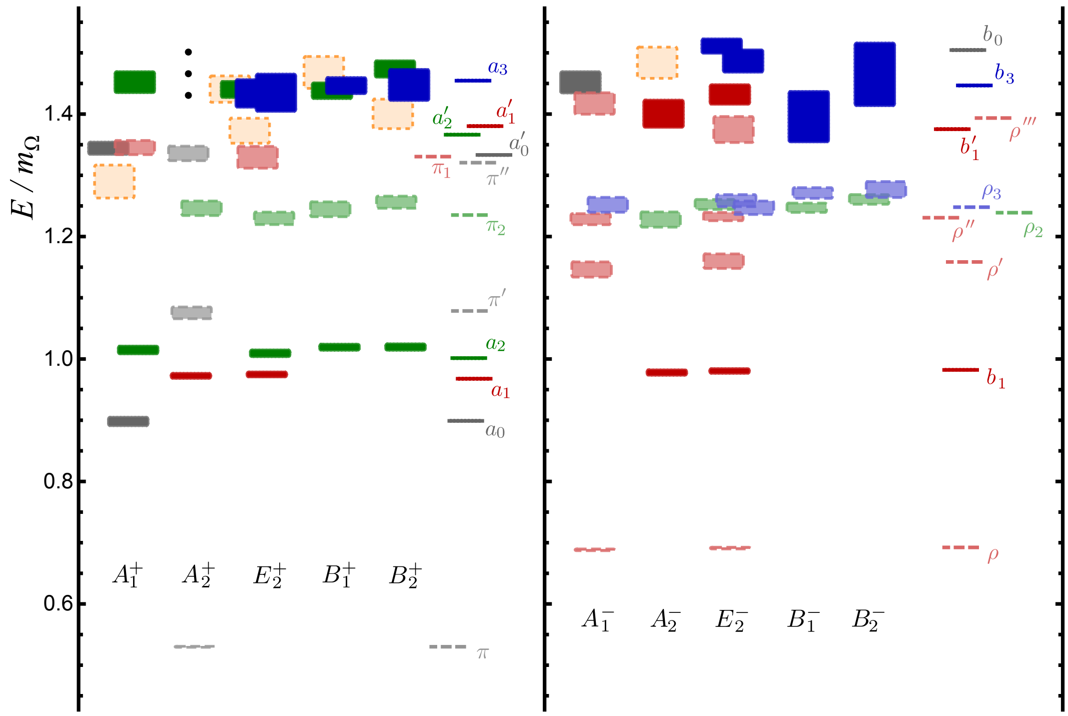

Figure 4: Spectrum of low lying isovector mesons with positive (left hand panel) and negative (right hand panel) charge conjugation parity in each irrep, Λ^C, for $|\vec{p}|^2 = 1$ (Dic$_4$). The box height shows the one sigma statistical uncertainty above and below the central value; the colour coding, indicating the J^P, is described in the text. Ellipses indicate that there are additional states within a given irrep in that energy range but that they are not well determined in this calculation. The lines in the right hand column show expected energies for the lower-lying states as described in the text.

in each lattice irrep for $|\vec{p}^2| = 1$ (Dic$_4$), with the spin identified as discussed above, together with the expected energies extracted from the spectrum at zero momentum.

The phase-shift of $I = 2$ $\pi\pi$ scattering

The investigation of phase shift in non-resonant $I = 2\pi\pi$ scattering is both of inherent interest for comparison with experiment, and as a theatre in which to apply and to develop some of the methodology needed to investigate resonances. One procedure is that proposed by Lüscher[8] which maps the discrete spectrum of eigenstates of QCD in a finite cubic volume to the phase shift for elastic scattering. By extracting multiple excited eigenstates within a given quantum number sector, one can map out the phase shift as a function of scattering momentum and, if present in that channel, observe resonant behaviour.

In 2010/2011, we applied the method to $I = 2\,\pi\pi$ scattering[9], using as an operator basis a pair of back-to-back pions with total momentum zero, but with definite relative momentum. We were able to extract the momentum-dependent phase shifts δ_0 and, for the first time, δ_2 using data at only a single lattice spacing; we note that the use of "distillation" was key in enabling us to project onto the back-to-back basis states not only at the sink, but also at the source, and hence to apply the variational method to precisely determine the energy levels.

Despite these achievements, the application of the method at zero total overall momentum provided a rather coarse resolution of the scattering momenta, and in particular only around five scat-

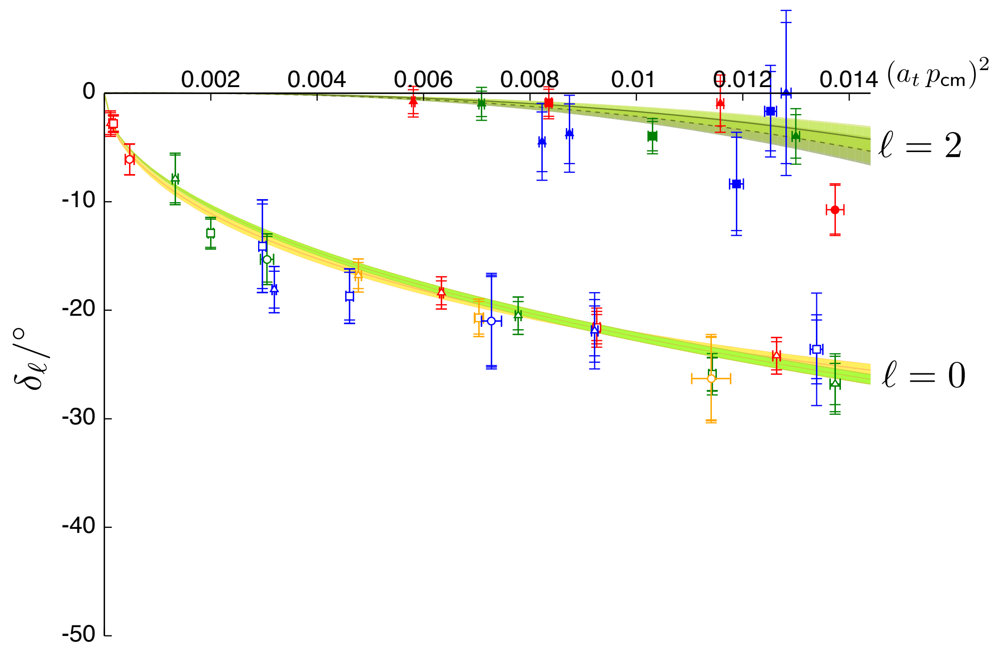

Figure 5: Extracted $I = 2$ $\pi\pi$ elastic S-wave and D-wave scattering phase shift (for $m_\pi = 396\,\mathrm{MeV}$); the bands correspond to scattering-length fits to the data for $l = 0$ and $l = 2$. Note that all the points shown are within the elastic regime at this value of the pion mass.

tering momenta below the inelastic threshold, the region of applicablity of the method. The solution to providing a greater range of scattering momenta is to apply the method to the case where the overall momentum of the two-pion system is non-zero; construction of subduced operators at non-zero momentum both for single-particle and two-particle states is a prerequisite for the calculation. The $l = 0$ and $l = 2$ phase shifts are shown in Figure 5, at a pion mass $m_\pi = 396$MeV, and at three lattice volumes; each of the lattice data on the plot corresponds to a point below the inelastic threshold at this value of the pion mass. The bands how scattering-length fits to the data for $l = 0$ and $l = 2$ respectively.

Charmonium Spectroscopy

The realization that a knowledge of the overlaps of interpolating operators could be used to identify the spins of states was first made in ref. [10] in a calculation of the charmonium spectrum in the quenched approximation. We have now applied the methodology developed for the light-quark spectrum, including the use of "distillation", to charmonium, using our the $N_f = 2 + 1$ anisotropic clover lattices, illustrated in Figure 6.

Plans for 2012/2013

The research plans for 2012/2013 will capitalize on the advances achieved over the previous years: the ability to efficiently include annihilation dynamics[11], the computation of momentum-dependent phase shifts[9], including in particular the ability to extract momentum-dependent phase shifts from systems in flight. In this proposal, we will investigate:

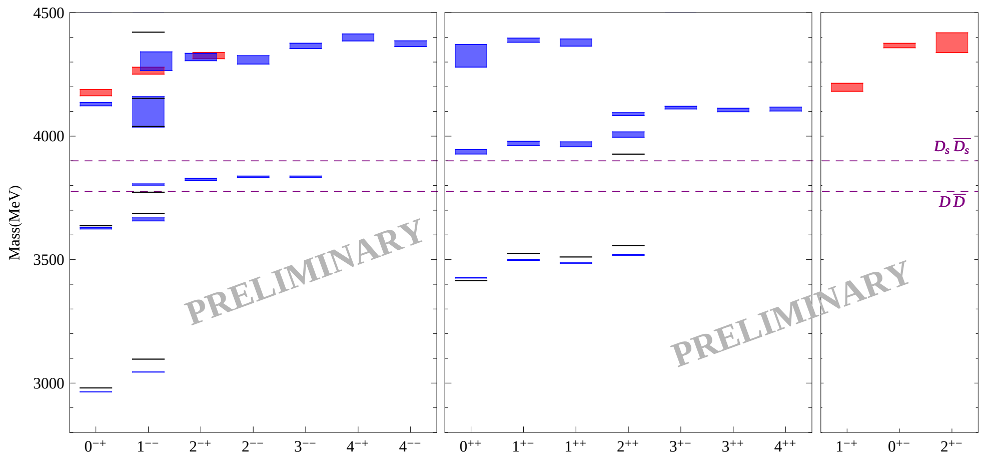

Figure 6: The spin-identified charmonium spectrum obtained on $24^3 \times 128$ lattices at a pion mass $m_\pi = 396$ MeV. The black lines denote the experimental determination, while the colored boxes denote the lattice calculations; boxes in red are those identified as "hybrid" states, including some of non-exotic quantum numbers.

1. The excited baryon spectrum on large lattices, including the contribution of the multi-hadron scattering states. In particular:
   - We will focus on the low-lying negative-parity spectrum including the πN channel, with the aim of extract the corresponding momentum-dependent phase shift.
   - We will calculate the spectrum of baryons containing one, two and three strange quarks, in anticipation of future experimental programs at JLab@12GeV
2. We apply our methods to compute the momentum-dependent phase shifts from systems in flight to channels exhibiting resonant behavior, including $I = 1\pi\pi$ scattering and the a_0.

In addition, the solution vectors and data generated under this proposal will be essential ingredients to other key calculations of our program, laid out in the proposal of *Edwards et al.*.

1. Charmonium spectroscopy, and the investigation of disconnected contributions near the $D\bar{D}$ threshold.
2. The spectrum of baryons containing a single heavy (c or b) quarks
3. Quark distribution amplitudes of light mesons and of some of the low-lying excited states.
4. Radiative transition form factors between mesons and between baryons.

Early Science Program Our previous calculations of the meson spectrum spectrum suggest that the lightest exotic has an excitation energy of around 1 GeV, but this observation arise from calculations with pion masses down to 400 MeV. We have been invited to participate in the Blue Waters *Early Science Program*, and will be generating around 200 trajectories on a $48^3 \times 512$ lattice at the physical pion mass. The aim will be to determine the mass of the anticipated lightest hybrid at the physical light-quark masses, and thereby confirm or refute the hypothesis that this state persists and will be accessible at GlueX at the 12GeV Upgrade of JLab; we request time for the calculation of the solution vectors and the construction of the correlation functions.

Computational Strategy

Actions and Parameters

We will employ the $N_f = 2 + 1$ anisotropic clover gauge configurations that are being generated as part of the proposal of *Edwards et al.*. Our calculations will use $32^3 \times 256$ lattices at a pion mass $m_\pi = 230$ and 380 MeV, and $40^3 \times 256$ lattices at $m_\pi = 230$ MeV; for the study of the mass of the lightest expected exotic meson, we will use $48^3 \times 512$ lattices at the physical pion mass.

Calculation of correlation functions

We will continue to exploit the "distillation" method. The number of eigenvectors employed has to be sufficient to explore the low-lying states of interest. In order to overcome the increase in the number of eigenvectors $N_{\rm vec}$ with increasing volume, we will use a stochastic sampling of the eigenvectors[12]. This not only reduces the computational costs of the computation of the solution vectors, but also reduces the memory and computational requirements for computing the correlators; for the quark annihilation contributions, we will use temporal dilution.

Software

We propose to exploit both GPUs and clusters, with the former used for the solution of the Dirac equation, and the latter for the construction of the hadron correlation functions.

We will use the Chroma software system in conjunction with the QUDA library[13]. The performance of the inverter for the $32^3 \times 256$ lattices and the Wilson-clover action is shown in Figure 7, showing the efficiency of code on the large GPU partitions that would be required for our largest $48^3 \times 512$ lattice[14].

The construction of the elementals, and the contractions of those elements to form the correlation matrices, will continue to be performed on the clusters. We have developed a new package, *Red-Star*, that automates operator construction and the many Wick contractions to reliably calculate the matrices of correlation functions.

Requested Resources

Our calculations require both GPUs for solutions of the Dirac equation, and conventional clusters for the construction of the hadron correlation functions.

GPUs

During 2011/2012, we have developed a new implementation of the stochastic variant of distillation in which the building blocks are the solution vectors: vectors

$$\hat{\tau}^{(n)}_{\alpha\beta}(\vec{x}, t; t_0) = M^{-1}_{\alpha\beta}(\vec{x}, t; t_0) V^{(n)}(t_0) \tag{4}$$

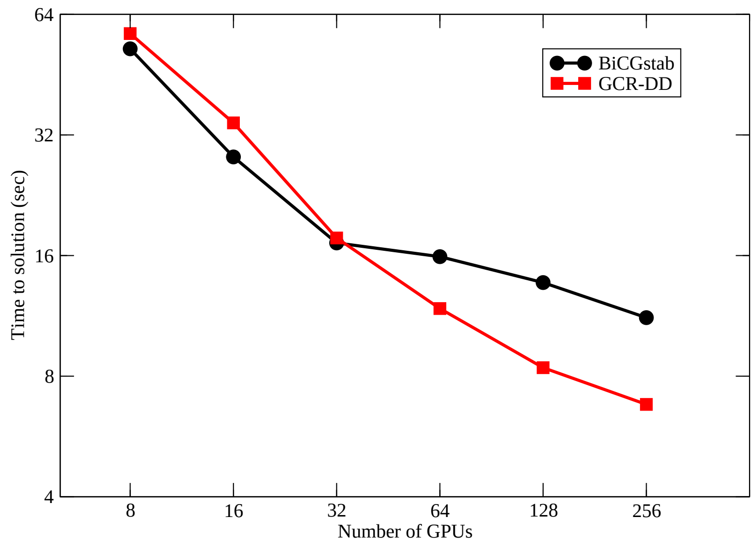

Figure 7: The figure shows the performance of the mixed-precision BiCGStab and GCR-DD Wilson-clover inverters on a $32^3 \times 256$ lattice.

where M is the Dirac operator, and $V^{(n)}(t_0), n = 1 \ldots N_{\rm samp}$, is a stochastic sampling of the distillation eigenvectors. This new implementation has the benefit of enabling us to compute local or quasi-local interpolating operators at t, in addition to smeared operators at the sink admitted by the "perambulator" construction.

Based on the observed volume scaling of the number of eigenvectors with the (spatial) volume, we will use 384 eigenvectors on the 32^3 volumes, 750 eigenvectors on the 40^3 volume, and 1200 eigenvectors on the 48^3 volume; in each case we will choose $N_{\rm samp} = 32$ stochastic samplings, noting the observation that the number of stochastic samplings needed is independent of the volume despite the increase in the number of eigenvectors required[12]. However, we need an *independent* sampling for each quark line beginning at a given time slice. For the connected contributions, we consider the case of at most five quark lines, corresponding to, for example, $\pi N \to \pi N$ scattering. For the disconnected contributions, we will use temporal dilution with $N_{\rm dil} = 32$.

From our analysis of the meson and baryon spectrum at pion masses down to 400 MeV, we find that correlation functions separated from time slices separated by four or greater are statistically independent. We will exploit this to generate solultion vectors from $N_{t_0} = 16$ time slices on the $32^3 \times 256$ and $40^3 \times 256$ lattices, and from $N_{t_0} = 64$ time slices on the $48^3 \times 512$ lattices reflecting the small ensemble of configurations in this case.

We base our time request on the observation that the time to compute solution vectors on the $32^3 \times 128$ lattices at $m_\pi = 230$ MeV from a single time slice for 16 samplings and for all spin components is 40 minutes on 16 Tesla GPUs, corresponding to 10.7 GPU-hours. The time to compute the solution vectors is shown in Table 1; **we request 2.67M GPU-hours, preferably at Jefferson Laboratory**.

Task	Volume	m_π	$N_{\rm samp}$	N_{t0}	$N_{\rm line}$	$N_{\rm dil}$	Cost/config	$N_{\rm cfg}$	TOTAL
u/d quark	$32^3 \times 256$	230	32	16	5	1	2048	350	717K
s quark	$32^3 \times 256$	230	32	16	3	1	627	350	219K
u/d quark	$32^3 \times 256$	380	32	16	5	1	926	250	232K
s quark	$32^3 \times 256$	380	32	16	3	1	627	250	157K
u/d quark	$40^3 \times 256$	230	32	16	5	1	4000	200	800K
s quark	$40^3 \times 256$	230	32	16	3	1	1261	200	252K
u/d quark	$48^3 \times 512$	140	32	64	2	0	14380	20	288K
TOTAL									**2665K**

Table 1: The table shows the total cost of computing the solution vectors in GPU-hours, as described in the text.

Volume	m_π	$N_{\rm samp}$	N_{t0}	N_t	$N_{\rm cfg}$	Cost (Jpsi core-hours)
$32^3 \times 256$	230	32	16	24	350	17.28M
$32^3 \times 256$	380	32	16	24	250	12.35M
$40^3 \times 256$	230	32	16	24	200	9.88M
$48^3 \times 512$	380	32	64	48	20	0.08M
TOTAL						**39.6M**

Table 2: The cost of computing the correlation functions in JPsi core-hours. Note that on the lattice at the physical light-quark mass, we will compute only the single-hadron correlation functions.

Clusters

We propose to construct the necessary correlation functions on the clusters at Jefferson Laboratory. We note first that the cost of the correlator construction is independent of the spatial size of the lattice, depending on the number of eigenvector samples, $N_{\rm samp}$, the number of source points N_{t_0} and the number of sink points N_t on which the correlator is constructed; the construction of the "perambulators", formed by contracting the solution vectors with the eigenvectors at the sink, scales with the spatial volume but is a negligible part of the cost.

The cost of the correlator construction is dominated by that of the baryons, for which the cost scales as $N_{\rm samp}^4$. The focus of the baryon work proposed here is the investigation, for the first time, of baryon decays on the lattice for systems both at rest and in flight; we will perform this calculation for the N and Δ channels. For the other isospins and strangeness, we will compute only the single-hadron operators, and multi-hadron operators for a limited range of momenta.

For the lattices at the physical light-quark mass, our focus is on the nature of the lightest 1^{-+} exotic channel, and therefore we will compute only the single-hadron correlation functions.

Our estimates are based on the resources needed to compute the single-hadron baryon spectrum on three ensembles, corresponding to the SU(3) point, and to $m_\pi = 524$ and 396 MeV, using 56 unsampled eigenvectors with around 500 configurations on each ensemble for which we used 11M core-hours. The cost of work proposed herein is listed in Table 2; **We request 39.6M "J/Psi" equivalent core hours, preferably at Jefferson Laboratory; it is essential that this allocation be at the same location as the GPUs**.

Storage

The spectrum project is currently storing 464 TByte of data. The tape storage requirements for the work proposed this yeart are shown in Table 3. Our program of computations require that we store

Object	Volume	m_π	Storage/cfg (GBytes)	$N_{\rm cfg}$	Storage (TBytes)
Eigenvectors	$32^3 \times 256$	230	144	350	50
Eigenvectors	$32^3 \times 256$	380	144	250	35
Eigenvectors	$40^3 \times 256$	230	550	200	107
Eigenvectors	$48^3 \times 512$	140	3038	20	59
Solution Vectors	$32^3 \times 256$	230	384	350	131
Solution Vectors	$32^3 \times 256$	380	384	250	94
Solution Vectors	$40^3 \times 256$	230	750	200	146
Solution Vectors	$32^3 \times 256$	140	1301	20	25
Correlation functions					20
TOTAL					**667 TBytes**

Table 3: The archival storage requirements for the various components of our calculation. We request 251 TBytes to store the eigenvectors of the spatial Laplacian, 396 TBytes to store the solution vectors, and 20 TBytes to store the correlation functions, yielding 667 TBytes.

the following:

- The $N_{\rm eigen}$ eigenvectors (note not the sampled eigenvectors) on each timeslice, in double precision.
- The "solution vectors" $\hat{\tau}^{(n)}_{\alpha\beta}(\vec{x}, t; t_0)$ of Eq. 4, are of use for both the calculation of radiative-transition matrix elements, and for the distribution amplitudes. Furthermore, they enable us to include additional operators for subsequent analysis. We will store the solution vectors in single precision from $N_{t_0} = 4$ timeslices ($N_{t_0} = 16$ for the $48^3 \times 512$ lattices), and for $N_t = 32$ timeslices where we find we can fit the data.
- In addition, we request 20 TByte for the storage of the correlation functions.

Thus we request tape storage of **667 TBytes**, equivalent to **2M J/Psi-equivalent core-hours**.

Since we will not be storing most of the solution vectors on tape, we need sufficient storage disk storage to enable us to pipe-line the calculation between the calculation of the solution vectors on the GPU, and the subsequent correlator construction on the clusters storage of **120 TBytes** equivalent to **3.6M J/Psi-equivalent core-hours**.

Data sharing

The solution vectors are of general use, except for the exclusive projects outlined below.

Exclusivity

The computation of the meson and baryon excited-state spectra and resonances, using the continuum-derived interpolating operators, are exclusive elements of the proposal. The following calculations are also exclusive elements of the program: radiative transitions between mesons and between baryons, quark distribution amplitudes, and charmomium and charm spectroscopy using distillation.

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