Towards the hadron spectrum using spatially-extended operators in lattice QCD

Colin Morningstar

Carnegie Mellon University

3rd Topical Workshop on Lattice Hadron Physics

Jefferson Lab

July 31, 2006

Lattice Hadron Physics Collaboration

- Lattice Hadron Physics Collaboration (LHPC) formed in 2000
- LHPC has several broad goals
  - compute QCD spectrum (baryons, mesons,...)
  - hadron structure (form factors, structure functions,...)
  - hadron-hadron interactions
- current members of spectroscopy effort:
  - Robert Edwards, George Fleming, Jimmy Juge, Adam Lichtl, CM, Nilmani Mathur, 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
- efforts divide into two categories
  - operator technology
  - Monte Carlo updating technology (light quark loops)
- this talk is an interim status report
  - focus on baryons

Outline

- how to extract excited-state energies from Monte Carlo computations
  - need for multi-hadron operators
- operator construction
  - spatially-extended operators
  - symmetry channels
- field smearing
- operator pruning
- milestone reached: extraction of nine or more levels in a symmetry channel!!
- outlook and conclusion

Excited states, resonances in lattice Monte Carlo

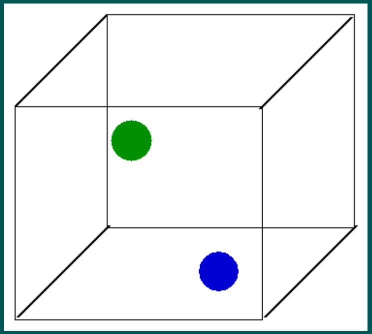
Principal correlators

- extracting excited-state energies described in
  - C. Michael, NPB **259**, 58 (1985)
  - Luscher and Wolff, NPB **339**, 222 (1990)
- exploits the variational method
- for $N \times N$ correlator matrix $C_{\alpha\beta}(t) = \langle 0 | O_\alpha(t) O_\beta^+(0) | 0 \rangle$ define N *principal correlators* $\lambda_\alpha(t, t_0)$ as 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 $\lim_{t\to\infty} \lambda_\alpha(t, t_0) = e^{-(t-t_0)E_\alpha}(1 + e^{-t\Delta E_\alpha})$
- N *principal effective masses* $\Omega_\alpha(t) = \ln\left(\frac{\lambda_\alpha(t, t_0)}{\lambda_\alpha(t+1, t_0)}\right)$ now tend (plateau) to N lowest-lying stationary-state energies

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)
- first goal: get finite-box spectrum
  - must extract multi-hadron state energies
  - check volume dependences
  - know masses of decay products → placement and pattern of multi-particle states roughly known

Operator construction

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
- must project onto definite spin polarizations or will observe many degeneracies

Three stage approach

- 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 $(\tilde{D}_j^{(p)}\tilde{\psi}(x))_{Aa\alpha}$ p - link displacement ($j = 0, \pm1, \pm2, \pm3$)
- (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

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

  - Grassmann package in Maple to do these calculations
- details in PRD72, 094506 (2005)

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

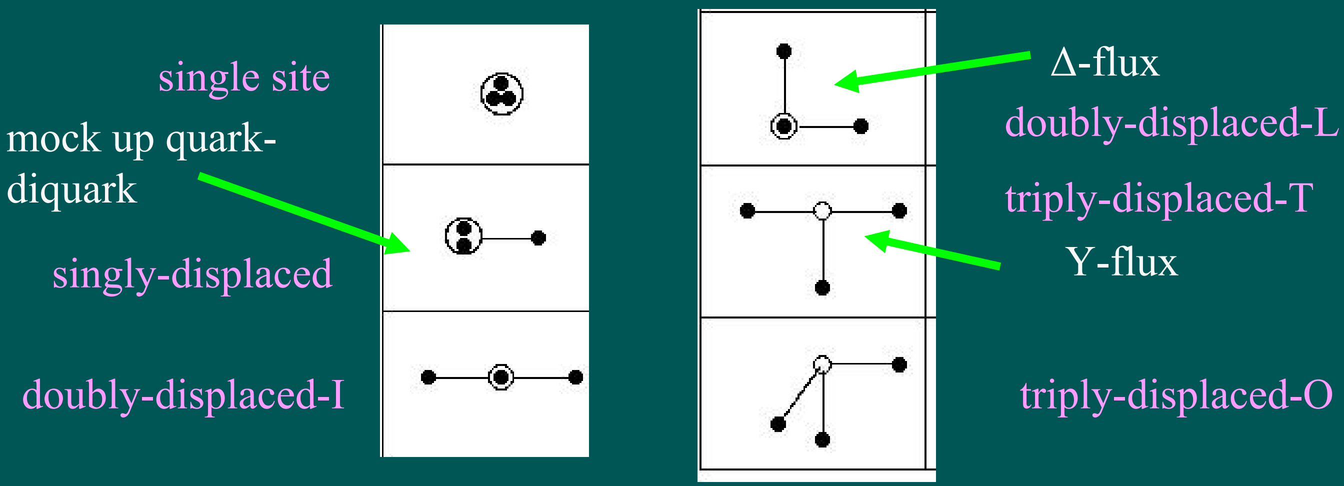
$$\tilde{D}_j^{(p)}(x,x') = \tilde{U}_j(x)\,\tilde{U}_j(x+\hat{j}) \cdots \tilde{U}_j(x+(p-1)\hat{j})\,\delta_{x',x+p\hat{j}} \qquad (j = \pm 1, \pm 2, \pm 3)$$

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

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



- 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:

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

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

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

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

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

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

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

$\Delta++$ 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	$-\sqrt{3}\, N_{113}$

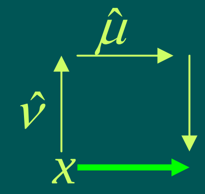
Quark-field and link-variable smearing issues

Run parameters

- run parameters for all results presented here
  - $12^3 \times 48$ anisotropic lattice
  - Wilson gauge, Wilson fermion actions
  - lattice spacings $a_s \sim 0.1\,\mathrm{fm}, \quad a_s/a_t \sim 3.0$
  - quark masses such that $m_\pi \sim 700\,\mathrm{MeV}$
  - quenched
  - correlator matrices averaged over irrep rows
  - use of opposite-parity time-reversed propagators to double statistics
  - number of configurations used
    - 50 for operator smearing tests
    - 200 for operator prunings

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

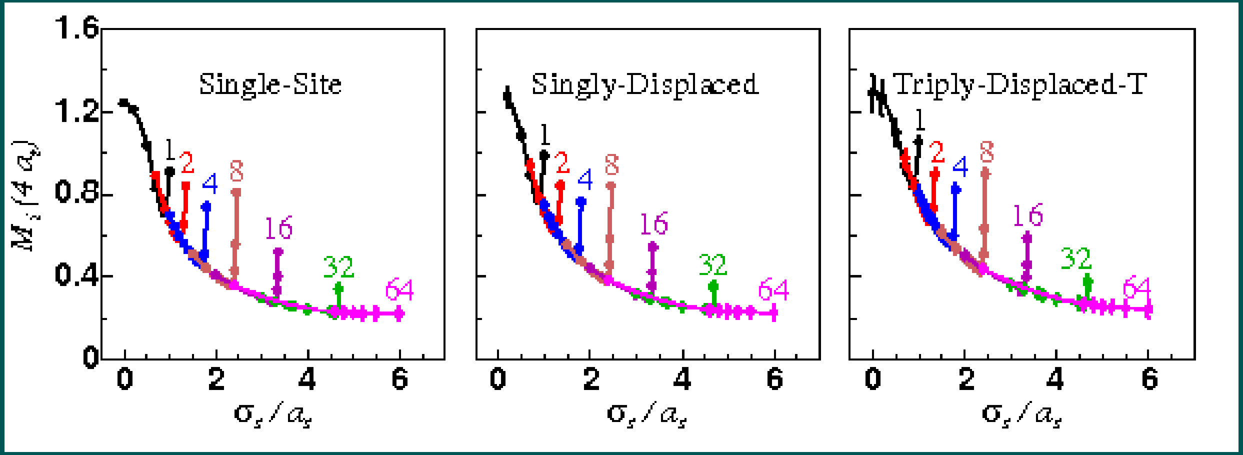
$$U_\mu \to U_\mu^{(1)} \to \cdots \to U_\mu^{(n)} \equiv \widetilde{U}_\mu$$

- quark-field smearing (covariant Laplacian uses smeared gauge field) $\tilde{\psi}(x) = \left(1 + \frac{\sigma_s^2}{4n_\sigma}\tilde{\Delta}^2\right)^{n_\sigma} \psi(x)$
- parameters to tune: $\sigma_s, n_\sigma, \rho, n_\rho$

Quark-field smearing tuning

- focus on three particular operators for smearing tests
  - a single-site operator O_{SS} in the G_{1g} irrep
  - a singly-displaced operator O_{SD} with a particular choice of Dirac indices and 3-link displacement length
  - a triply-displaced-T operator O_{TDT} with a particular choice of the Dirac indices (3-link displacement lengths)
- define effective mass as usual $M_i(t) = \ln\left(\frac{C_{ii}(t)}{C_{ii}(t+a_t)}\right)$
- use $M_i(t=4a_t)$ to compare different quark-field smearings
- smeared links $\rho n_\rho = 2.5, n_\rho = 16$ since displaced operators noisy

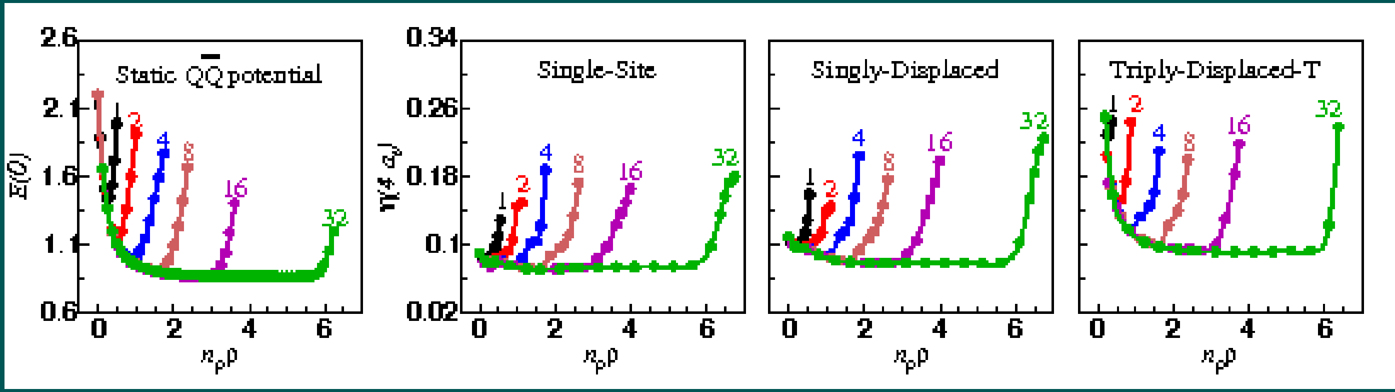
$n_\sigma = 1,2,4,8,$
$16,32,64$



Link-variable smearing tuning

- first, used the effective mass $E(t=0)$ associated with the static quark-antiquark potential at spatial separation $R=5a_s \sim 0.5\ \mathrm{fm}$
- found that link-smearing did not appreciably alter values of baryon effective masses, but had dramatic effect on *variance*
- compared relative jackknife error $\eta_i(t=4a_t)$ of $M_i(t=4a_t)$ for different link-smearing parameters $(\sigma_s=4.0, n_\sigma=32)$
- lesson learned: preferred parameters from static potential produce smallest errors in baryon effective masses

$$n_\rho = 1,2,4,8,16,32$$



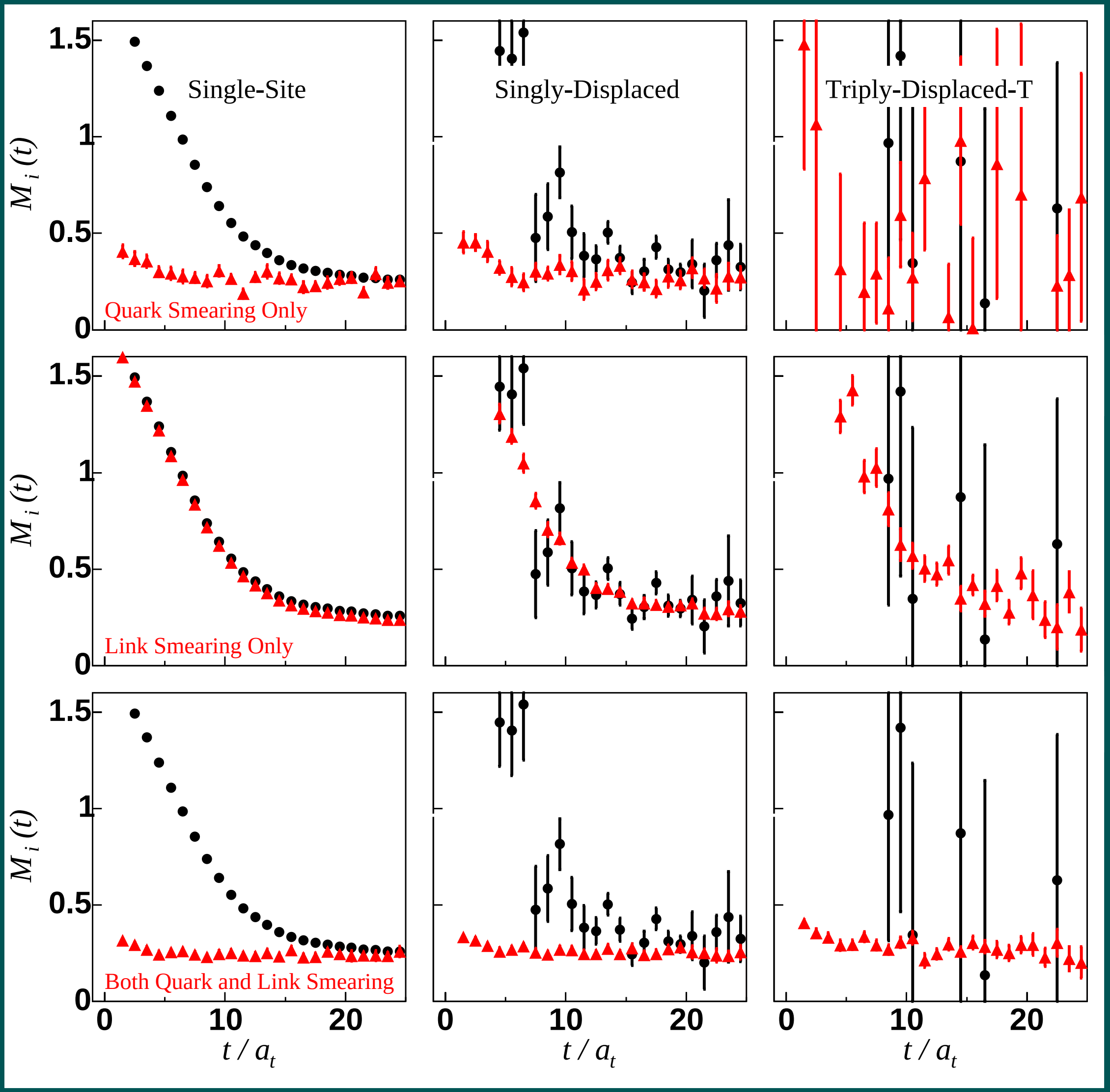
Importance of smearing

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

$$\sigma_s = 4.0, \quad n_\sigma = 32$$

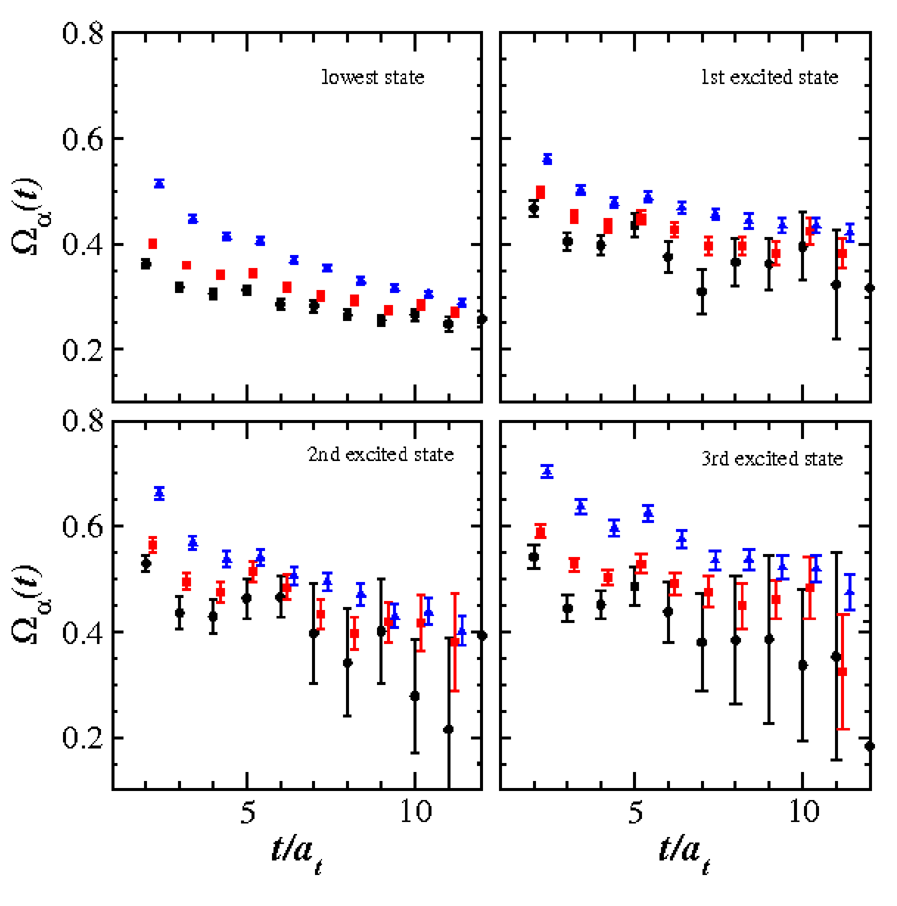
$$n_\rho \rho = 2.5, \quad n_\rho = 16$$

- effect on excited states shows $\sigma_s = 3.0$ better



Smearing and excited states

- previous tests involved lowest state only
- important to tune smearing for excited states as well
- lowest 4 principal effective masses for 10x10 matrix of DDI G_{1g} operators shown
  - same link smearing
    $\rho n_\rho = 2.5, n_\rho = 16$
  - quark-field smearings
    $\sigma_s = 2.0$ (blue), 3.0 (red), 4.0 (black) $\quad n_\sigma = 32$
  - $\rho n_\rho = 5.0, n_\rho = 32$ with $\sigma_s = 4.0$ did not reduce errors
- preferred: $n_\sigma = 32, \sigma_s = 3.0$



Smearing summary

- From our quenched study of the G_{1g} nucleon channel on small lattices $12^3 \times 48$ for $a_s \sim 0.1\,\mathrm{fm}$ and $a_s / a_t \sim 3.0$ and $m_\pi \sim 700\,\mathrm{MeV}$, the preferred smearing parameters are

$$\boxed{\rho n_\rho = 2.5, n_\rho = 16} \qquad \boxed{n_\sigma = 32, \sigma_s = 3.0}$$

- factors still to consider:
  - evidence for same smearing for other irreps
  - expect same smearing for other isospin channels
  - dependence on lattice spacing
  - dependence on quark mass

Operator pruning issues

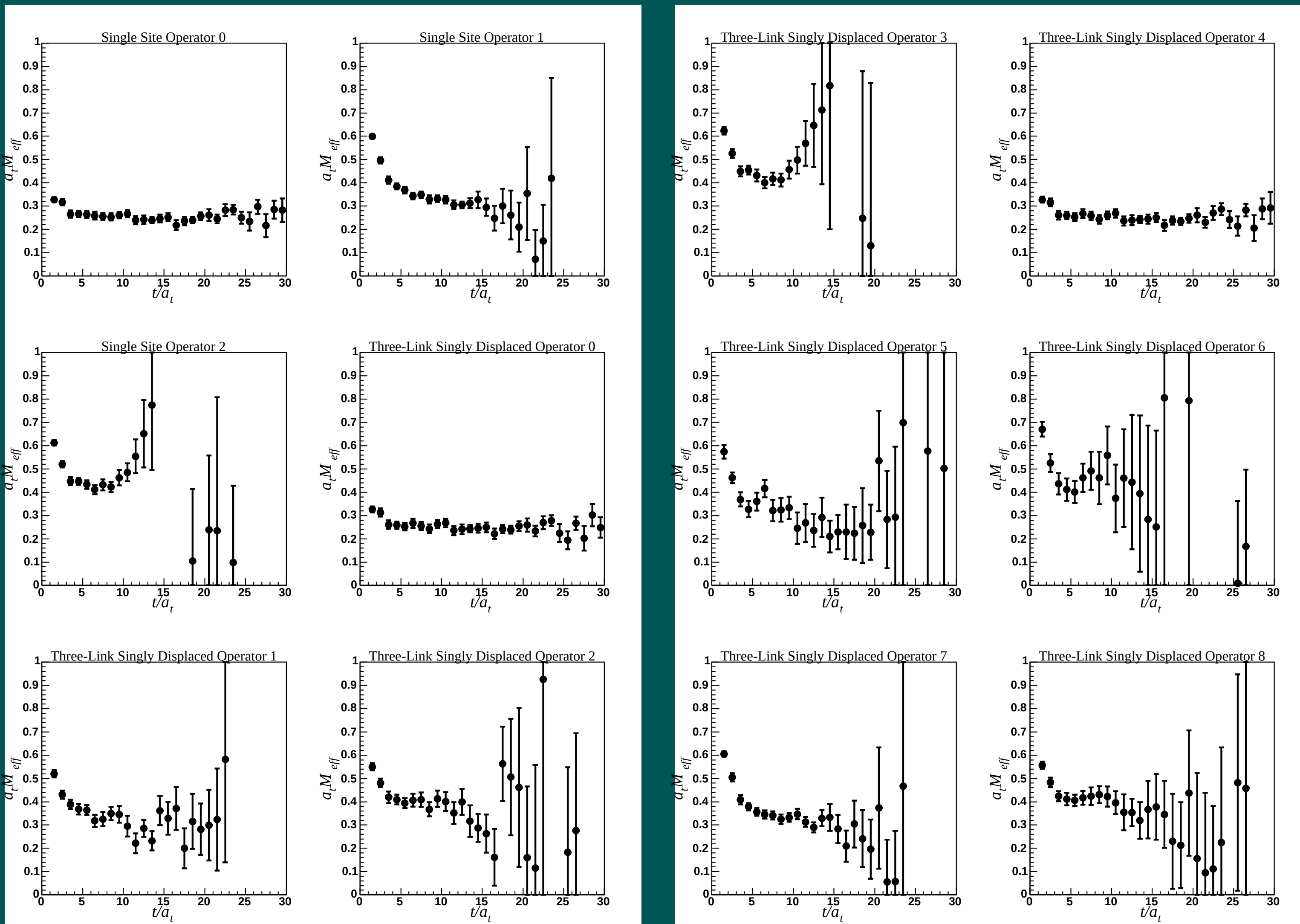
Operator plethora

- Number of N^+ operators given below (1 displacement length)
  - total of 179 operators in G_{1g} channel

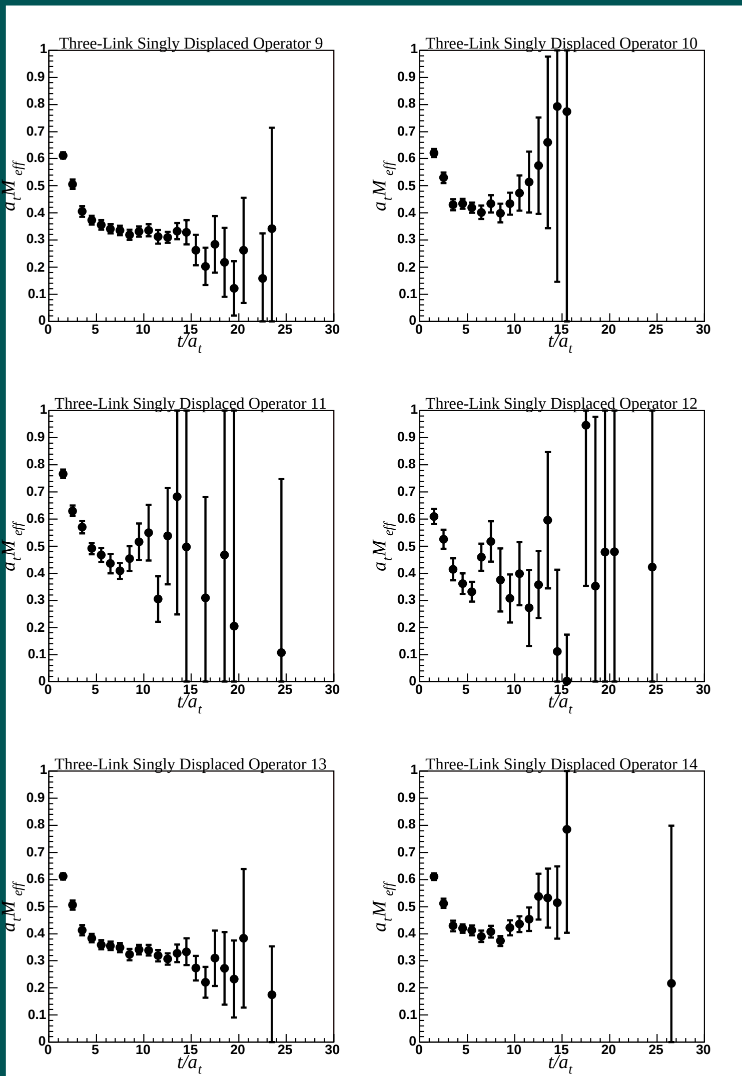
	G_{1g}	G_{2g}	H_g
Single-site	3	0	1
Singly-displaced	24	8	32
Doubly-displaced-I	24	8	32
Doubly-displaced-L	64	64	128
Triply-displaced-T	64	64	128

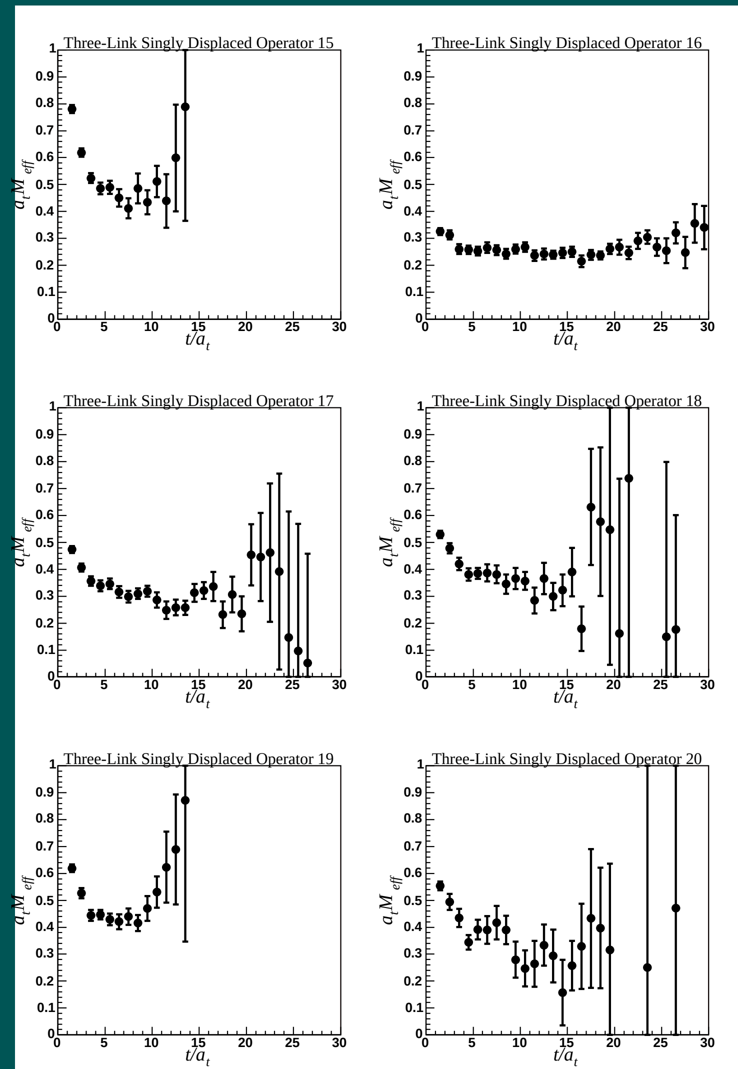
- since 179x179 matrix too large to be practical, operator pruning is clearly necessary
- will focus on G_{1g} channel first

Operator plethora (G1g Nucleon)

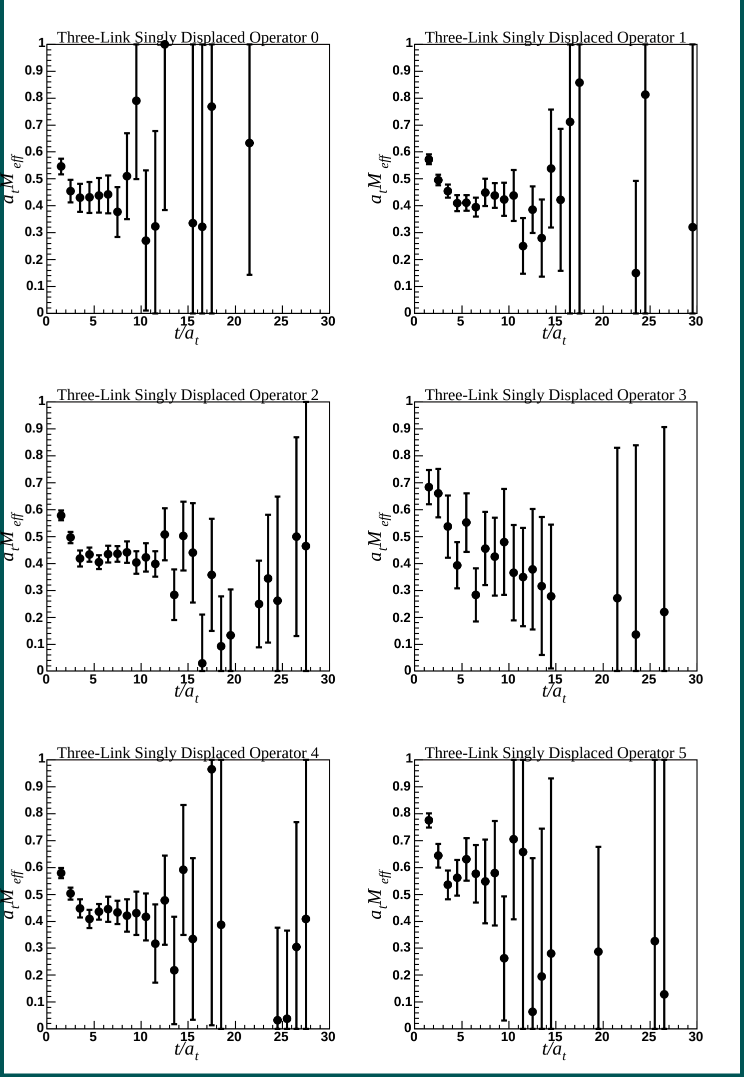


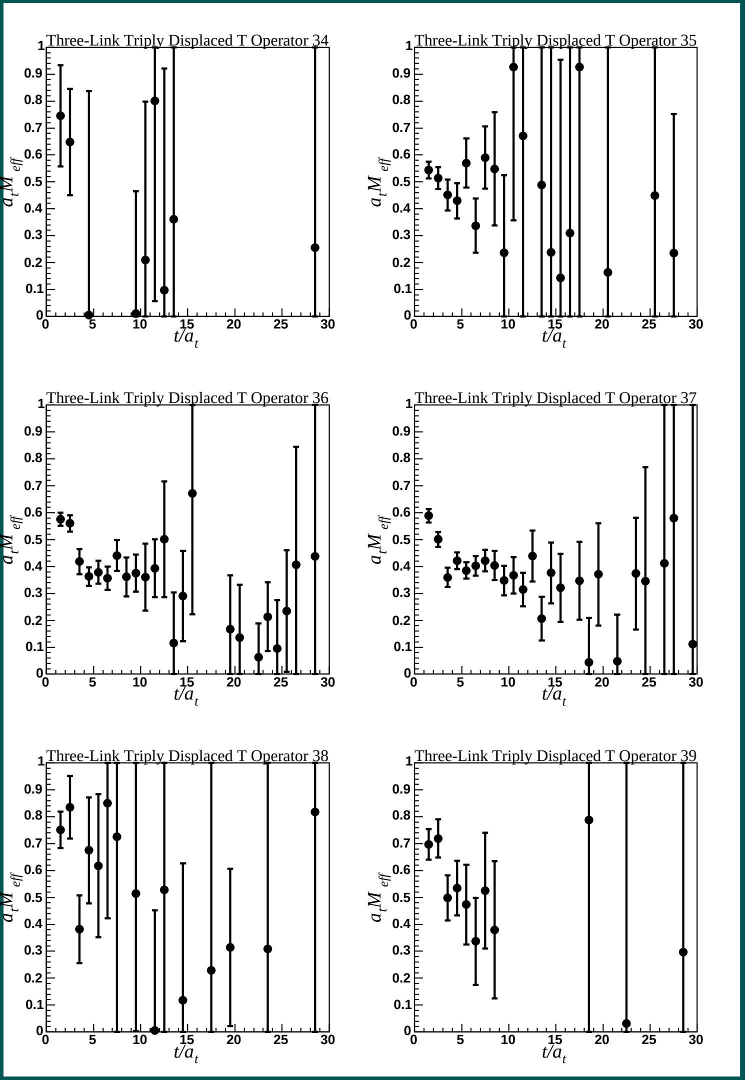
G1g nucleon operators



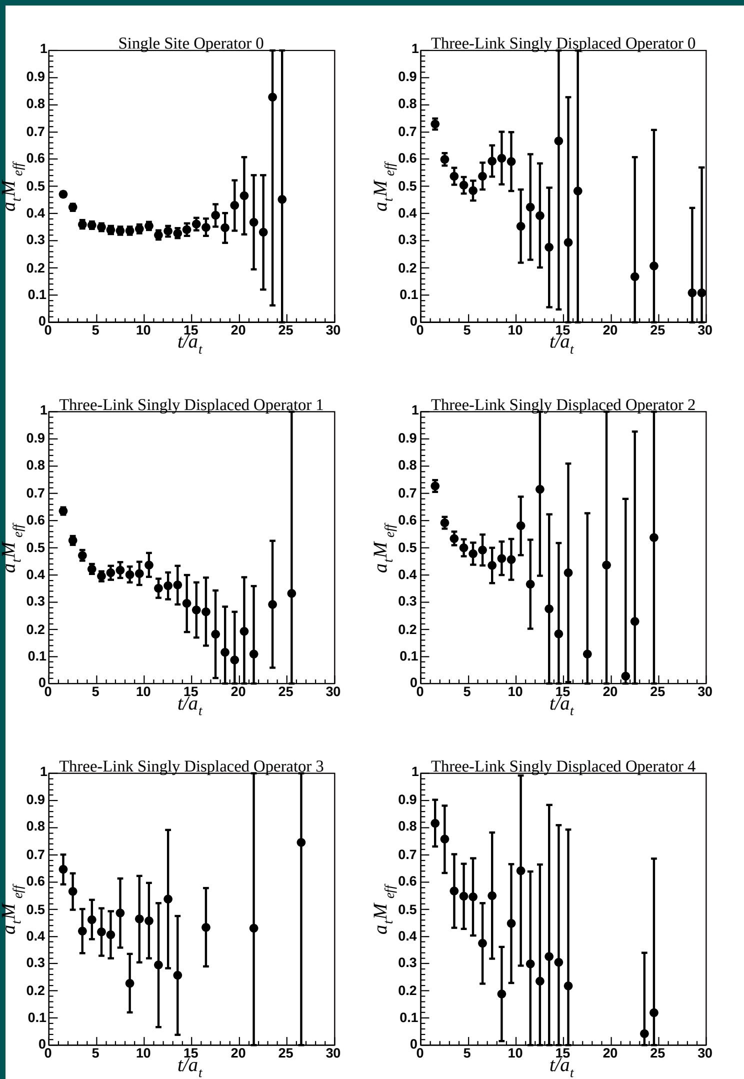


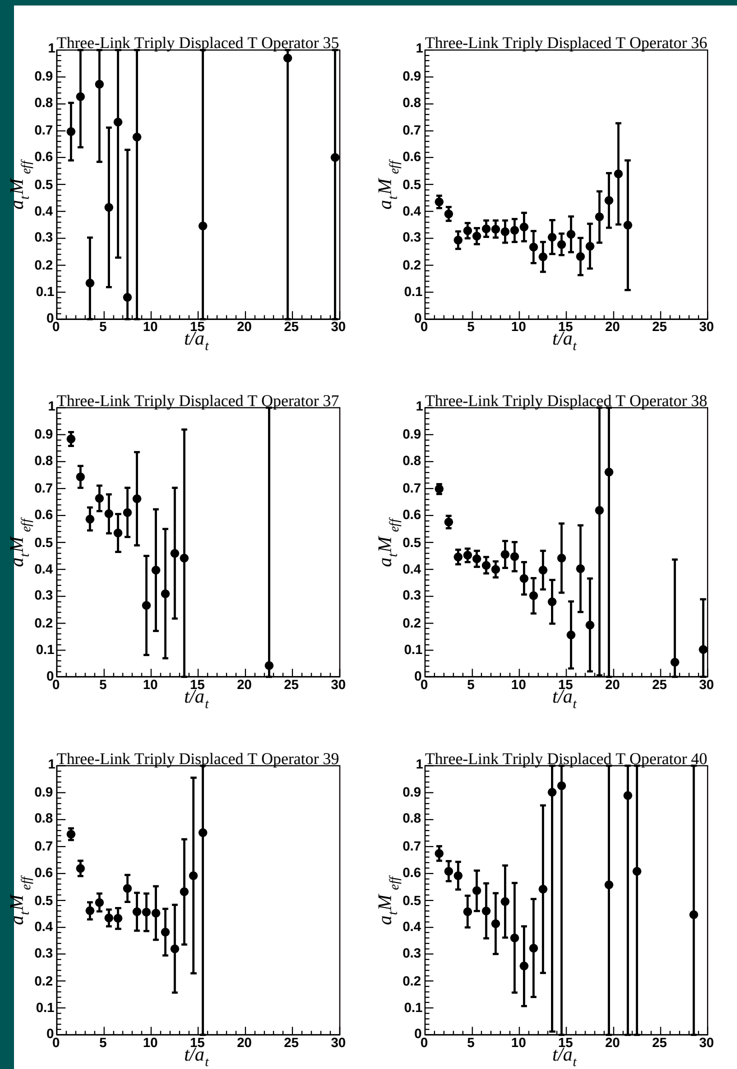
G2g nucleon operators





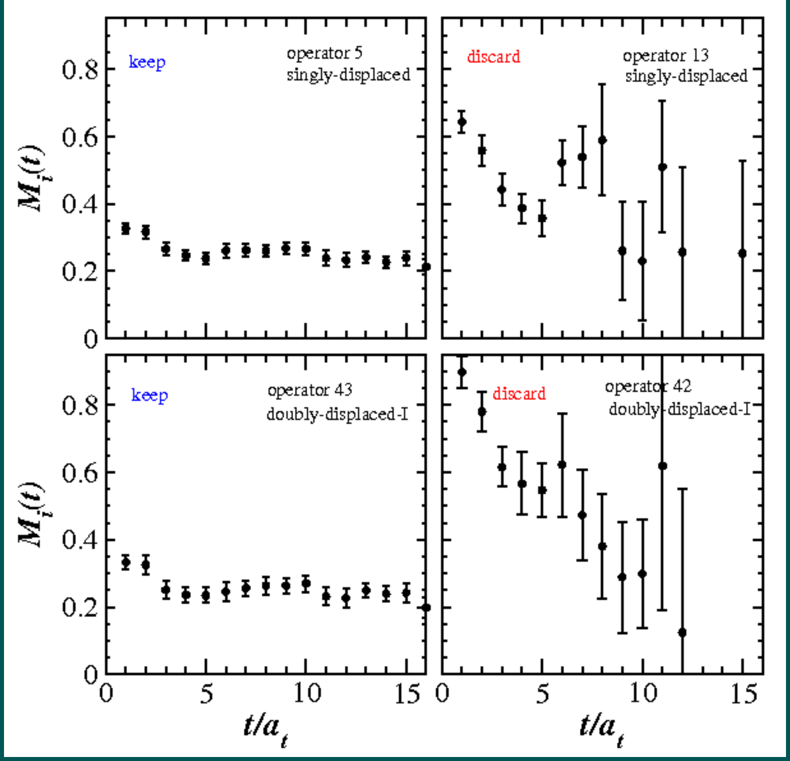
Hu nucleon operators

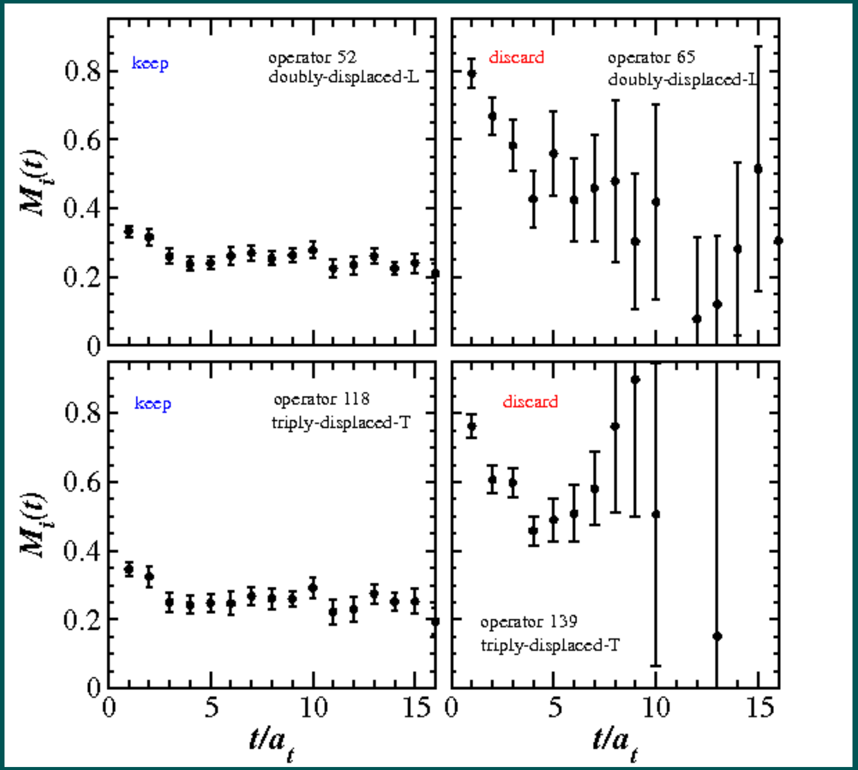




Pruning: step one

- look at effective masses of diagonal elements of correlation matrix and discard noisy operators
- examples shown below $(\rho n_\rho = 2.5, n_\rho = 16, n_\sigma = 32, \sigma_s = 4.0 \text{ used})$
- all 179 effective masses





Pruning: step one (continued)

- retain 64 operators out of the 179
  - SS: 0, 1, 2
  - SD: 3, 5, 6, 8, 10, 12, 14, 17, 19, 20, 22, 24, 25
  - DDI: 27, 29, 30, 31, 33, 36, 38, 41, 43, 44, 45, 48
  - DDL: 52, 54, 56, 57, 58, 59, 60, 61, 62, 72, 74, 76, 78, 85, 88, 94, 97, 98, 105, 110
  - TDT: 116, 118, 119, 124, 125, 126, 132, 134, 136, 138 149, 158, 162, 163, 169, 174

Noise, noise, noise, noise

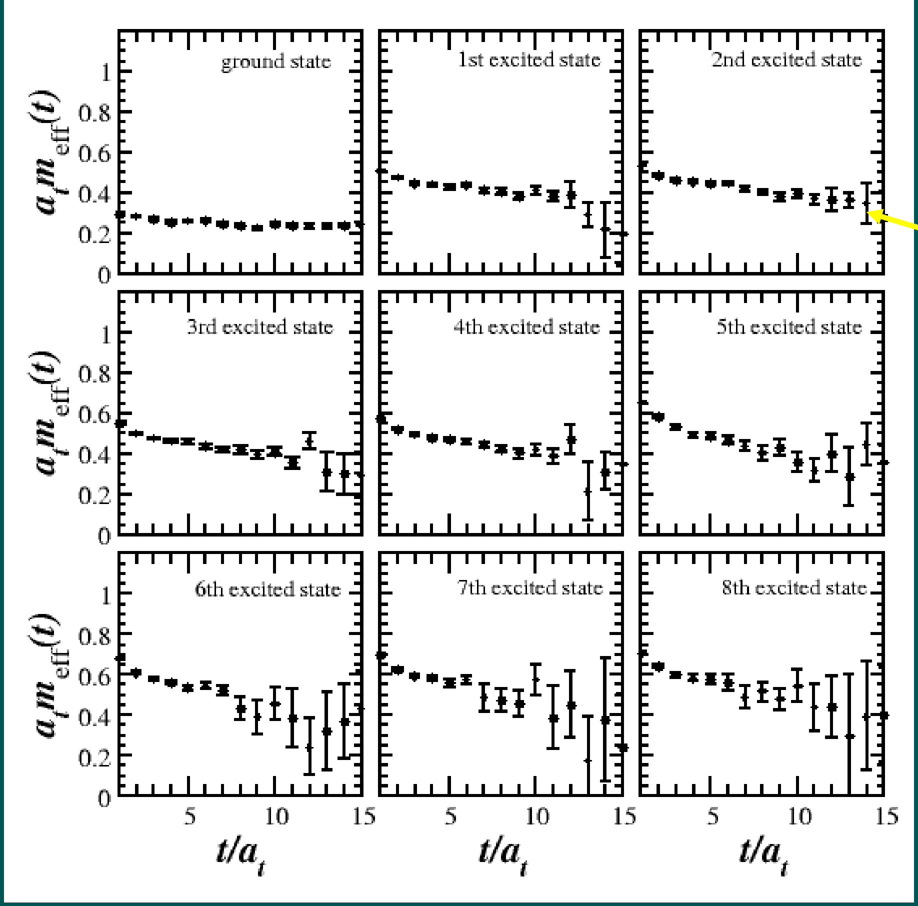
- noise is the enemy!!
  - intrinsic noise in each operator
  - presence of small singular values indicates operator set not "independent enough" → noise can creep in
- examine renormalized matrix at early time *t=1*

$$\hat{C}_{ij}(1) = C_{ij}(1) / \sqrt{C_{ii}(1) C_{jj}(1)}$$

- sort operators in order of increasing noise
- keep 6 least noisiest operators of each kind (SD,DDI,...) which yield acceptable matrix condition number
- from above set, choose 25 operators which still yield acceptable matrix condition number
- try to keep different operator types if condition number allows

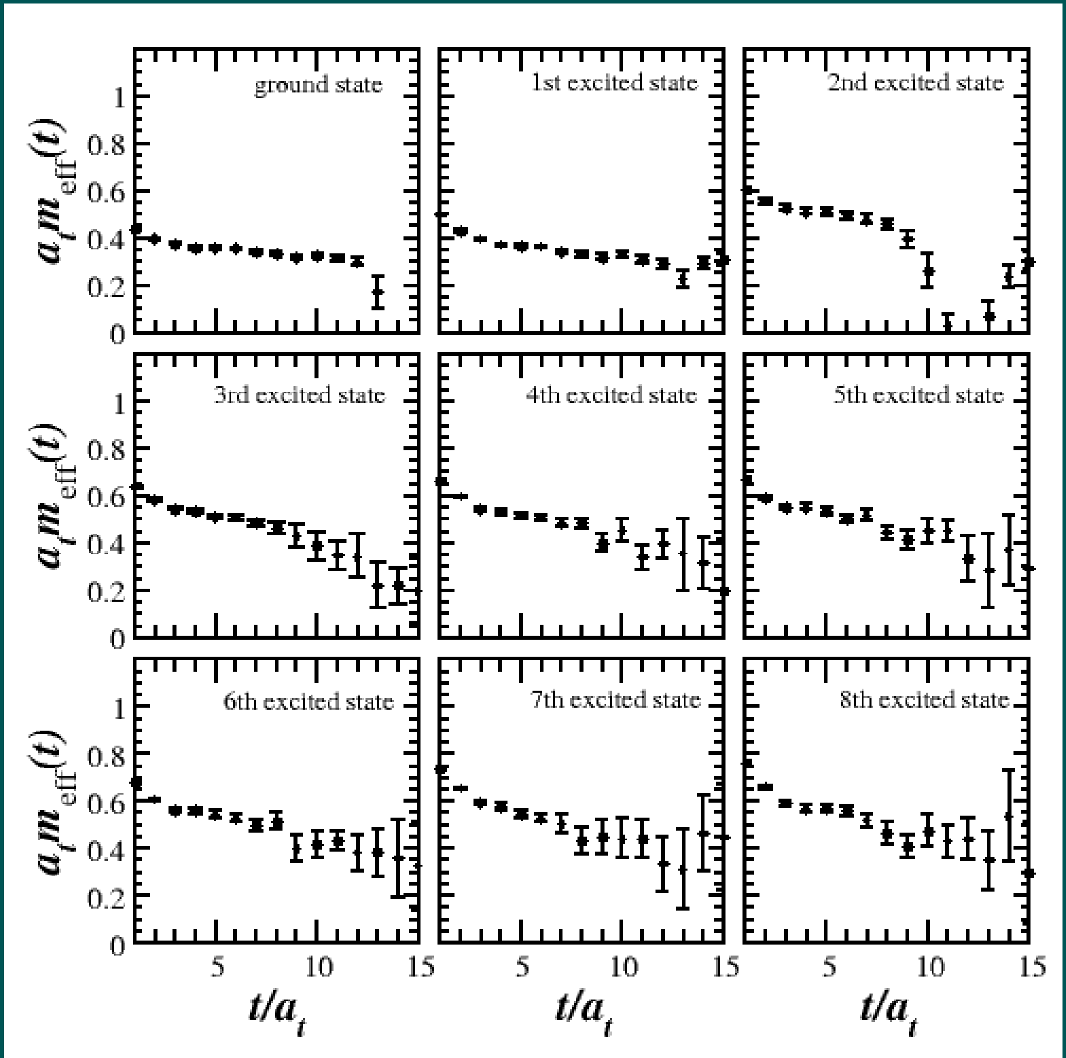
Milestone: principal effective masses

- G1g nucleons (16x16 matrix) using 200 configurations
- world record: 9 levels extracted (even more possible!)



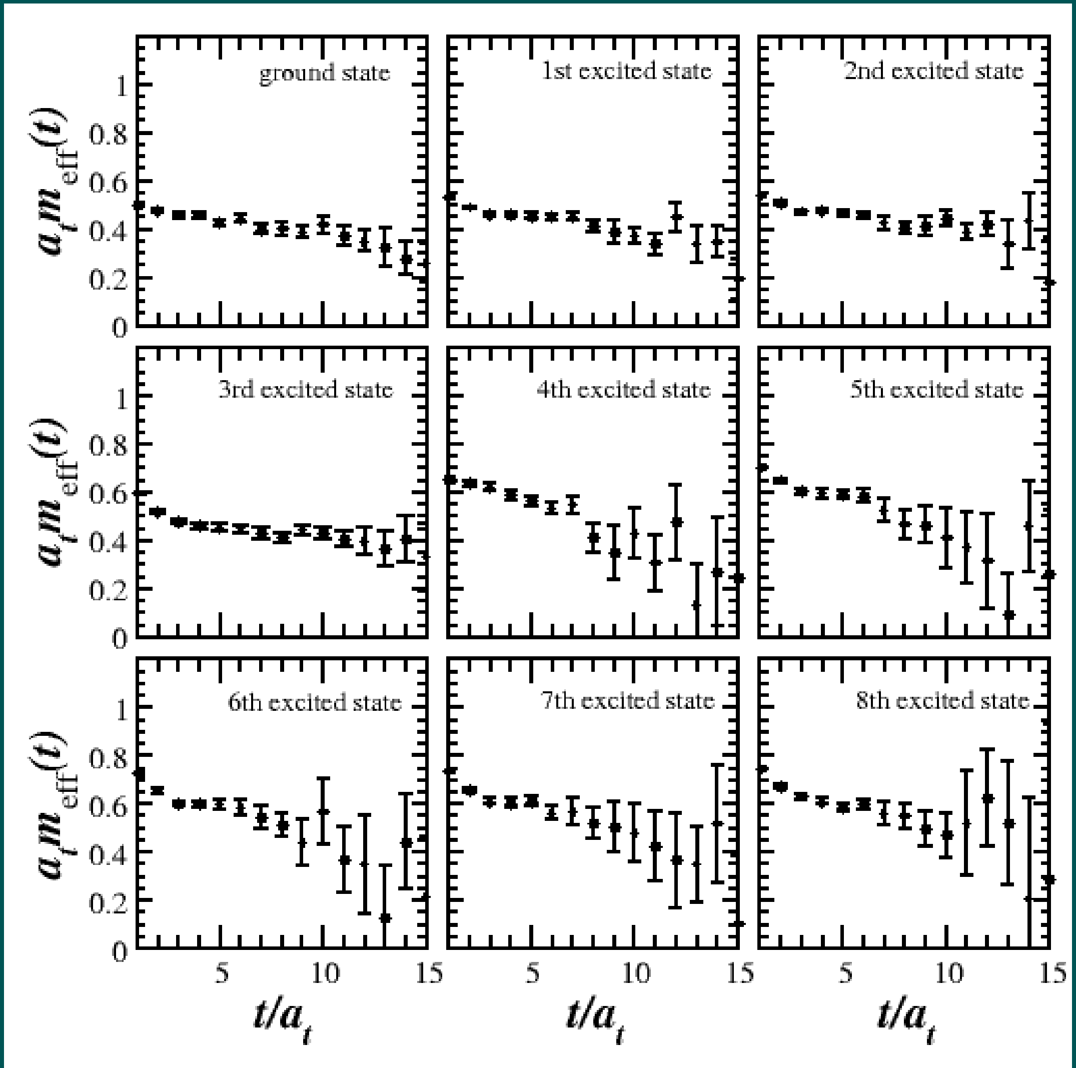
effect of time-backward propagation of anti-baryons

G1u Nucleon channel

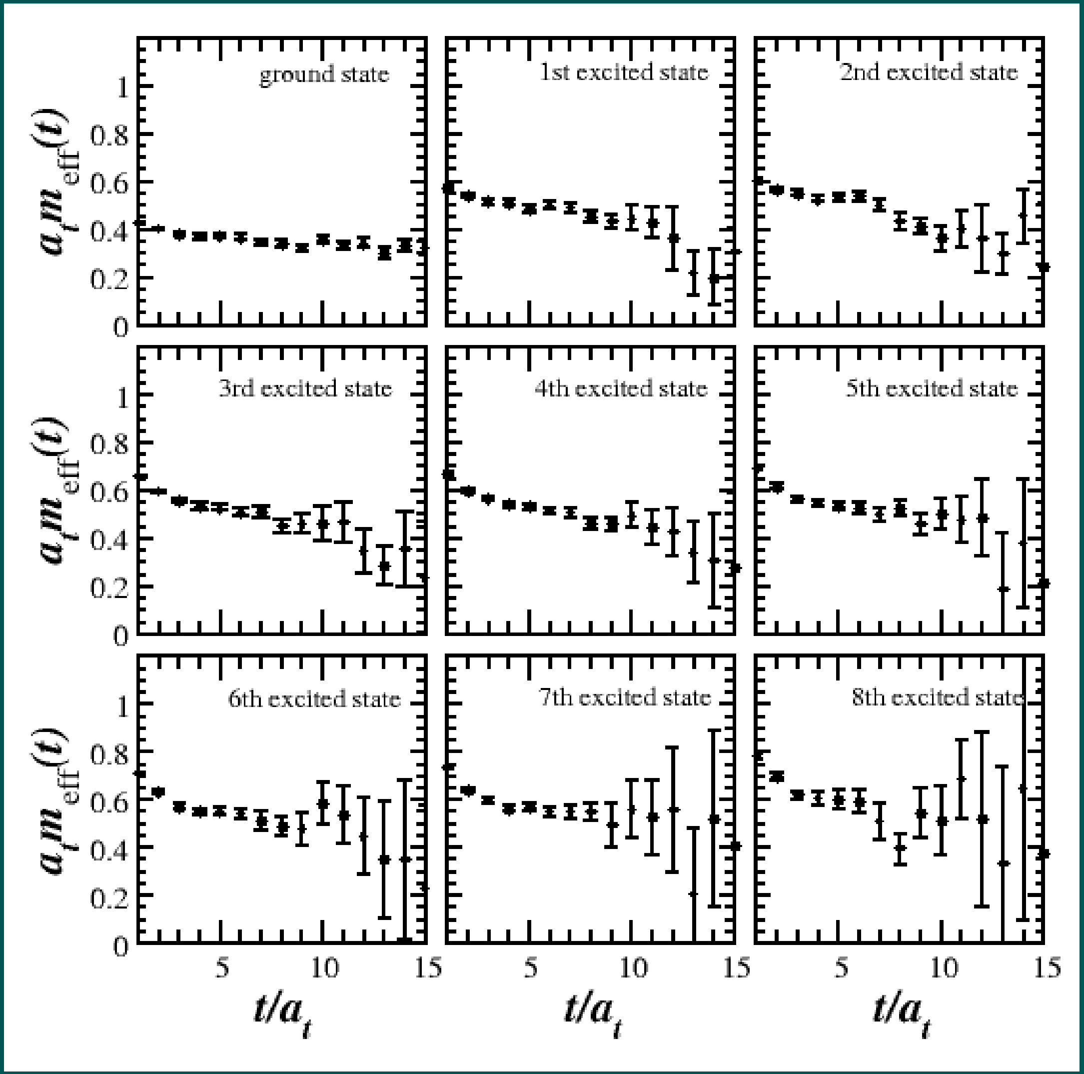


can see effect of time-backward propagation of anti-baryons

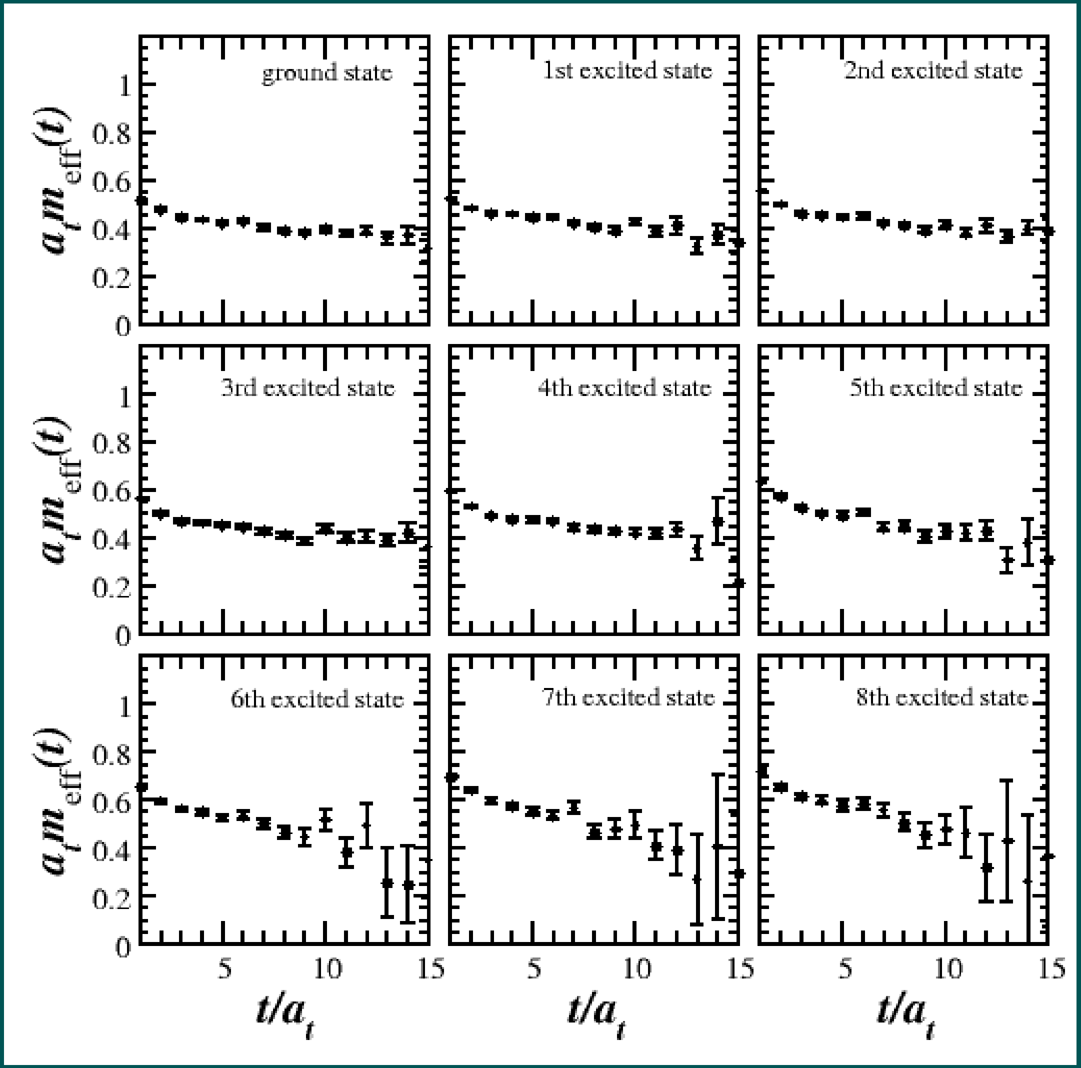
G2g nucleon channel



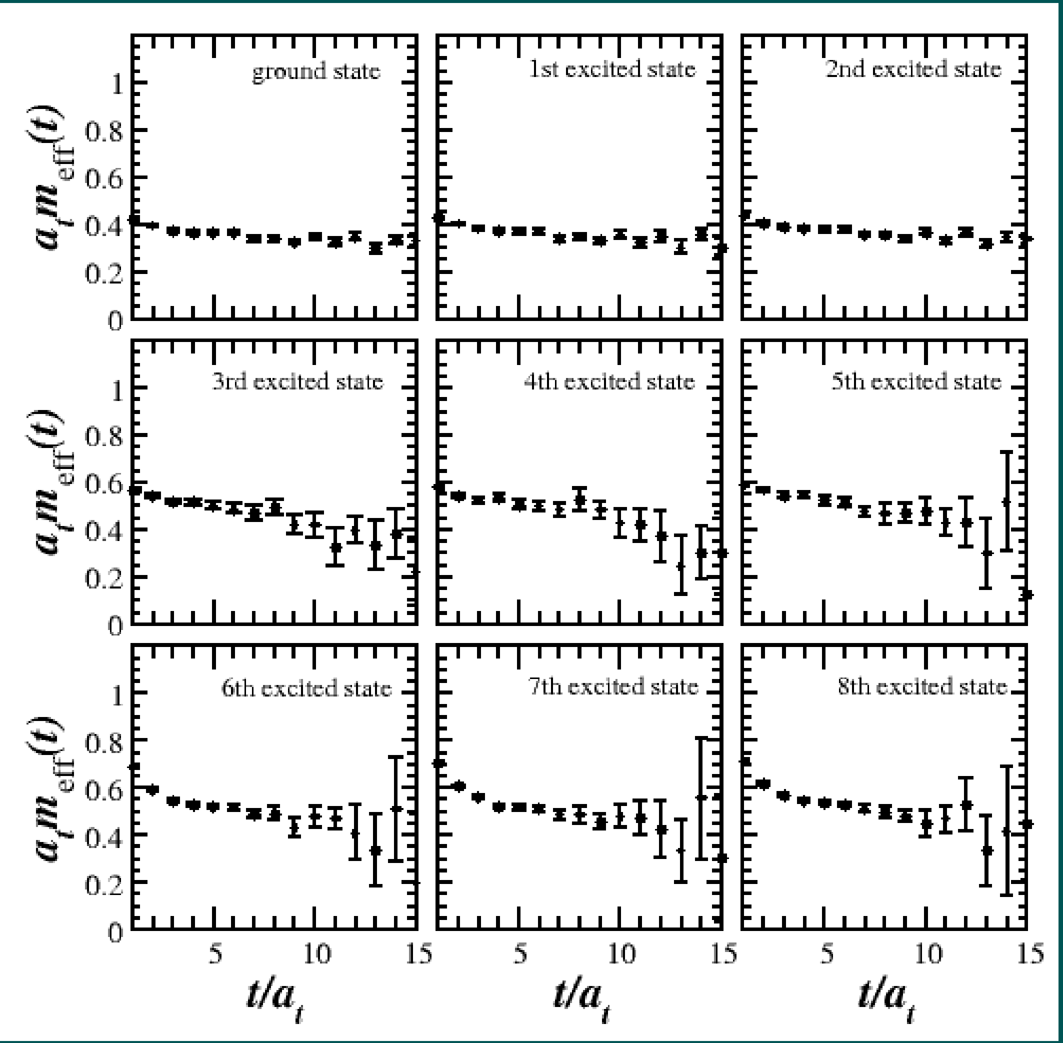
G2u nucleon channel



Hg nucleon channel



Hu nucleon channel



Future work

- three-quark operator pruning to be completed
  - all irreps, all isospin channels
  - different displacement lengths
- include mesons (in progress)
- include multi-hadron operators
  - stochastic all-to-all propagators with dilution, low eigenvectors
  - will also facilitate disconnected diagrams
- goal: operator technology ready to go when unquenched simulations near realistically-light quark masses become possible
- LHPC recently was awarded 1/6 of QCDOC to generate configurations on large lattices with dynamical quarks such that pion mass around 300 MeV

Summary

- progress report on ongoing efforts of LHPC to extract hadron spectrum with large sets of extended operators
  - need for correlation matrices of good operators
  - spin identification must be addressed
  - multi-hadron operators will become important
- exploration of 3-quark baryon operators nearly done
- study of meson operators beginning
- major milestone reached: can extract 9 or more states!!
- ultimately, MC updating with realistically light quark masses needed
- very challenging calculations
  - will keep hammering at it!