Towards a determination of the spectrum of QCD using a space-time lattice

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Lattice Hadron Physics Collaboration

- charge from Nathan Isgur to use Monte Carlo method to extract the spectrum of baryon resonances (Hall B at JLab)
- formed the Lattice Hadron Physics Collaboration (LHPC) in 2000
- acquired funding through DOE SciDAC to build large computing cluster at JLab (also at Fermilab and Brookhaven), develop software
- LHPC has several broad goals
  - compute QCD spectrum (baryons, mesons,…)
  - hadron structure (form factors, structure functions,…)
  - hadron-hadron interactions
- current members of spectroscopy effort:
  - Subhasish Basak, Robert Edwards, George Fleming, Jimmy Juge, Adam Lichtl, CM, David Richards, Ikuro Sato, Steve Wallace

LHPC spectroscopy efforts

- extracting spectrum of resonances is big challenge!!
  - need sets of extended operators (correlator matrices)
  - multi-hadron operators needed too
  - deduce resonances from finite-box energies
  - anisotropic lattices $(a_t < a_s)$
  - inclusion of light-quark loops at realistically light quark mass
- long-term project
- this talk is a brief status report
  - discuss how to extract excited-state energies from Monte Carlo estimates of correlation functions in Euclidean lattice field theory
  - baryon operator construction
    - smearing and pruning

Energies from correlation functions

- stationary state energies extracted from asymptotic decay rate of temporal correlations of the fields (imaginary time formalism)
- evolution in Heisenberg picture $\phi(t) = e^{Ht}\ \phi(0)\ \ e^{-Ht}$ ($H =$Hamiltonian)
- spectral representation of a simple correlation function
  - assume transfer matrix, ignore temporal boundary conditions
  - focus only on one time ordering

$$\langle 0|\ \phi(t)\phi(0)\ |0\rangle = \sum_n \langle 0|e^{Ht}\phi(0)\ e^{-Ht}\ |n\rangle\langle n|\phi(0)|0\rangle$$

$$= \sum_n \left|\langle n|\phi(0)\ |0\rangle\right|^2 e^{-(E_n - E_0)t} = \sum_n A_n e^{-(E_n - E_0)t}$$

insert complete set of energy eigenstates (discrete and continuous)

- extract A_1 and $E_1 - E_0$ as $t \to \infty$

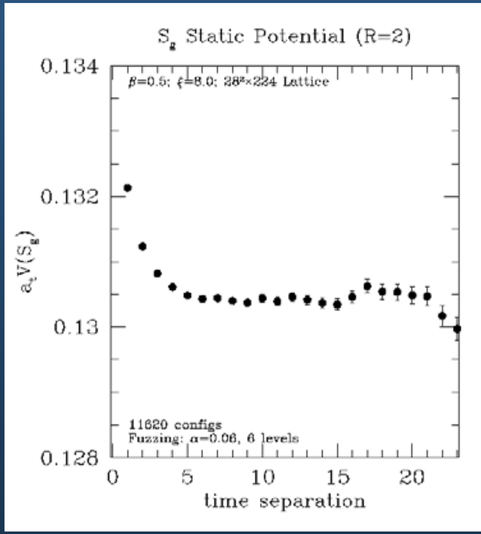
  (assuming $\langle 0|\phi(0)\ |0\rangle = 0$ and $\langle 1|\phi(0)\ |0\rangle \neq 0$)

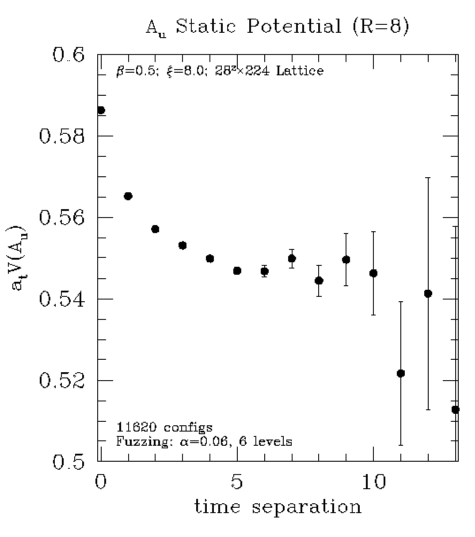
Effective mass

- the "effective mass" is given by $m_{\text{eff}}(t) = \ln\left(\frac{C(t)}{C(t+1)}\right)$
- notice that (take $E_0 = 0$)

$$\lim_{t\to\infty} m_{\text{eff}}(t) = \ln\left(\frac{A_1 e^{-E_1 t} + A_2 e^{-E_2 t} + \cdots}{A_1 e^{-E_1(t+1)} + \cdots}\right) \to \ln e^{-E_1} = E_1$$

- effective mass tends to the actual mass (energy) asymptotically
- effective mass plot is convenient visual tool to see signal extraction
  - seen as a plateau
- plateau sets in quickly for good operator
- excited-state contamination before plateau





Reducing contamination

- statistical noise generally increases with temporal separation t
- effective masses associated with correlation functions of simple local fields often do not reach a plateau before noise swamps the signal
  - need better operators
  - better operators have reduced couplings with higher-lying contaminating states
- recipe for making better operators
  - crucial to construct operators using *smeared* fields
    - link variable smearing
    - quark field smearing
  - spatially extended operators
  - use large *set* of operators (variational coefficients)

Principal correlators

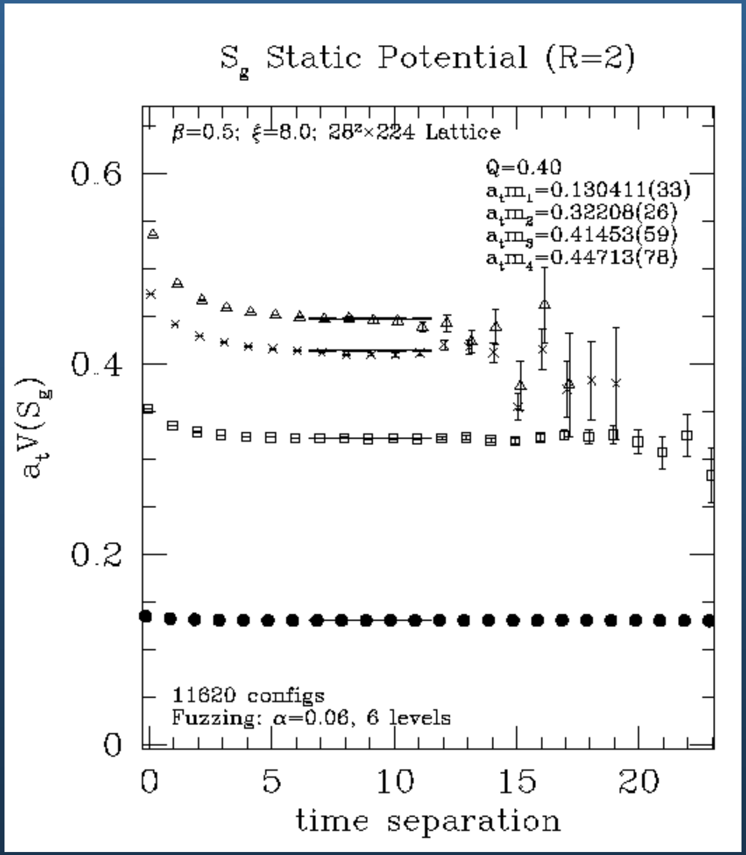
- extracting excited-state energies described in
  - C. Michael, NPB **259**, 58 (1985)
  - Luscher and Wolff, NPB **339**, 222 (1990)
- can be viewed as exploiting the variational method
- for a given $N \times N$ correlator matrix $C_{\alpha\beta}(t) = \langle 0 | O_\alpha(t) O_\beta^+(0) | 0 \rangle$ one defines the N *principal correlators* $\lambda_\alpha(t, t_0)$ as the eigenvalues of

$$C(t_0)^{-1/2} C(t) \, C(t_0)^{-1/2}$$

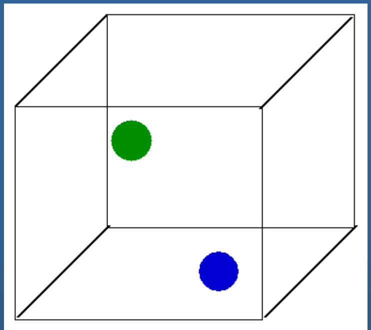
  where t_0 (the time defining the "metric") is small
- can show that $\lim_{t\to\infty} \lambda_\alpha(t, t_0) = e^{-(t-t_0)E_\alpha}(1 + e^{-t\Delta E_\alpha})$
- N principal effective masses defined by $m_\alpha^{\text{eff}}(t) = \ln\left(\frac{\lambda_\alpha(t, t_0)}{\lambda_\alpha(t+1, t_0)}\right)$ now tend (plateau) to the N lowest-lying stationary-state energies

Principal effective masses

- single-exponential fit to each principal correlator to extract spectrum!
  - two-exponentials to minimize sensitivity to t_{min}
- principal effective masses can cross, approach asymptotic behavior from below
- final results independent of t_0, but larger values of this reference time can introduce larger errors



Unstable particles (resonances)



- our computations done in a periodic box
  - momenta quantized
  - discrete energy spectrum of stationary states → single hadron, 2 hadron, …
- scattering phase shifts → resonance masses, widths (in principle) deduced from finite-box spectrum
  - B. DeWitt, PR **103**, 1565 (1956) (sphere)
  - M. Luscher, NPB**364**, 237 (1991) (cube)
- more modest goal: "ferret" out resonances from scattering states
  - must differentiate resonances from multi-hadron states
  - avoided level crossings, different volume dependences
  - know masses of decay products → placement and pattern of multi-particle states known
  - resonances show up as extra states with little volume dependence

Resonance in a toy model (I)

- O(4) non-linear σ model (Zimmerman et al, NPB(PS) **30**, 879 (1993))

$$S = -2\kappa \sum_x \sum_{\mu=1}^{4} \Phi_a(x)\Phi_a(x+\hat{\mu}) + J\sum_x \Phi^4(x), \qquad \sum_{a=1}^{4} \Phi_a^2(x) = 1$$

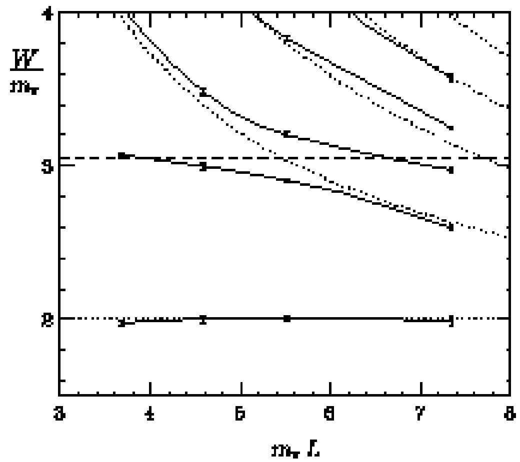


Figure 2. *Two-particle energy spectrum*

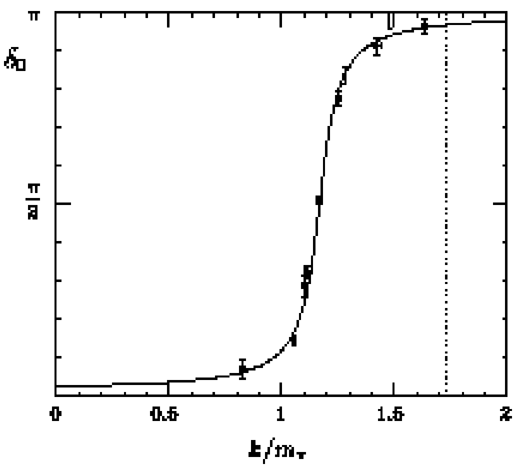


Figure 3. *Scattering phase shift δ_0 in the isospin 0 channel*

Resonance in a toy model (II)

- coupled scalar fields: (Rummukainen and Gottlieb, NPB**450**, 397 (1995))

$$S=\frac{1}{2}\int d^4x\left(\left(\partial_\mu\phi\right)^2+m_\pi^2\phi^2+\lambda\phi^4+\left(\partial_\mu\rho\right)^2+m_\pi^2\rho^2+\lambda_\rho\rho^4+g\rho\phi^2\right)$$

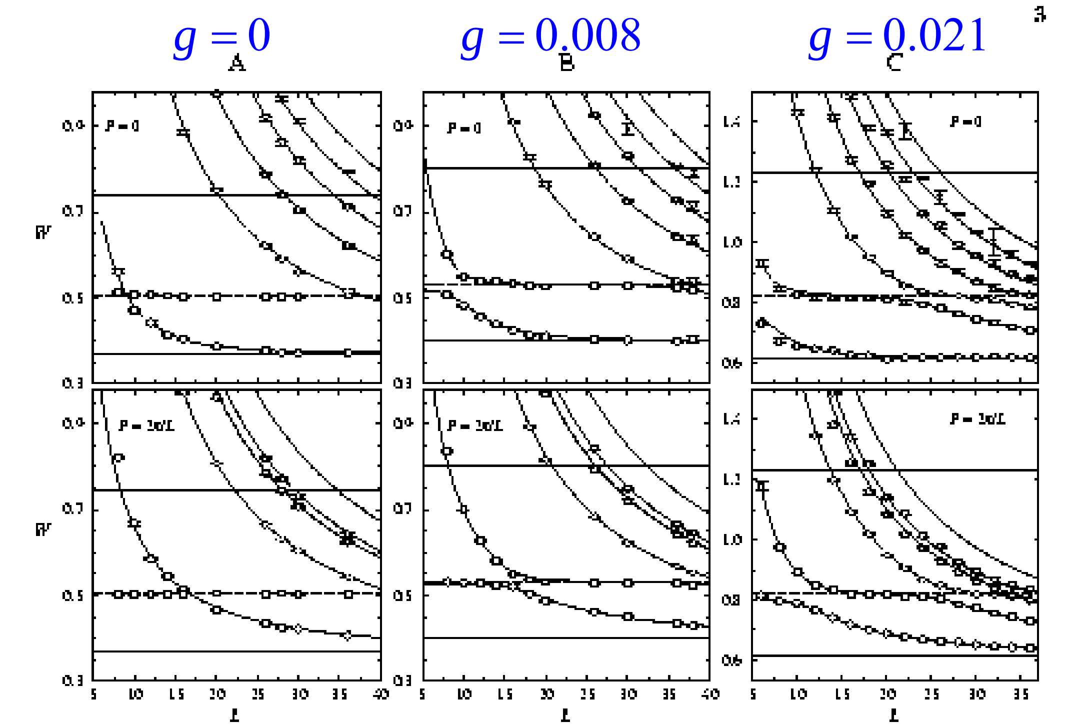


Figure 2. The center of mass energy levels for sectors $\vec{P}=0$ (top row) and $\vec{P}=2\pi/L$ (bottom) for cases A, B and C (see table 1).

Operator design issues

- must facilitate spin identification
  - shun the usual method of operator construction which relies on cumbersome continuum space-time constructions
  - focus on constructing operators which transform irreducibly under the symmetries of the lattice
- one eye on maximizing overlaps with states of interest
- other eye on minimizing number of quark-propagator sources
- use building blocks useful for baryons, mesons, multi-hadron operators

Three stage approach (hep-lat/0506029)

- concentrate on baryons at rest (zero momentum)
- operators classified according to the irreps of O_h

$$G_{1g}, G_{1u}, G_{2g}, G_{2u}, H_g, H_u$$

- (1) basic building blocks: smeared, covariant-displaced quark fields

$$(\widetilde{D}_j^{(p)}\widetilde{\psi}(x))_{Aa\alpha} \qquad p\text{-link displacement } (j = 0, \pm 1, \pm 2, \pm 3)$$

- (2) construct elemental operators (translationally invariant)

$$B^F(x) = \phi^F_{ABC}\varepsilon_{abc}(\tilde{D}_i^{(p)}\tilde{\psi}(x))_{Aa\alpha}(\tilde{D}_j^{(p)}\tilde{\psi}(x))_{Bb\beta}(\tilde{D}_k^{(p)}\tilde{\psi}(x))_{Cc\gamma}$$

  - flavor structure from isospin, color structure from gauge invariance

- (3) group-theoretical projections onto irreps of O_h

$$B_i^{\Lambda\lambda F}(t) = \frac{d_\Lambda}{g_{O_h^D}} \sum_{R\in O_h^D} D_{\lambda\lambda}^{(\Lambda)}(R)^* U_R B_i^F(t) U_R^+$$

  - wrote Grassmann package in Maple to do these calculations

Three-quark elemental operators

- three-quark operator

$$\Phi^{ABC}_{\alpha\beta\gamma,ijk}(t) = \sum_{\vec{x}} \varepsilon_{abc} (\tilde{D}_i^{(p)} \tilde{\psi}(\vec{x},t))^A_{a\alpha} \; (\tilde{D}_j^{(p)} \tilde{\psi}(\vec{x},t))^B_{b\beta} \; (\tilde{D}_k^{(p)} \tilde{\psi}(\vec{x},t))^C_{c\gamma}$$

- covariant displacements

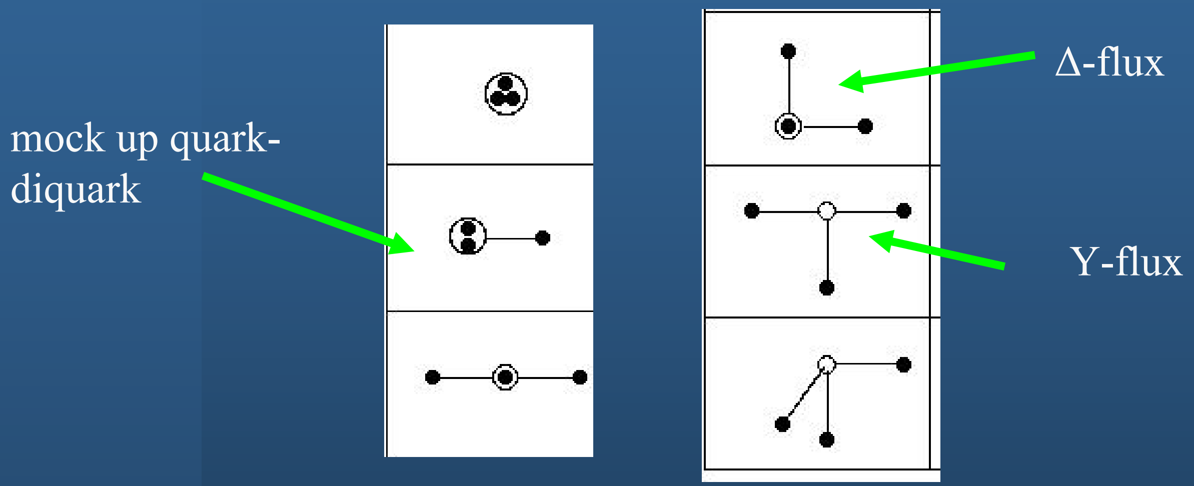
$$\tilde{D}_j^{(p)}(x,x') = \tilde{U}_j(x)\,\tilde{U}_j(x+\hat{j}) \cdots \tilde{U}_j(x+(p-1)\hat{j})\,\delta_{x',x+p\hat{j}} \qquad (j = \pm 1, \pm 2, \pm 3)$$

$$\tilde{D}_0^{(p)}(x,x') = \delta_{x',x}$$

Baryon	Operator
Δ^{++}	$\Phi^{uuu}_{\alpha\beta\gamma,ijk}$
Σ^{+}	$\Phi^{uus}_{\alpha\beta\gamma,ijk}$
N^{+}	$\Phi^{uud}_{\alpha\beta\gamma,ijk} - \Phi^{duu}_{\alpha\beta\gamma,ijk}$
Ξ^{0}	$\Phi^{ssu}_{\alpha\beta\gamma,ijk}$
Λ^{0}	$\Phi^{uds}_{\alpha\beta\gamma,ijk} - \Phi^{dus}_{\alpha\beta\gamma,ijk}$
Ω^{-}	$\Phi^{sss}_{\alpha\beta\gamma,ijk}$

Incorporating orbital and radial structure

- displacements of different lengths build up radial structure
- displacements in different directions build up orbital structure



- operator design minimizes number of sources for quark propagators
- useful for mesons, tetraquarks, pentaquarks even!
- can even incorporate hybrid mesons operator (in progress)

Enumerating the three-quark operators

- lots of operators (too many!)

	Δ^{++}, Ω^{-}	Σ^{+}, Ξ^{0}	N^{+}	Λ^{0}
Single-site	20	40	20	24
Singly-displaced	240	624	384	528
Doubly-displaced-I	192	572	384	576
Doubly-displaced-L	768	2304	1536	2304
Triply-displaced-T	768	2304	1536	2304
Triply-displaced-O	512	1536	1024	1536

Spin identification and other remarks

- spin identification possible by pattern matching

J	$n^J_{G_1}$	$n^J_{G_2}$	n^J_H
$\frac{1}{2}$	1	0	0
$\frac{3}{2}$	0	0	1
$\frac{5}{2}$	0	1	1
$\frac{7}{2}$	1	1	1
$\frac{9}{2}$	1	0	2
$\frac{11}{2}$	1	1	2
$\frac{13}{2}$	1	2	2
$\frac{15}{2}$	1	1	3
$\frac{17}{2}$	2	1	3

total numbers of operators assuming two different displacement lengths

Irrep	Δ, Ω	N	Σ, Ξ	Λ
G_{1g}	221	443	664	656
G_{1u}	221	443	664	656
G_{2g}	188	376	564	556
G_{2u}	188	376	564	556
H_g	418	809	1227	1209
H_u	418	809	1227	1209

- total numbers of operators is huge → uncharted territory
- ultimately must face two-hadron scattering states

Single-site operators

- choose Dirac-Pauli convention for γ-matrices

- 20 independent single-site Δ^{++} elemental operators:

$$\Delta_{\alpha\beta\gamma} = \epsilon_{abc}\, \bar{u}_{a\alpha}\, \bar{u}_{b\beta}\, \bar{u}_{c\gamma}, \qquad (\alpha \le \beta \le \gamma)$$

- 20 independent single-site N^{+} elemental operators:

$$N_{\alpha\beta\gamma} = \epsilon^{abc}\left(\bar{u}_{a\alpha}\, \bar{u}_{b\beta}\, \bar{d}_{c\gamma} - \bar{d}_{a\alpha}\, \bar{u}_{b\beta}\, \bar{u}_{c\gamma}\right), \qquad (\alpha \le \beta,\ \alpha < \gamma)$$

- 40 independent single-site Σ^{+} elemental operators:

$$\Sigma_{\alpha\beta\gamma} = \epsilon_{abc}\, \bar{u}_{a\alpha}\, \bar{u}_{b\beta}\, \bar{s}_{c\gamma} \qquad (\alpha \le \beta)$$

- 24 independent single-site Λ^{0} elemental operators:

$$\Lambda_{\alpha\beta\gamma} = \epsilon_{abc}\left(\bar{u}_{a\alpha}\, \bar{d}_{b\beta}\, \bar{s}_{c\gamma} - \bar{d}_{a\alpha}\, \bar{u}_{b\beta}\, \bar{s}_{c\gamma}\right) \qquad (\alpha < \beta)$$

Δ++ single-site operators

Irrep	Row	DP Operators
G_{1g}	1	$\Delta_{144} - \Delta_{234}$
G_{1g}	2	$-\Delta_{134} + \Delta_{233}$
G_{1u}	1	$\Delta_{124} - \Delta_{223}$
G_{1u}	2	$-\Delta_{114} + \Delta_{123}$
H_g	1	Δ_{222}
H_g	2	$-\sqrt{3}\,\Delta_{122}$
H_g	3	$\sqrt{3}\,\Delta_{112}$
H_g	4	$-\Delta_{111}$
H_g	1	$\sqrt{3}\,\Delta_{244}$
H_g	2	$-\Delta_{144} - 2\Delta_{234}$
H_g	3	$2\Delta_{134} + \Delta_{233}$
H_g	4	$-\sqrt{3}\,\Delta_{133}$

Irrep	Row	DP Operators
H_u	1	$\sqrt{3}\,\Delta_{224}$
H_u	2	$-2\Delta_{124} - \Delta_{223}$
H_u	3	$\Delta_{114} + 2\Delta_{123}$
H_u	4	$-\sqrt{3}\,\Delta_{113}$
H_u	1	Δ_{444}
H_u	2	$-\sqrt{3}\,\Delta_{344}$
H_u	3	$\sqrt{3}\,\Delta_{334}$
H_u	4	$-\Delta_{333}$

Single-site $N+$ operators

Irrep	Row	DP Operators
G_{1g}	1	N_{122}
G_{1g}	2	$-N_{112}$
G_{1g}	1	$N_{144} - N_{243}$
G_{1g}	2	$-N_{134} + N_{233}$
G_{1g}	1	$N_{144} - 2N_{234} + N_{243}$
G_{1g}	2	$N_{134} - 2N_{143} + N_{233}$
G_{1u}	1	N_{142}
G_{1u}	2	$-N_{132}$
G_{1u}	1	N_{344}
G_{1u}	2	$-N_{334}$
G_{1u}	1	$2N_{124} - N_{142} - 2N_{223}$
G_{1u}	2	$-2N_{114} + 2N_{123} - N_{132}$

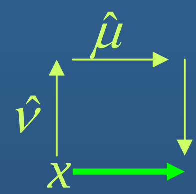
Irrep	Row	DP Operators
H_g	1	$\sqrt{3}\, N_{244}$
H_g	2	$-N_{144} - N_{234} - N_{243}$
H_g	3	$N_{134} + N_{143} + N_{233}$
H_g	4	$-\sqrt{3}\, N_{133}$
H_u	1	$\sqrt{3}\, N_{224}$
H_u	2	$-2N_{124} + N_{142} - N_{223}$
H_u	3	$N_{114} + 2N_{123} - N_{132}$
H_u	4	$-\sqrt{3}\, N_{113}$

Current status and next step

- Development of software to carry out the baryon computations has been completed and thoroughly tested (at long last!)
  - gauge-invariant three-quark propagators as intermediate step
  - baryon correlators are superpositions of *qqq*-propagator components → superposition coefficients precalculated
  - source-sink rotations to minimize source orientations
- Next step: smearing optimization and operator pruning
  - optimize link-variable and quark-field smearings
  - remove dynamically redundant operators
  - remove ineffectual operators
  - low statistics runs needed
  - monitor progress at http://enrico.phys.cmu.edu

Quark- and gauge-field smearing

- smeared quark and gluon fields fields → dramatically reduced coupling with short wavelength modes
- link-variable smearing (stout links PRD**69**, 054501 (2004))
  - define $C_\mu(x) = \sum_{\pm(\nu\neq\mu)} \rho_{\mu\nu} U_\nu(x) U_\mu(x+\hat{\nu}) U_\nu^+(x+\hat{\mu})$
  - spatially isotropic $\rho_{jk} = \rho, \quad \rho_{4k} = \rho_{k4} = 0$
  - exponentiate traceless Hermitian matrix



$$\Omega_\mu = C_\mu U_\mu^+ \qquad Q_\mu = \frac{i}{2}\left(\Omega_\mu^+ - \Omega_\mu\right) - \frac{i}{2N}\mathrm{Tr}\left(\Omega_\mu^+ - \Omega_\mu\right)$$

  - iterate $U_\mu^{(n+1)} = \exp\left(iQ_\mu^{(n)}\right) U_\mu^{(n)}$

$$U_\mu \rightarrow U_\mu^{(1)} \rightarrow \cdots \rightarrow U_\mu^{(n)} \equiv \widetilde{U}_\mu$$

- quark-field smearing (covariant Laplacian uses smeared gauge field)

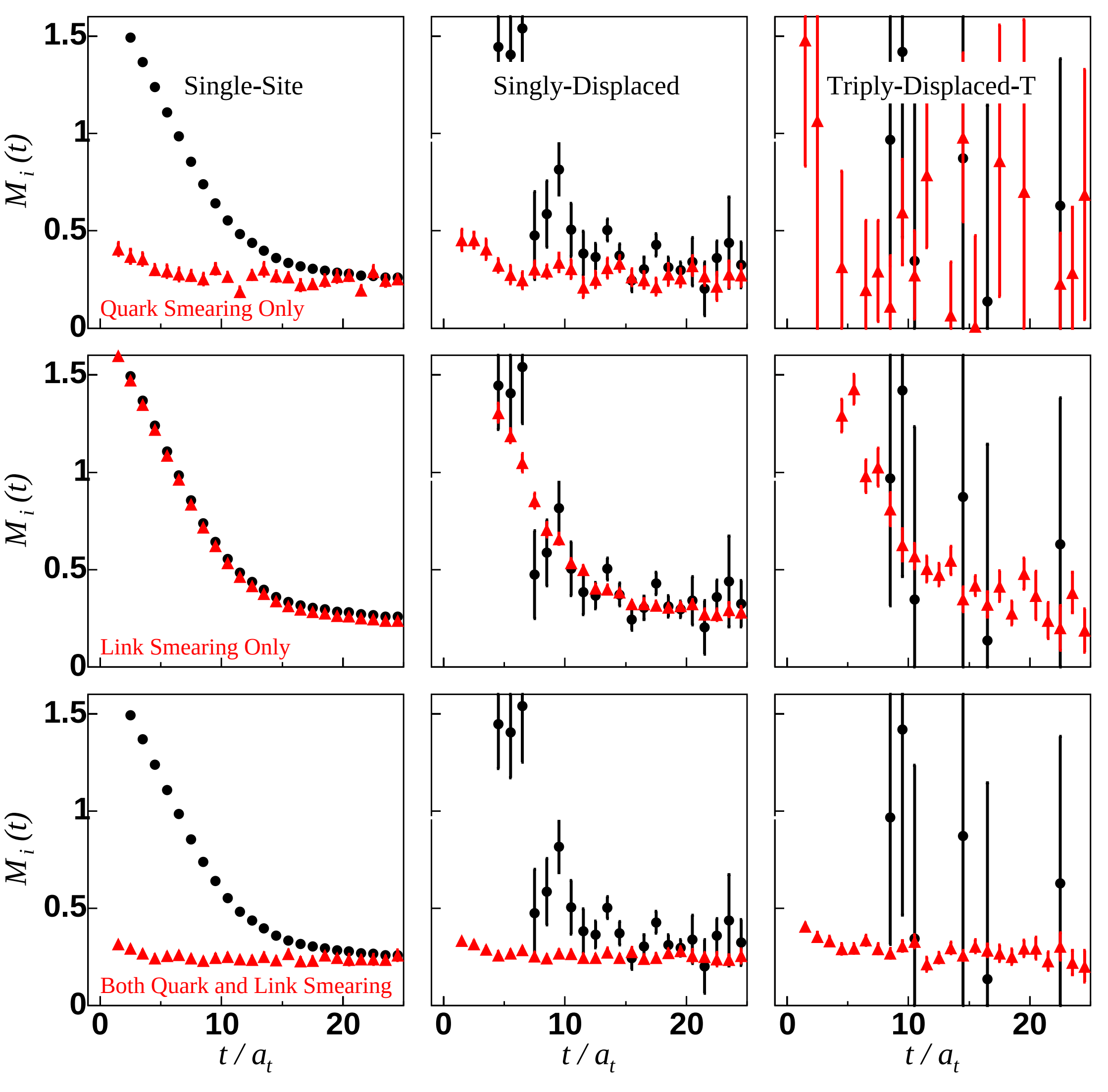
$$\tilde{\psi}(x) = \left(1 + \frac{\sigma_s}{4n_\sigma}\tilde{\Delta}^2\right)^{n_\sigma} \psi(x)$$

Importance of smearing

- Nucleon G1g channel
- effective masses of 3 selected operators
- noise reduction from link variable smearing, especially for displaced operators
- quark-field smearing reduces couplings to high-lying states

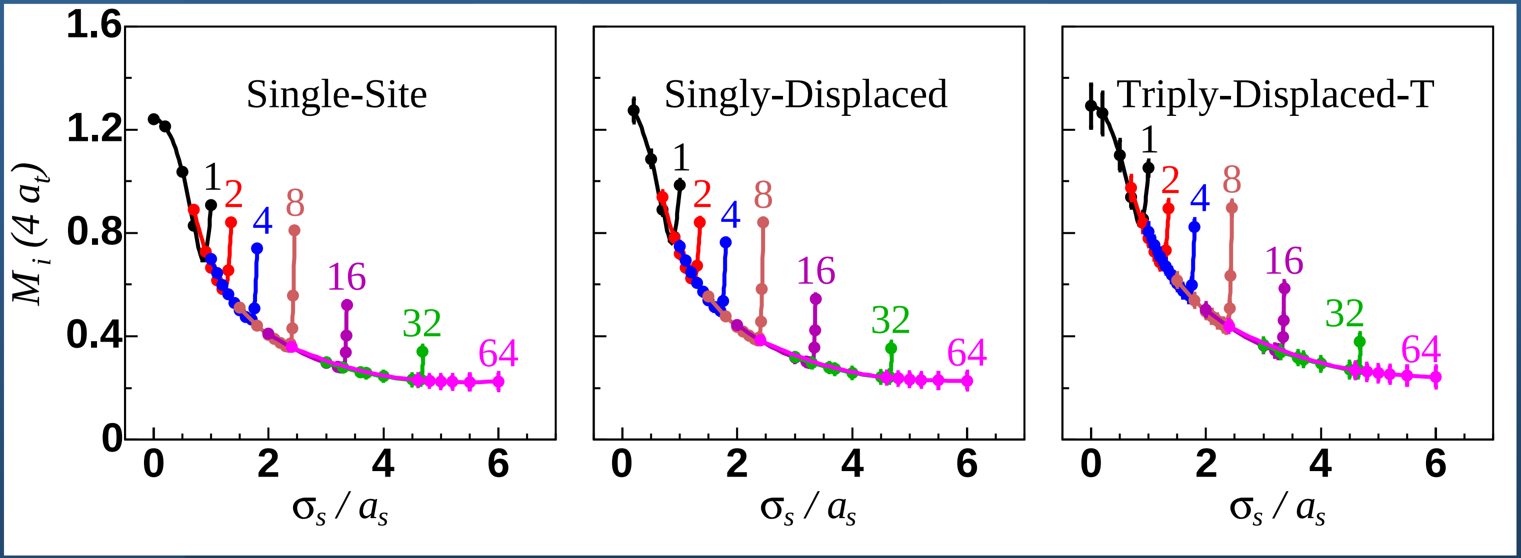
$$\sigma_s = 4.0, \quad n_\sigma = 32$$
$$n_\rho \rho = 2.5, \quad n_\rho = 16$$

- effect on excited states still to be studied

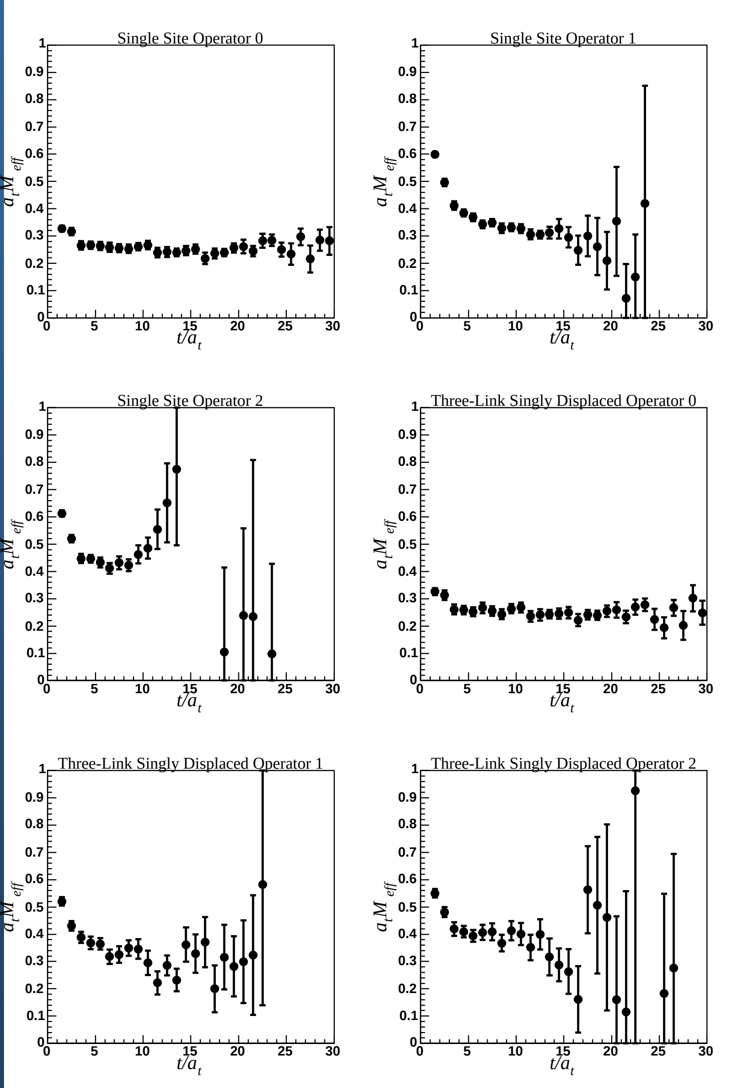


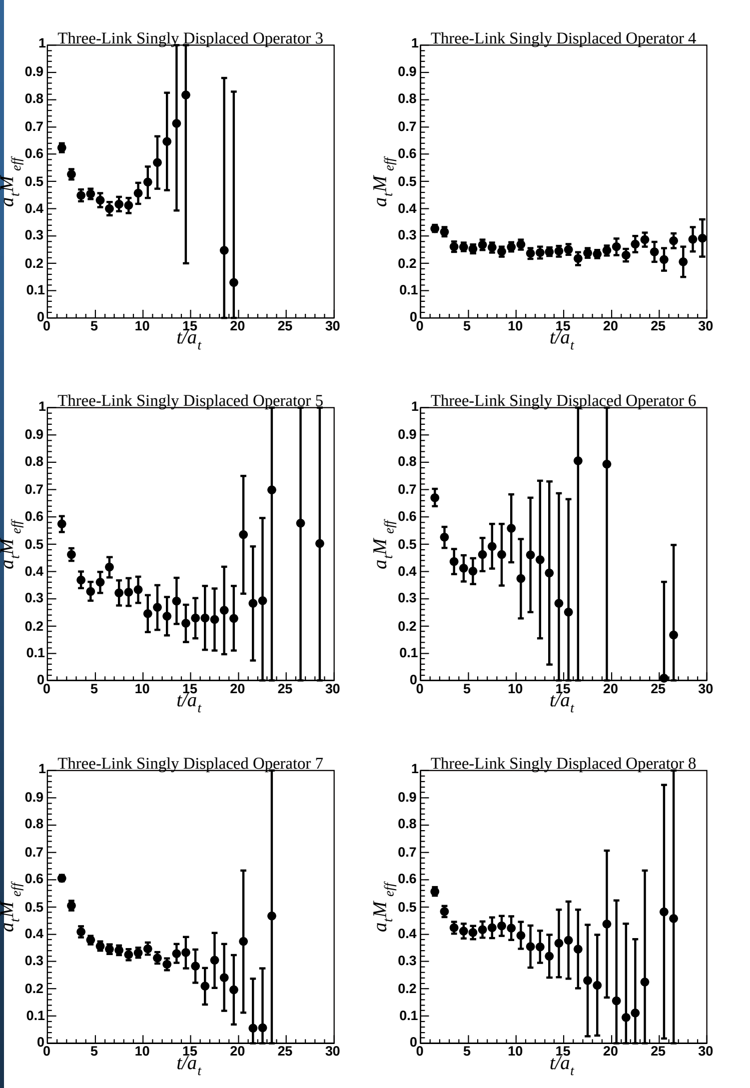
Tuning the smearing

- the effective mass at $t = 4a_t$ for three specific nucleon operators for different quark-field smearings (link smearing same as last slide)

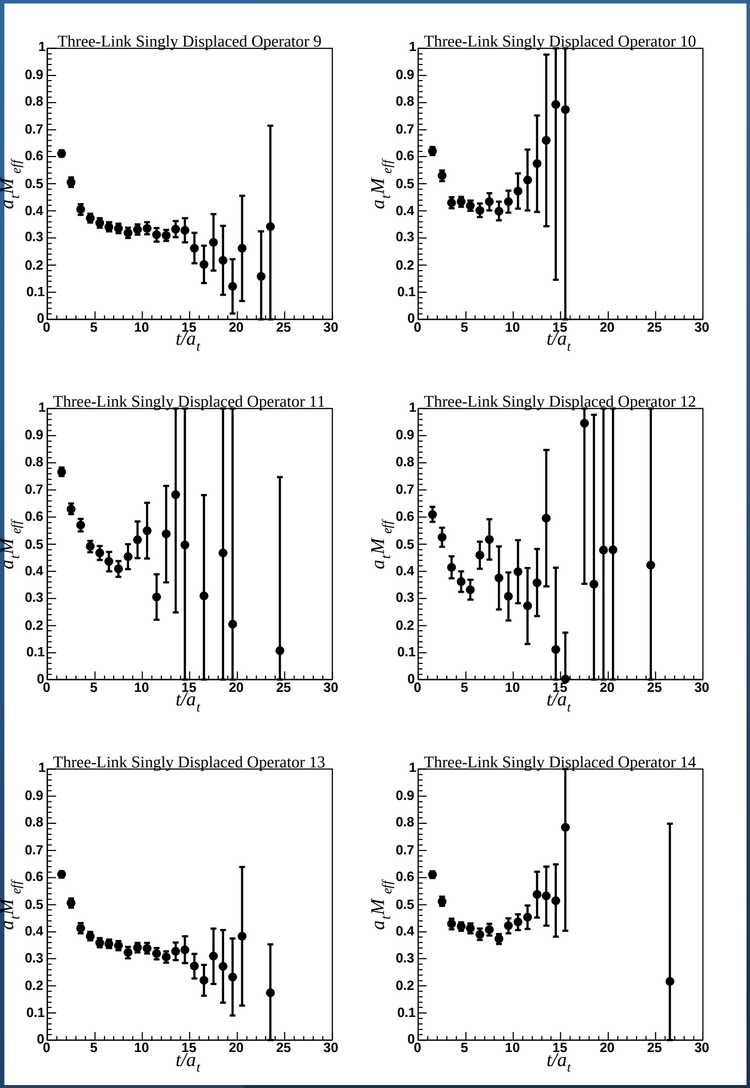


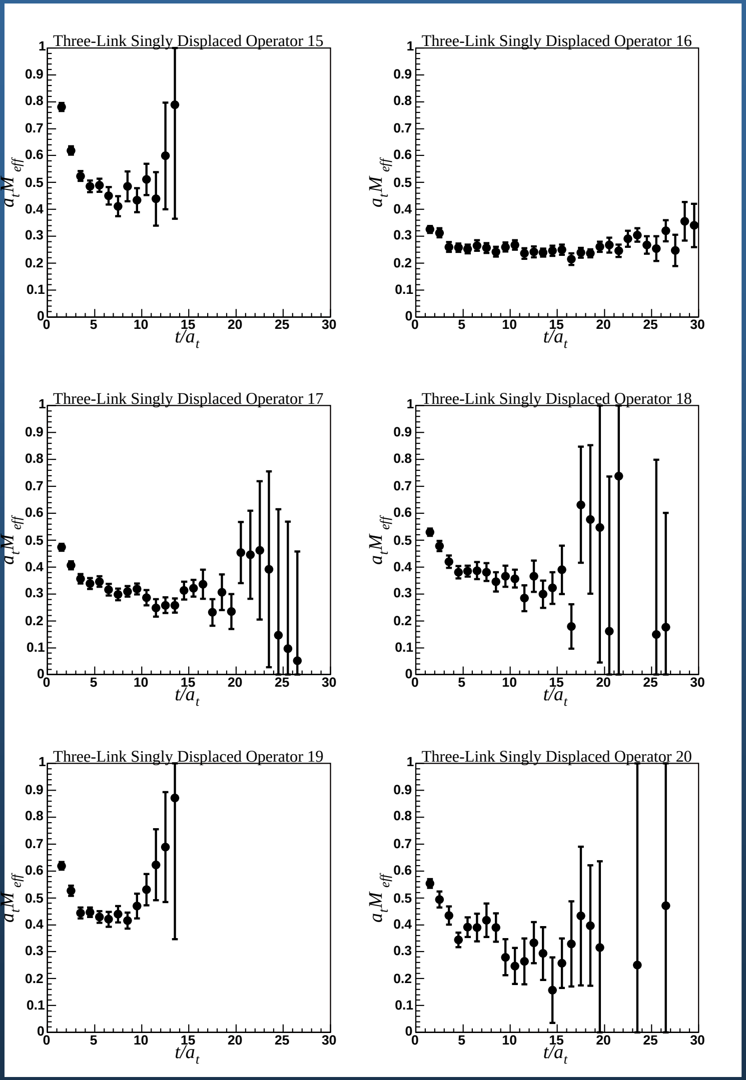
Operator plethora (G1g Nucleon)



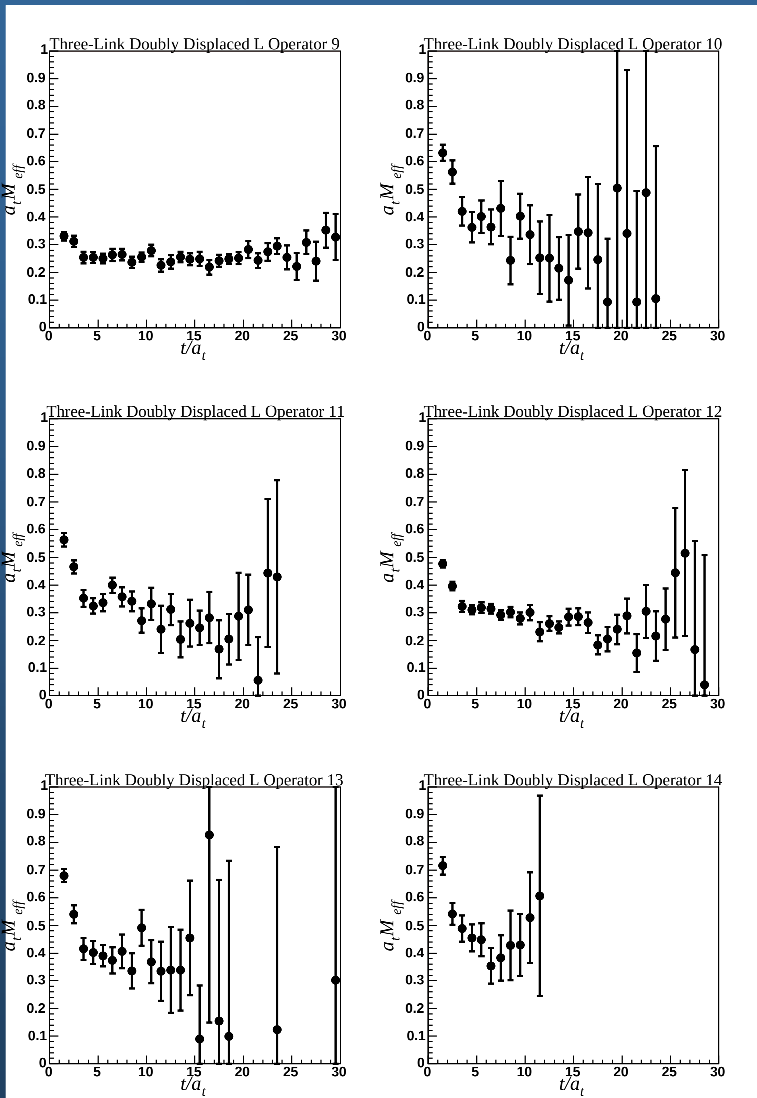


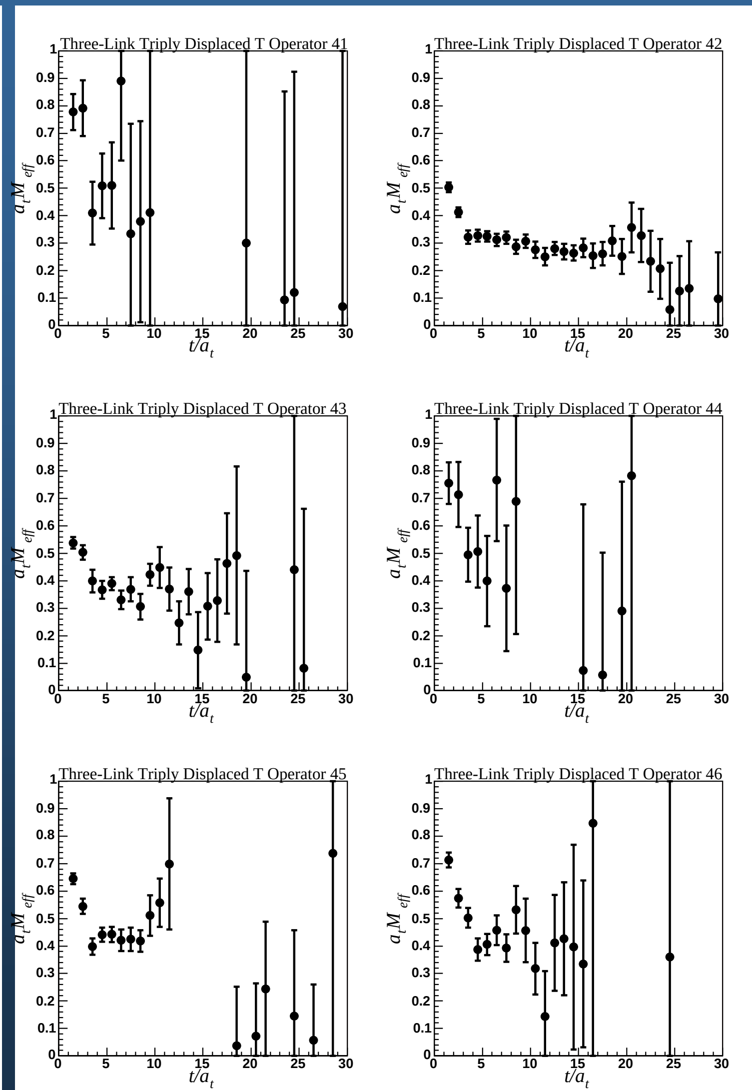
G1g nucleon operators



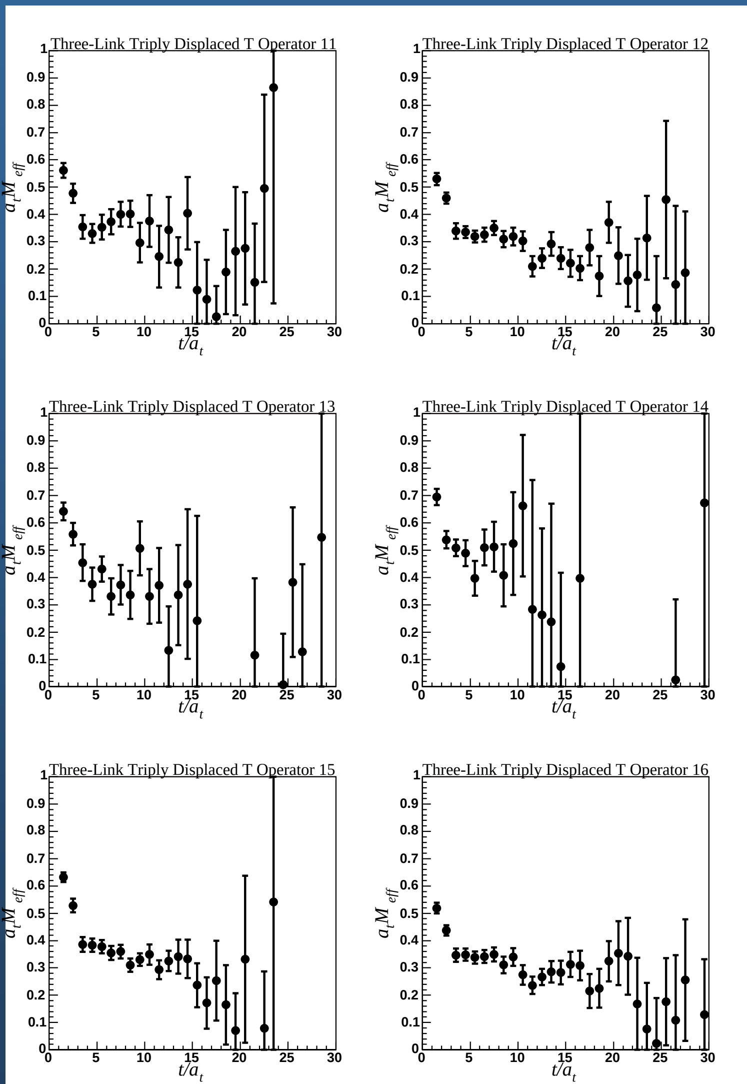


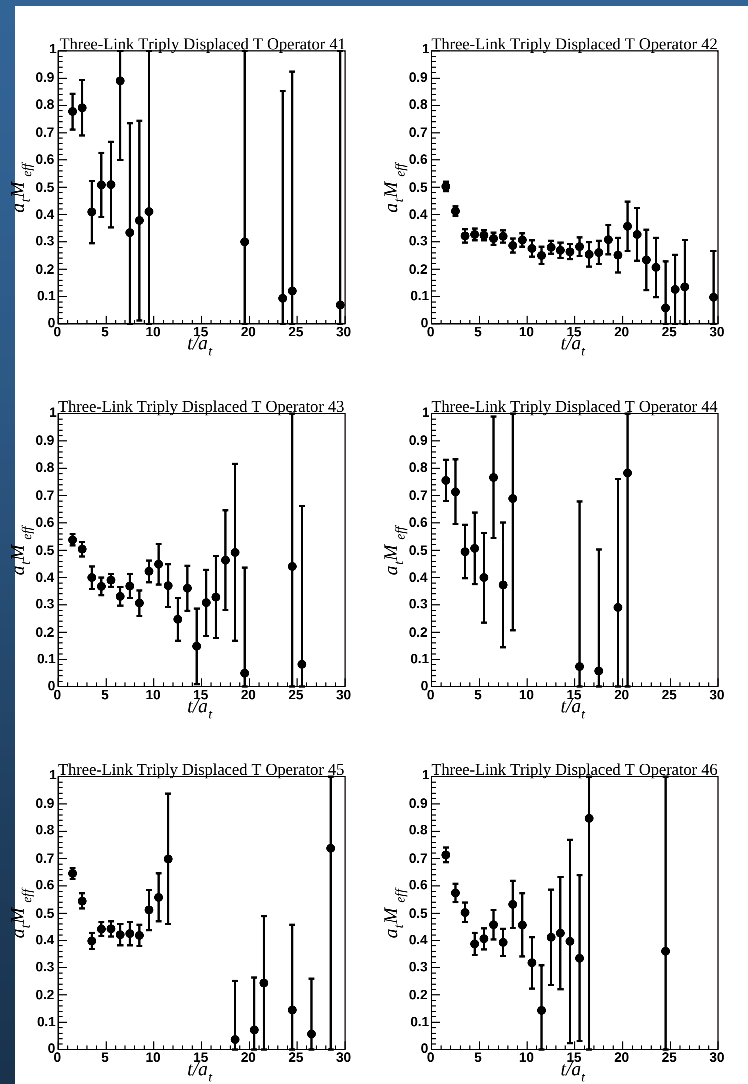
G1g nucleon operators



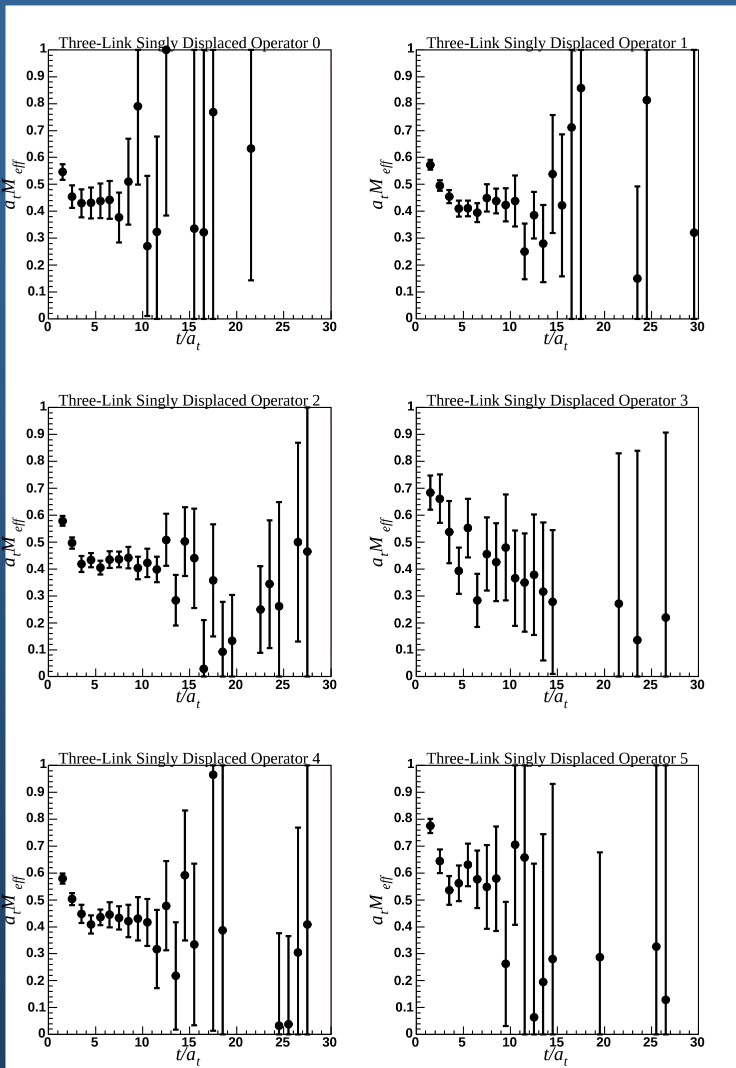


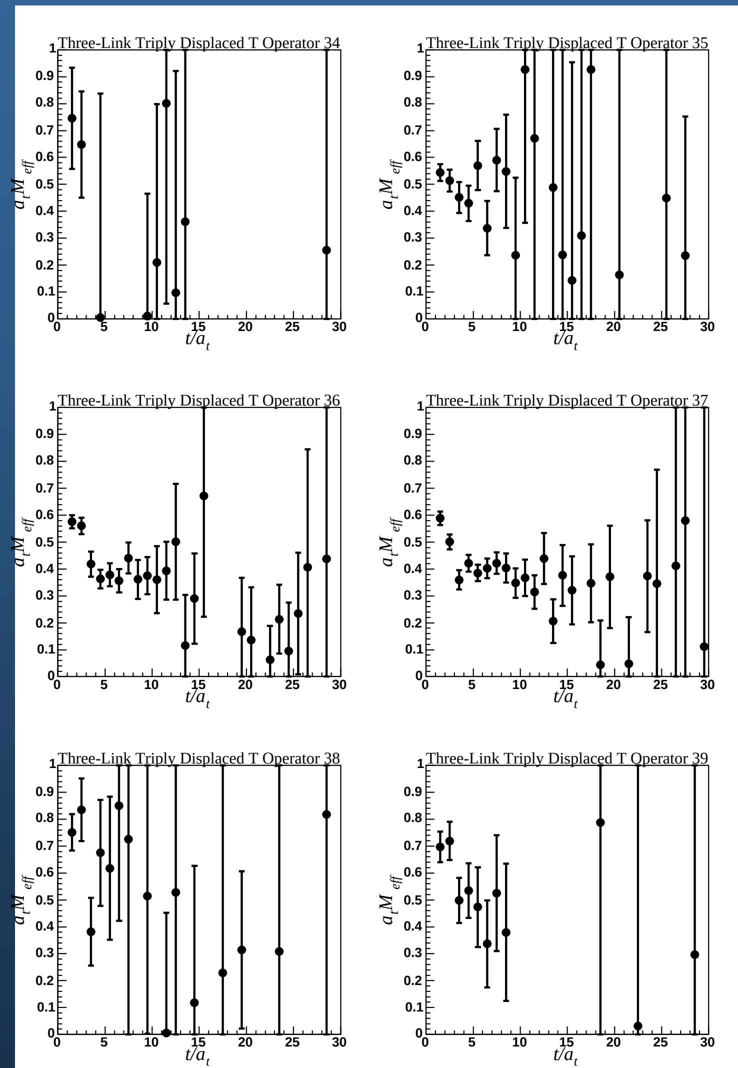
G1g nucleon operators



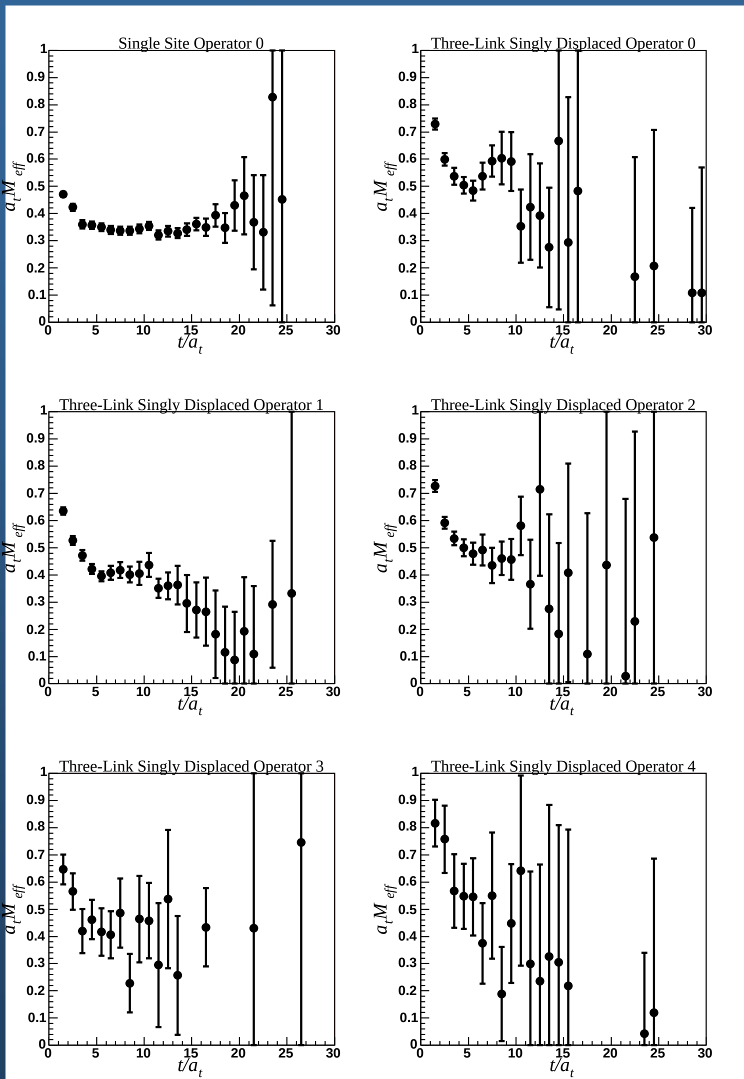


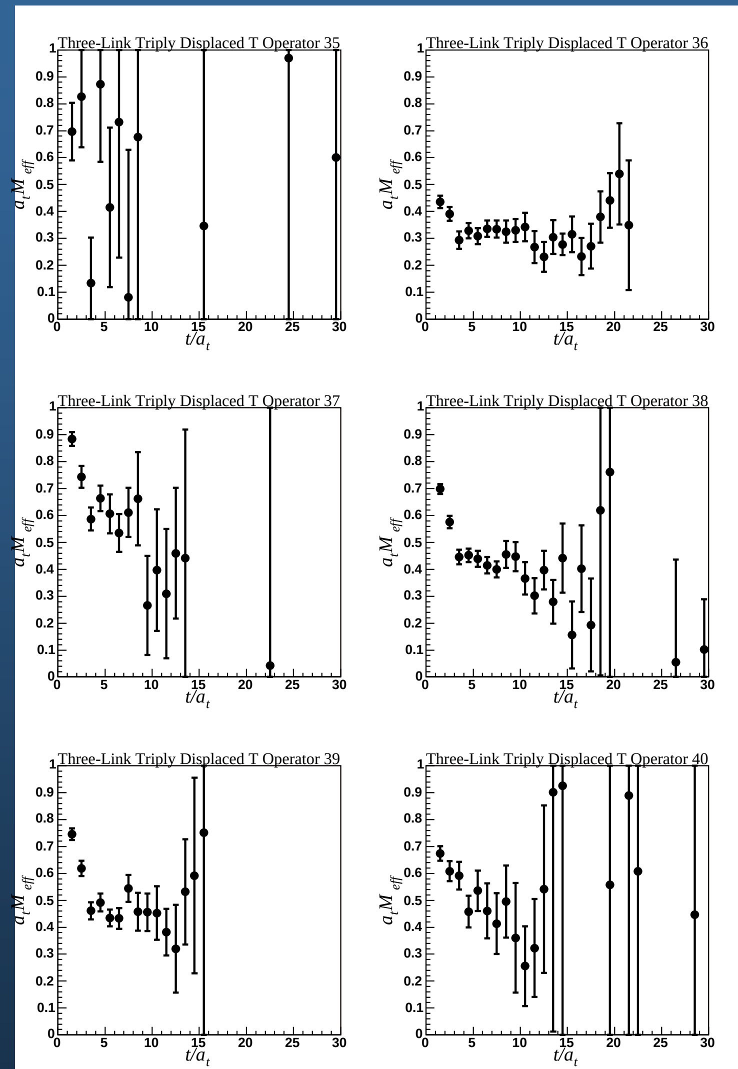
G2g nucleon operators





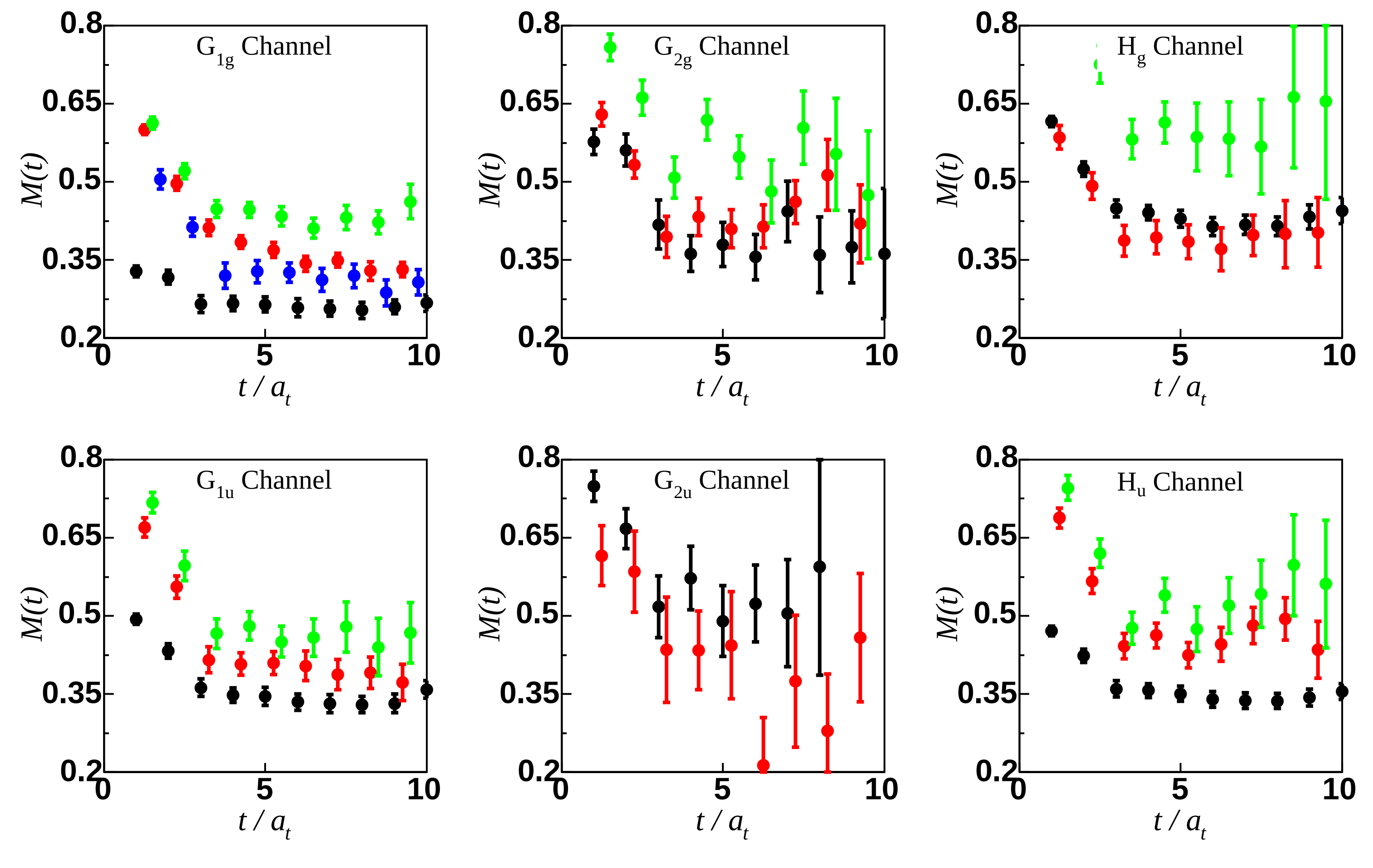
Hu nucleon operators





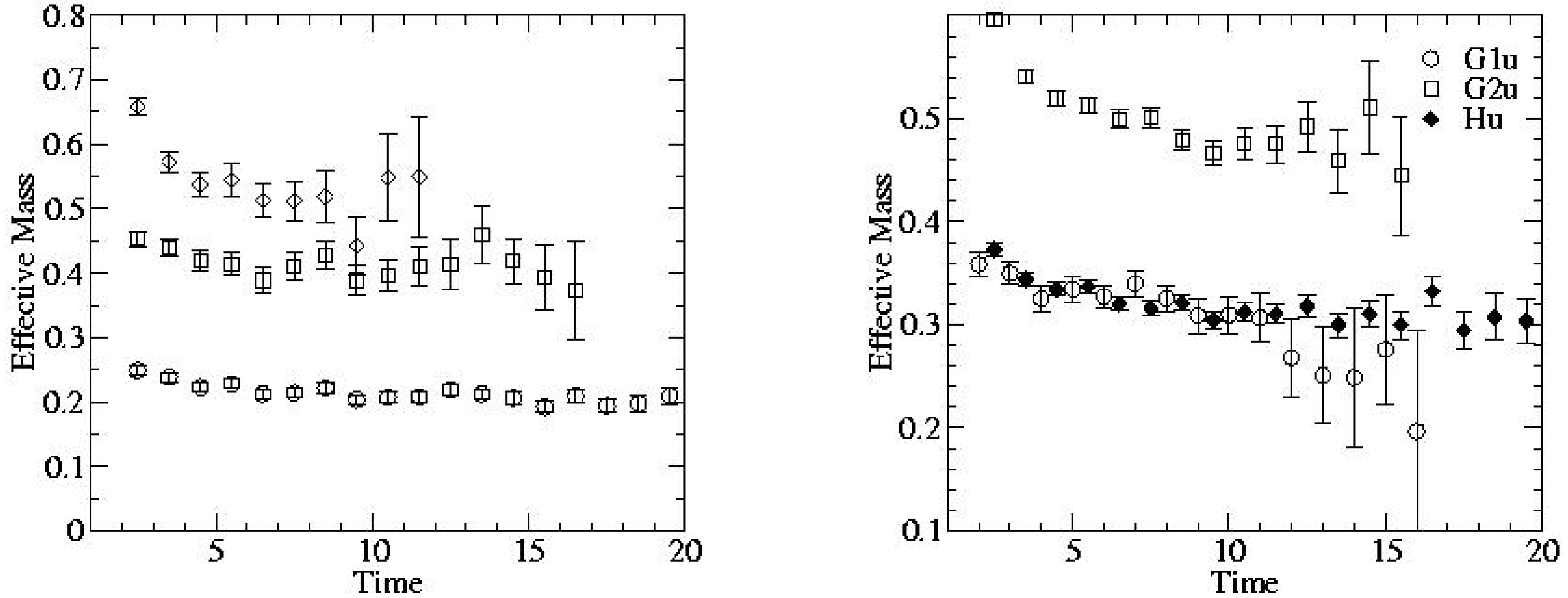
More effective masses

- single-site + triply-displaced-T operators (25 configurations)



Principal effective masses

- principal effective masses for small set of 10 operators



- G_{1g} on left, other irreps on right.

Summary

- outlined ongoing efforts of LHPC to extract baryon spectrum using Monte Carlo methods on a space-time lattice
  - mesons (and hybrids), tetraquarks, …to be studied as well
- emphasized need for correlation matrices to extract spectrum
- spin identification must be addressed
- as light-quark mass decreases, inclusion of multi-hadron operators will become important
- very challenging calculations
- …to be continued