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 work at two values of the pion mass, 485 and 380 MeV, and compute the spectrum on $24^3 \times 128$ lattices at $a_s = 0.1$ fm, with a renormalized anisotropy of three; a flavor SU(3)-symmetric computation on $N_f = 3$ lattices at the strange-quark mass, in a region where the resonances are stable, will also be performed. An important goal of the proposal is a demonstration that we can delineate single- and multi-particle states. Thus at the larger of the two pion masses, we will also perform the calculation on a $32^3 \times 128$ lattice. For the computation and analysis of the valence propagators for the resonance spectrum, we request 560,000 Processor-Hours on the JLab "6n" cluster, or its equivalent.

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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 know 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. This proposal is above the threshold for a Class-A proposal. 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 two criteria for a Class-A proposal. Furthermore, we propose to save the point-source propagators that will be of use in numerous projects.

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 with 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 delineate between the different masses

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

where $\Delta M_n = \min\{\mid M_n - M_i \mid : i \neq n\}$. 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 is to fix the basis at some reference time slice t_1, and then look at the evolution of these operators. We try both methods; for an $N \times N$ matrix the extent to which this second method is effective depends on the degree to which the $N \times N$ matrix is indeed dominated by only N states.

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. To facilitate rigorous spin identification, these operators should have the property that they respect the

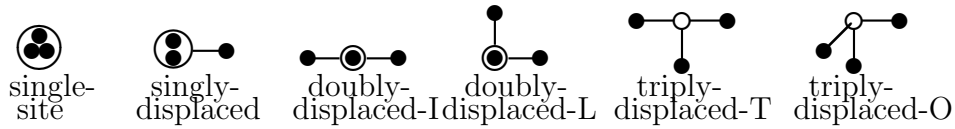

Figure 1: The spatial arrangements of the extended three-quark baryon operators. Smeared quark-fields are shown by solid circles, line segments indicate gauge-covariant displacements, and each hollow circle indicates the location of a Levi-Civita color coupling. For simplicity, all displacements have the same length in an operator.

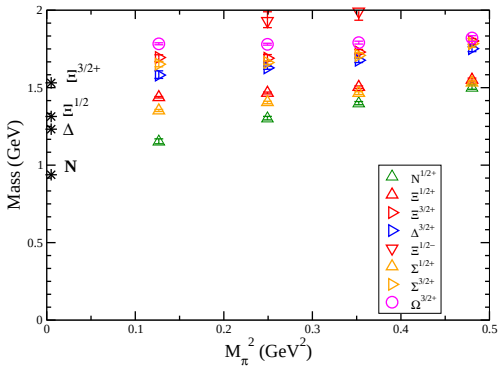

Figure 2: The figure shows the masses, in physical units, for the lowest-lying states extracted from single-particle fits to the smeared-source, point-sink data, as discussed in the text. The computations were performed on the $20^3 \times 64$ lattices generated by the MILC collaboration at $a = 0.124$ fm, with the u/d and s DWF valence propagators calculated at a mass corresponding to the Asqtad Goldstone boson.

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]; the extension to mesons is straightforward, and has been undertaken. The use of smeared quark and gauge fields is crucial in constructing good operators.

All of our hadronic operators are constructed using gauge-covariantly displaced smeared quark fields as the building blocks. 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 1. 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. The pattern of degeneracies in the approach to the continuum limit allows us to identify the continuum spins J of the states we extract.

1.2 Progress so far

An illustration of the applicability of our group-theoretic operator construction has been to the analysis of the hadron spectrum by the LHP Collaboration, using DWF propagators for the valence quarks on MILC Asqtad gauge configurations. All possible operators in each of the $G_{1g/u}$ and $H_{g/u}$ irreducible representations that can be constructed with the computed, smeared-source, valence quark propagators at the u/d and s quark masses were determined; note that, with a quasi-local quark source, the $G_{2g/u}$ irrep is not accessible demonstrating the need for the displaced propagators of this proposal. The spectrum of the lowest-lying states is shown in Figure 2; we see the emergence of the SU(3) flavour symmetry as the u/d-quark masses approach those of the s quark, and the SU(3) calculation provides a valuable benchamrk. We were unable to resolve excited states, both because of DWF non-localities manifiest in the correlators, and because the use of an *isotropic* lattice precluded the resolution of the higher eigenvalues.

We have recently 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. The spectrum is shown as the left-hand panel in Figure 3, and demonstrates our ability to isolate up to nine energy eigenvalues from the correlation functions[5]. The right-hand panel shows the experimental spectrum, but with the states assigned to their corresponding lattice irreps.. Even in this quenched calculation, at unphysical pion masses, there are tantalizing suggestions of the existence of a band of negative-parity states well separated from the higher excitations, as observed experimentally. A related computation, employing a smaller basis of operators, has demonstrated that the crucial need for such an analysis in order to correctly identify the spins of the states[6].

This study has important implications. Firstly, it demonstrates the ability to extract many energy eigenvalues in an anisotropic lattice calculation. Secondly, in order to perform this analysis, the extremely large basis of operators was first "pruned" to yield the basis of sixteen operators used in the variational analysis; this procedure was performed for each of $G_{1g/u}$, $G_{2g/u}$ and $H_{g/u}$. Therefore, an important observation is that the sixteen "important" operators included representatives of the single-site, doubly-displaced-I, doubly-displaced-L and triply-displaced-T configurations. Thus we conclude that a reliable variational method requires operators from all of these classes.

We are extending this study to full QCD, using the $N_f = 2$ anisotropic Wilson gauge configurations that have been generated under the 2006 SciDAC allocation, at $a_s \simeq$ 0.1fm and $a_s/a_t = 3$. Configurations have been generated on $16^3 \times 64$ lattices at $m_\pi \simeq 700$ MeV, and on $16^3 \times 64$ and $24^3 \times 64$ lattices at $m_\pi \simeq 460$ MeV. An analysis at the heavier pion mass will allow a straightforward comparison with the quenched results above, but at the lighter pion mass we are entering a regime in which we might expect the presence of multi-hadron states to contribute, for example in the $N^{1/2-}$. The first glimpses of our results at $m_\pi = 460$ MeV on the smaller of the lattices is revealed in Figure 4, where we show the results of a variational analysis using the same basis of operators as that used in the quenched study. Hints of the presence of multiparticle contributions are seen in the fall-off of the principal effective masses.

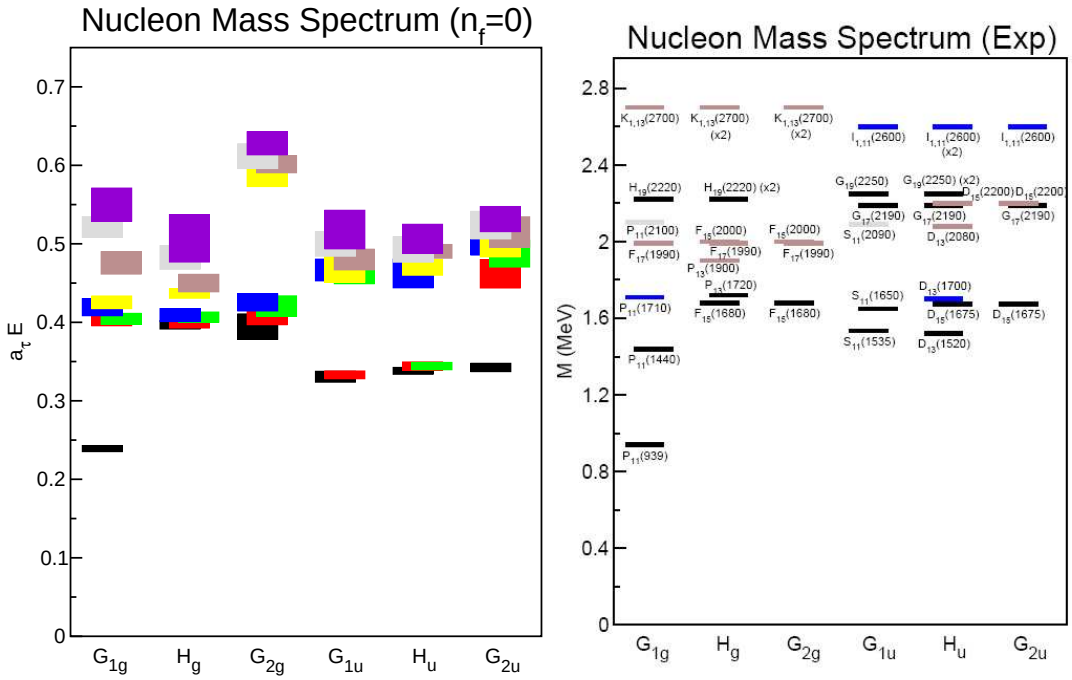

Figure 3: The left-hand panel shows the spectrum of energies, in lattice units, obtained in the quenched approximation to QCD on an anisotropic lattice with temporal lattice spacing $a_t \simeq 6$ GeV, and $m_\pi \simeq 700$ MeV. The right-hand model shows the experimentally measured spectrum, assigned to the irreducible representations of the cubic group.

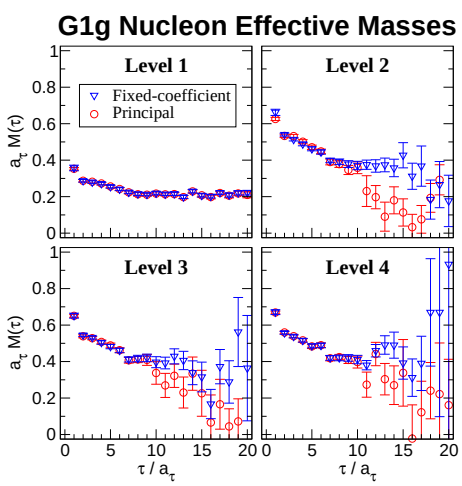

Figure 4: The figure shows the lowest four levels in the G_{1g} channel obtained on the $N_f = 2$ Wilson fermion gauge configurations on a $16^3 \times 64$ lattices at $m_\pi \simeq 460$. The points in red correspond to the principle eigenvalues introduced in equation 1, whilst the points in blue employ a basis fixed at seven temporal time units from the source.

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, 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".

With decreasing quark mass, baryonic resonances, including most ground states, become unstable, emphasising the need for a variational method to extract several energies, and two lattice volumes, to delineate between single- and multi-particle states. The proper treatment of multiparticle states[7], i.e. $N\pi$ etc., will require the use of stochastically-generated "all-to-all" propagators. The use of such propagators is part of an associated proposal (Juge *et al.*), but anticipating the eventual success of that method at our lightest pion masses, we are concentrating in this proposal on a more modest calculation at two pion masses, 465 and 380 MeV, and the smaller two lattices, 2.4 and 3.2 fm, that we expect to become available in time to complete this proposal. In addition, we will study the spectrum on $N_f = 3$ lattices, at a spatial volume of 2 fm; here the resonances we will be studying are stable, and this data will provide a benchmark for the subsequent calculations.

2 Computational Strategy

2.1 Actions and Parameters

The use of an anisotropic lattice has proved essential. Experimental data on the excited baryon states are dense and extend to around 3 GeV. Using conventional isotropic lattices, with spacings around 2 GeV^{-1}, one can expect significant lattice discretization errors. Using a highly anisotropic lattice, e.g. with temporal lattice spacing of 6 GeV^{-1}, the discretization errors are reduced as well as providing more signal of excited states. Therefore we propose to use the anistropic clover lattices being generated as described in the proposal of Robert Edwards *et al.*, and being generated under the INCITE award.

The non-perturbative Clover action was chosen since spectrum scaling violations of masses are quite small - at the target lattice spacing of $a = 0.1$ fm, the scaling violations are about 1% in $am_{vector}/\sqrt{a^2\sigma}$ [8]. These previous scaling studies used an isotropic quenched action. We have verified that anisotropic versions of the quenched Wilson fermion action and tadpole-improved Clover action follow the expected scaling forms, as shown in Figure 5.

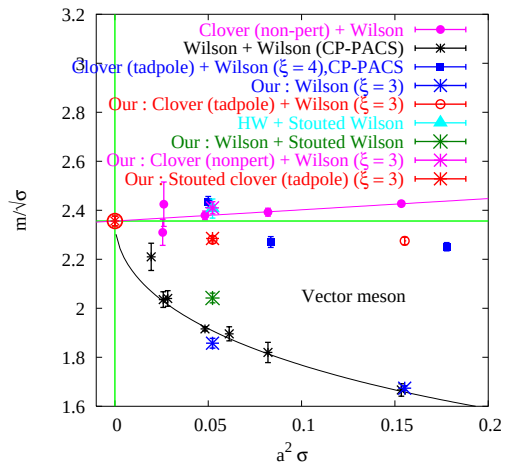

Figure 5: The figure shows the scaling behavior of various actions. Our studies are shown as the crosses for Wilson action (blue), Wilson with stout links (green) and clover (red); the anisotropic clover action shows the good scaling behavior required for studies of the spectrum.

2.2 Correlator construction

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

$$B_{\alpha\beta\gamma,\bar{\alpha}\bar{\beta}\bar{\gamma}}(t;0) = \sum_{\vec{x}} \epsilon^{abc}\epsilon^{\bar{a}\bar{b}\bar{c}} P^{a\bar{a}}_{\alpha\bar{\alpha}}(x;0) Q^{b\bar{b}}_{\beta\bar{\beta}}(x;0) R^{c\bar{c}}_{\gamma\bar{\gamma}}(x;0), \tag{2}$$

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 performed subsequently on a workstation.

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 large basis of interpolating operators, and in particular the *generalized baryon correaltors* of eqn. 2, 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. Whilst the relatively heavy computational cost for these measurements was acceptable in the exploratory study on the smaller lattices, it is clearly necessary to improve the computational efficiency for this production study. This we are doing in three ways:

1. Saving diquark temporaries in the evaluation of eqn. 2 immediately reduces the number of operators by a factor 3.2

2. Identification of common diquarks across the different qqq's yields a further factor of two in cost

3. Finally, the evaluation of the generalized baryon correlators for only those Dirac components needed in the construction of the final operators yields a further factor of around three.

Thus we base our cost estimates on the assumption that the number of floating-point operations per site required to compute eqn. 2 is reduced by a factor of ten to 200k, and that the limited communication demands will allow us to attain a performance comparable to that of the clover solver.

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. The solver is implemented in *Chroma*, and we adopt the benchmark figure of 1.4 Gflop/node on the dual-core "6n" cluster in constructing our time estimates. The generalized-baryon-correlator construction is also implemented in *Chroma*; so far optimization efforts have concentrated on the solver, but we estimate the purely local nature of the computation will enable us to attain a performance comparable to that of the solver. Finally, the reduction of the generalized baryon correlators to form the irreducible matrix of operators is performed using *adat*, and can be accomplished, albeit slowly, on workstations.

4 Required Resources

4.1 Quark propagators

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 required to compute the clover fermion propagators is based on a corresponding quenched computation of the propagators, using the anisotropic clover action with "stout" links, on a $16^3 \times 64$ lattice at the same lattice spacing and renormalized anisotropy proposed here. We find that for $m_\pi = 390$ MeV, 1300 CG iterations are required per colour-spin component, whilst for $m_\pi = 650$ MeV, around 850 CG iterations are required. We therefore assume the behaviour

$$N_{\rm iter} = A + \frac{B}{m_\pi^2}, \tag{3}$$

with the number of iterations independent of the volume.

The exploratory studies of baryon spectroscopy outlined earlier demonstrated the need to compute propagators from four sources: single-site, displaced in the $\pm x$ directions, and in the $+y$ direction. The single-site, "S-wave" propagators are of general use, and are therefore these will be saved. Thus we require three additiional propagators, at each of the u/d and s quark masses, that will not be saved; note that, in estimating the cost of propagator generation, we conservatively assume an $\bar{s}s$ "pseudoscalar masss" of 650 MeV. The cost of computing these propagators is shown in Table 1.

Size	m_π	$N_{\rm it}$	6n Proc-Hours
$20^3 \times 128$	650	847	22491
$24^3 \times 128$	650	847	38865
	485	1050	48173
	380	1338	61383
	300	1788	82061
$32^3 \times 128$	650	847	92124
	485	1050	114190
	380	1338	145500
	300	1788	194516
	254	2261	245908

Table 1: The number of processor-hours on the 6n cluster required to compute **four propagators** at a given quark mass, on a total of **700 configurations**.

Size	N_t	N_{qqq}	6n Proc-hours
$20^3 \times 128$	40	671	5964
$24^3 \times 128$	40	2000	30720
$32^3 \times 128$	40	2000	72818

Table 2: The cost of generating generalized baryon propagators on 700 configurations for a given $m_{u/d}$ and m_s. Note that for the degenerate $N_f = 3$ theory, a smaller number of generalized baryon correlators are needed.

Given the number of operators needed for a successful study of the spectrum, the construction of hadronic correlators in the baryon sector is a substantial undertaking; on each configuration, we propose computing a total of 2,000 generalized baryon correlators, enabling us to measure the lowest-lying energies for each isospin. We find that we can observe a signal only over the first 20 time slices. Since we employ anti-periodic boundary conditions in the temporal direction, we propose to compute the generalized baryon correlators for only 40 time slices. The cost of constructing these is, of course, independent of the quark masses employed, and therefore we show in Table 2 the cost of computing 2,000 qqq correlators on 700 configurations for a fixed pion mass at each of our two lattices sizes

Finally, in Table 3, we show the aggregate cost of performing our program at each value of the pion mass, and it is this table that encapsulates our request for resources. Performing the full analysis is sufficiently demanding that we would anticipate that future INCITE or early-use proposals include sufficient computational resources to accomplish a reasonable fraction of the measurement. The most urgent task of this program is demonstrating that we can delineate the single- and multi-particle states. Therefore, our proposal centers on an analysis of the spectrum at $m_\pi = 485$ MeV on both lattice sizes, together with an analysis at $m_\pi = 380$ MeV on the smaller lattice, which should be sufficient to allow a finite-volume analysis to delineate multiparticle states at the 485 MeV pion mass. In addition, we will perform an analysis of the $N_f = 3$ data at $m_\pi = 650$ MeV. Thus our request is for **560,000** Processor-Hours on the 6n cluster at Jefferson Lab, or the equivalent on any of the other

Size	m_π	$N_{\rm cfg}$	Propagators	qqq	Total
$20^3 \times 128$	650	700	22491	5964	**28455**
$24^3 \times 128$	485	700	87038	30720	**117758**
$24^3 \times 128$	380	700	100248	30720	**130968**
$24^3 \times 128$	300	700	120926	30720	151646
$32^3 \times 128$	485	700	206314	72817	**279131**
$32^3 \times 128$	380	700	237624	72817	310441
$32^3 \times 128$	300	700	286640	72817	359457
$32^3 \times 128$	254	700	338032	72817	410849

Table 3: The table shows the cost of the computation of three u/d and three s quark propagators at each value of m_π on 700 configurations, together with the cost of computing the qqq's; for the $N_f = 3$ calculation, only a single quark mass is used. The final column is the sum of the two previous columns; the entries in bold are used in constructing our time request.

clusters.

5 Data Sharing

We are proposing to save the single-site propagators, which would be of general use to the USQCD community, as part of this proposal, save for the exclusivity statements below, but are not proposing to save any of the displaced-source propagators. We would be prepared to store the latter should there be demand from other projects.

6 Exclusivity

The computation of the excited resonance spectrum using our lattice group-theory methods for baryons 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 in July 2009

7 Roadmap

The generation of anisotropic lattices is a multi-phase campaign, outlined in the proposal and presentation of Robert Edwards; the measurement of the baryon spectrum on those lattices is an essential component and motivator for the project. Should additional resources become available, we propose to advance the calculations listed in Table 3 of ths proposal, continuing in the outyears with calculations on the coarse $a = 0.125$ lattices, and at smaller quark masses and larger volumes; we have an active research effort aimed at establishing the efficacy of a stochastic approach, and hope to employ that in later

stages of the work. Note that these additional computations would entail only the transfer of the gauge configurations to USQCD resouces, and the storage of only the single-site propagators; thus we not envisage severe data-transfer impediments.

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