The excited hadron spectrum in lattice QCD using a new variance reduction method

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Overview

- overarching goal → obtain stationary state energies of QCD in cubic boxes (periodic b.c.) of various sizes using Monte Carlo method
- key points of talk:
  - good single hadron operators for various momenta now selected in nearly all light baryon and meson sectors
  - to get spectrum for lighter quark masses
    - multi-hadron operators needed → slice-to-slice quark propagators
    - recent technology breakthrough → new quark smearing with improved variance reduction
- interpretation of finite-volume energies
  - spectrum matching to construct effective hadron theory?

Dramatis Personae

- current collaborators:
  - Justin Foley, David Lenkner, Colin Morningstar, Ricky Wong (CMU)
  - Keisuke Jimmy Juge (U. of Pacific)
  - John Bulava (DESY, Zeuthen)
  - Mike Peardon, (Trinity Coll. Dublin)
  - Steve Wallace (U. Maryland)
  - B. Joo (JLab)

Excited-state energies from Monte Carlo

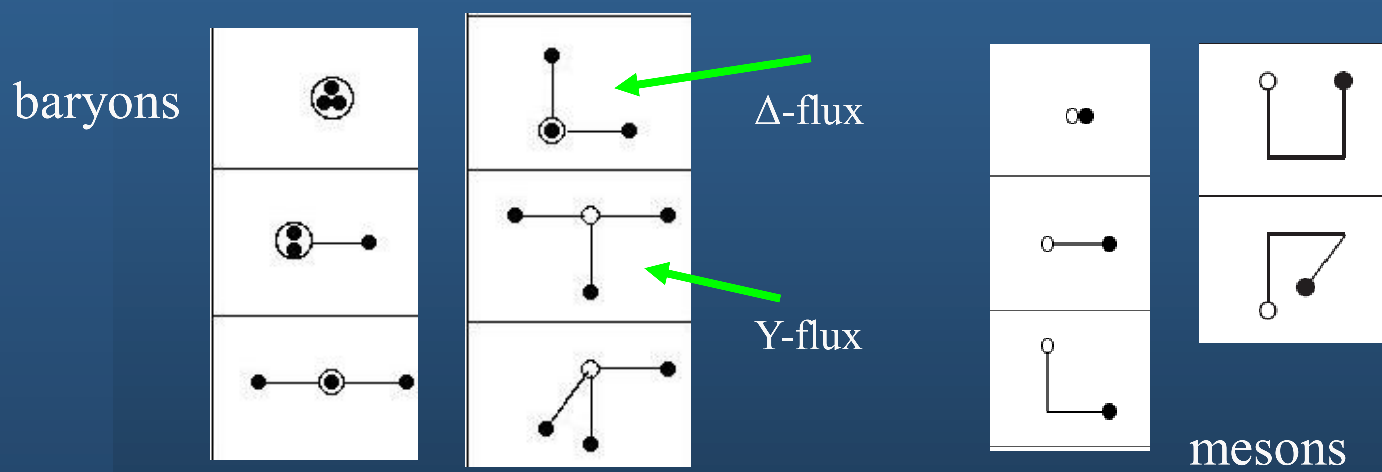
- extracting excited-state energies requires matrix of correlators
- for a given $N \times N$ correlator matrix $C_{\alpha\beta}(t) = \langle 0 | O_\alpha(t) O^{+}_\beta(0) | 0 \rangle$
  one defines the N *principal correlators* $\lambda_\alpha(t,t_0)$ as the eigenvalues of

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

  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 $m_\alpha^{\rm eff}(t) = \ln\left(\dfrac{\lambda_\alpha(t,t_0)}{\lambda_\alpha(t+1,t_0)}\right)$
  now tend (plateau) to the N lowest-lying stationary-state energies
- calculations done in cubic box (periodic boundary conditions)
  - all energies are *discrete*
  - zero-momentum states labeled by irreps of O_h point group even in *continuum* limit

Single-hadron operators

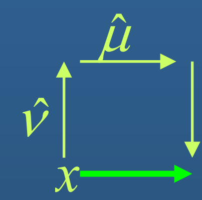
- covariantly-displaced quark fields as building blocks
- group-theoretical projections onto irreps of lattice symmetry group
- displacements of different lengths build up radial structure
- displacements in different directions build up orbital structure



- reference: PRD72, 094506 (2005)

Quark- and gauge-field smearing

- smeared quark and gluon fields fields → dramatically reduced coupling with short wavelength modes
- link-variable smearing (stout links PRD69, 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 $U_\mu^{(n+1)} = \exp\left(iQ_\mu^{(n)}\right) U_\mu^{(n)}$

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

- initial quark-field smearing (Laplacian using smeared gauge field)

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

Operator selection

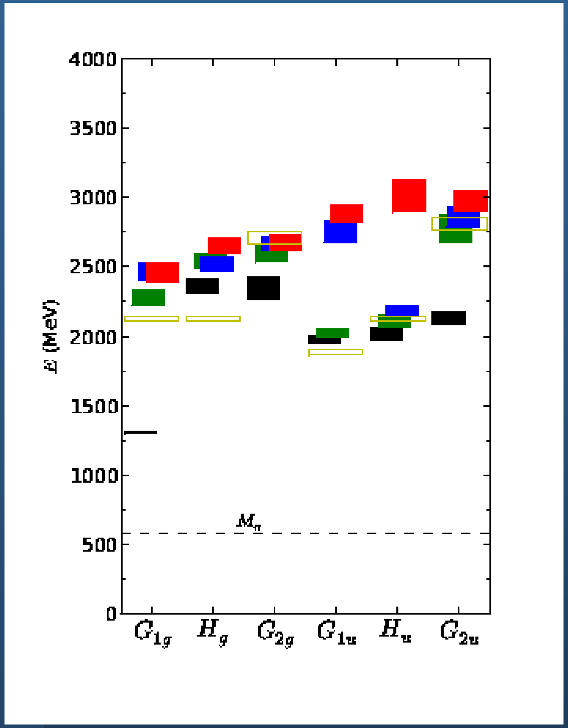
- operator construction leads to very large number of operators
- rules of thumb for "pruning" operator sets
  - noise is the enemy!
  - prune first using intrinsic noise (diagonal correlators)
  - prune next within operator *types* (single-site, singly-displaced, *etc.*) based on condition number of
  - prune across all operators based on condition number
- best to keep a variety of different types of operators, as long as condition numbers maintained

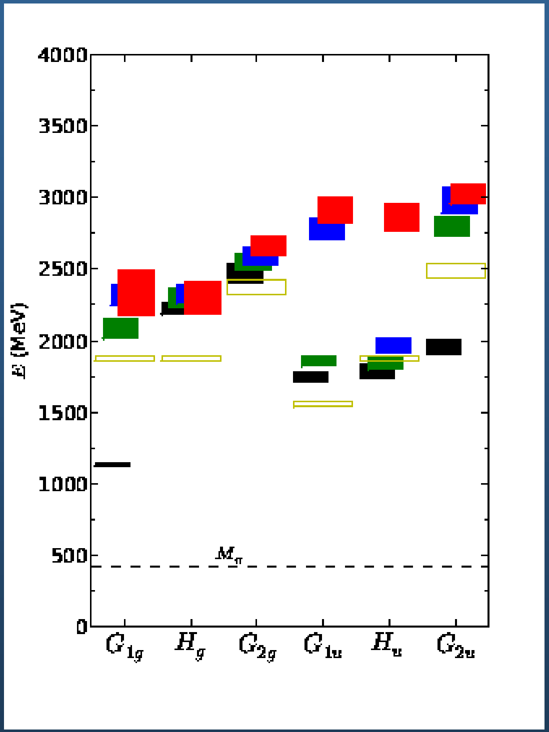
$$\hat{C}_{ij}(t) = \frac{C_{ij}(t)}{\sqrt{C_{ii}(t)C_{jj}(t)}}, \qquad t = 1$$

- typically use 16 operators to get 8 lowest lying levels

Nucleons

- N_f=2 on $24^3 \times 64$ anisotropic clover lattice, a_s~0.11 fm, a_s/a_t~3
- Left: m_π=578 MeV Right: m_π=416 MeV PRD 79, 034505 (2009)

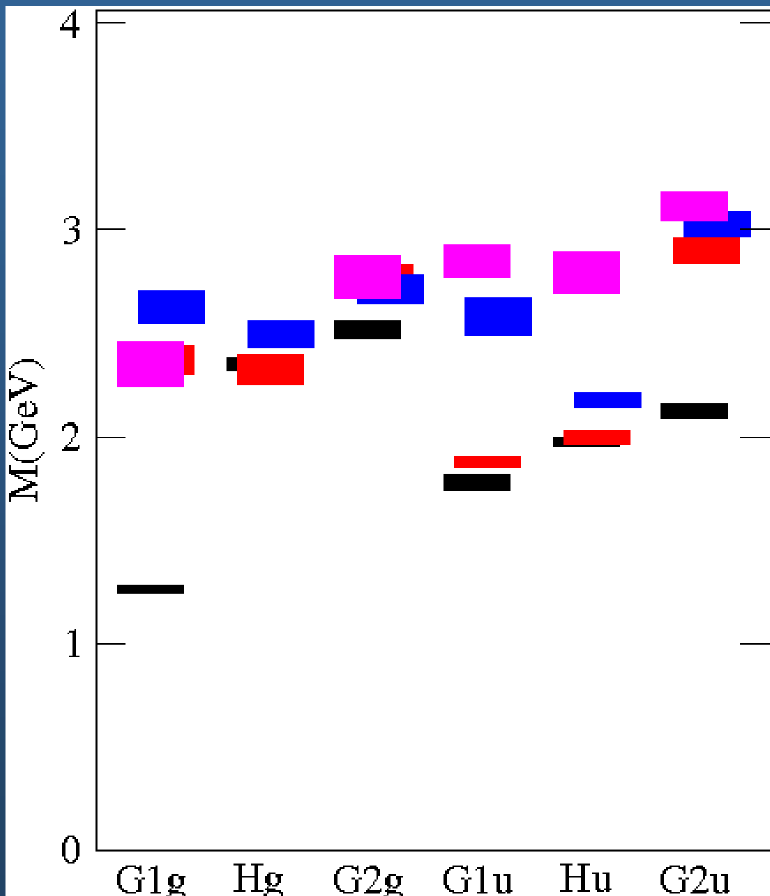


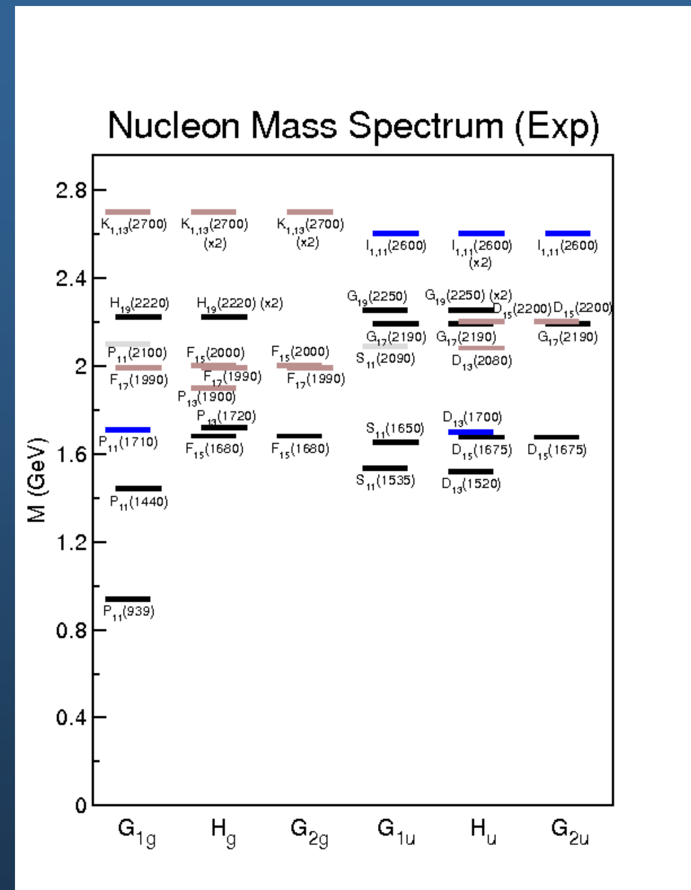


- multi-hadron thresholds above show need for multi-hadron operators to go to lower pion masses!!

Nucleon operator pruning

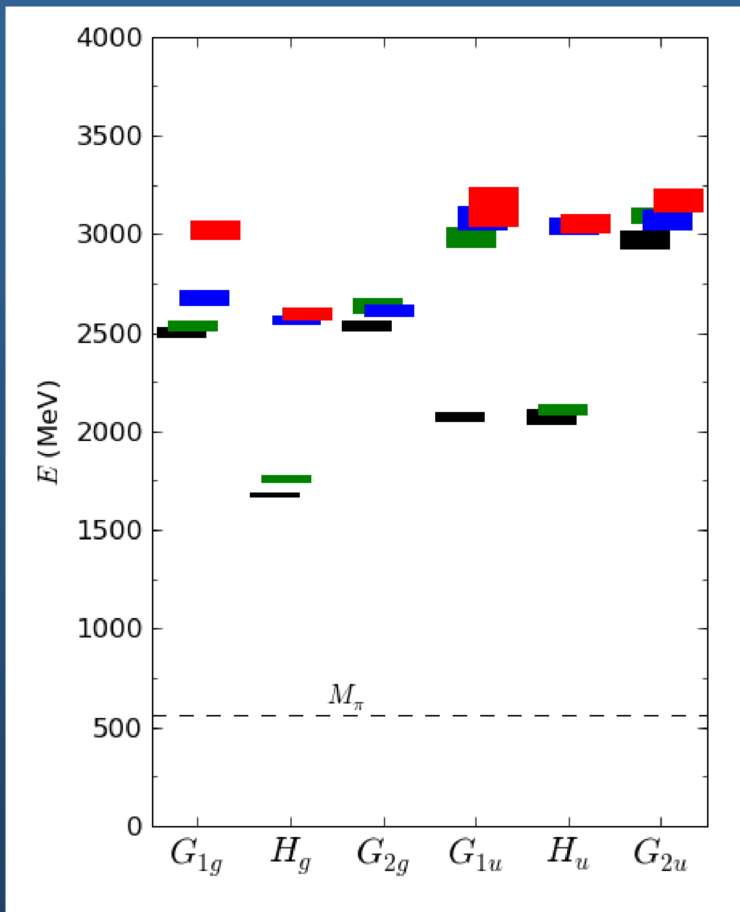
- N_f=2+1 on $16^3 \times 128$ lattice, m_π= 380 MeV (100 configs, 32 eigvecs)

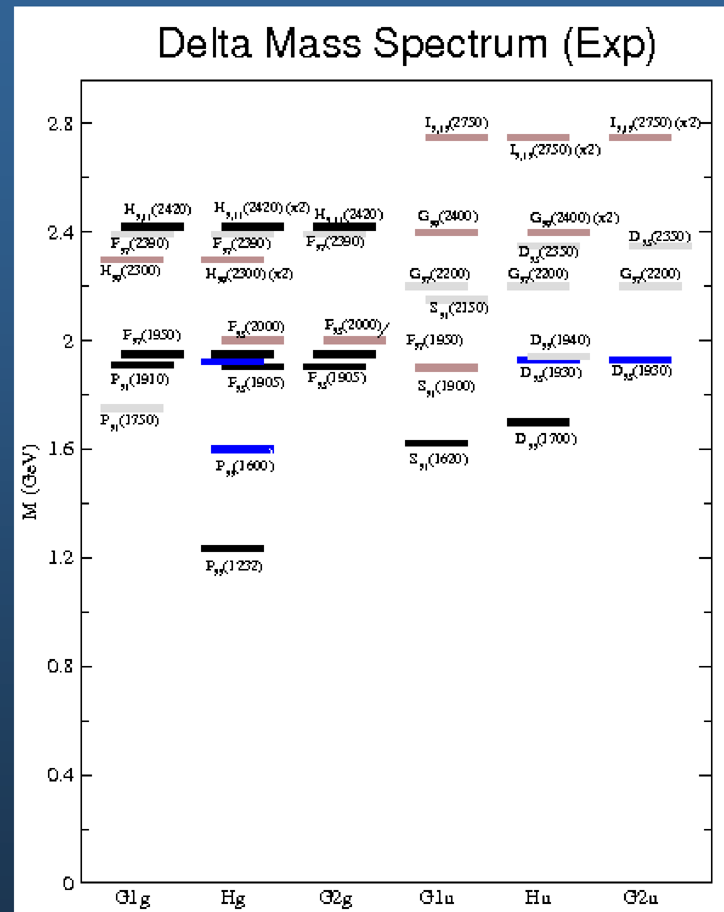




Delta operator pruning

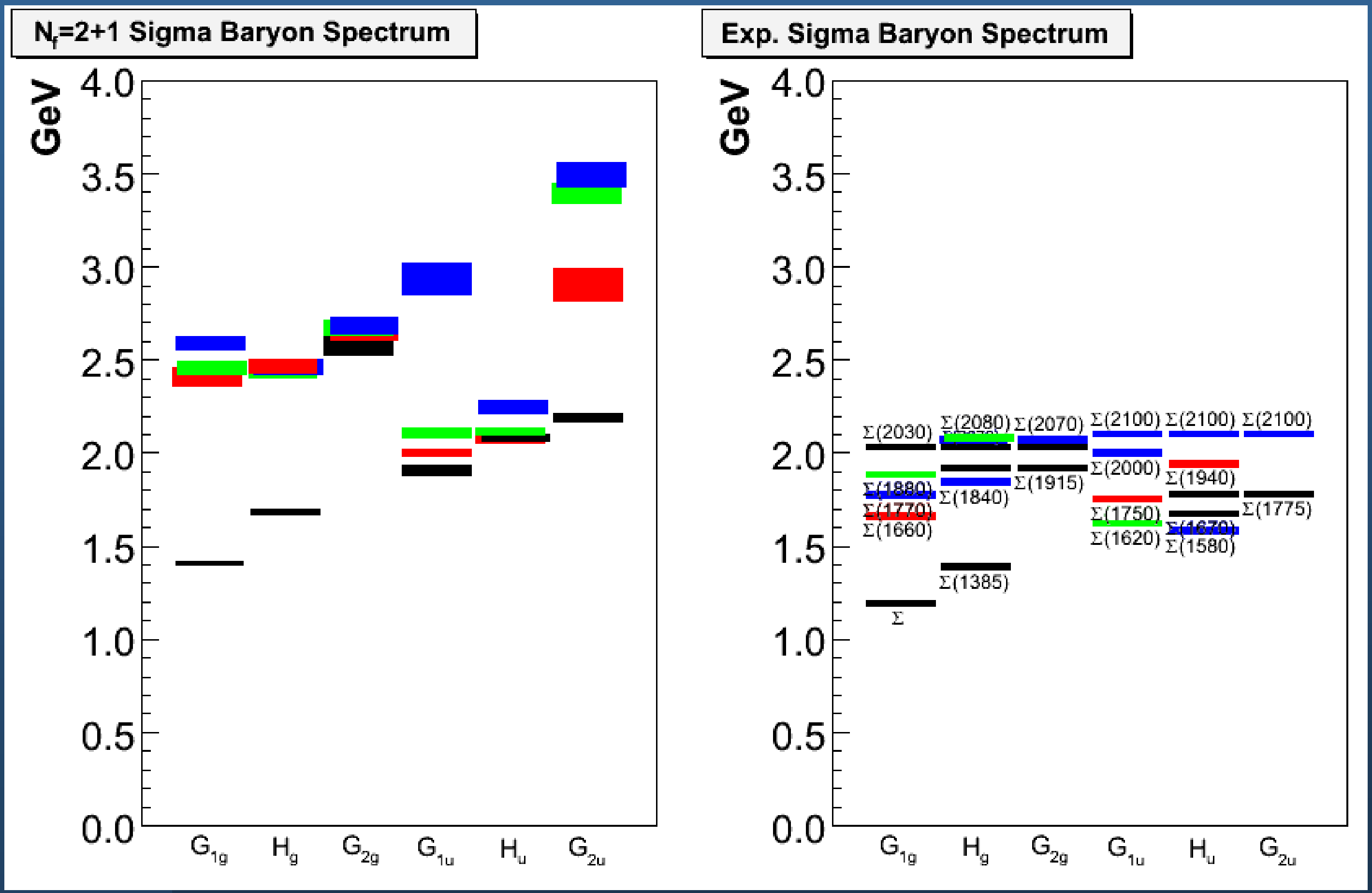
- N_f=2+1 on 16^3×128 lattice, m_π= 380 MeV (481 configs, 32 eigvecs)





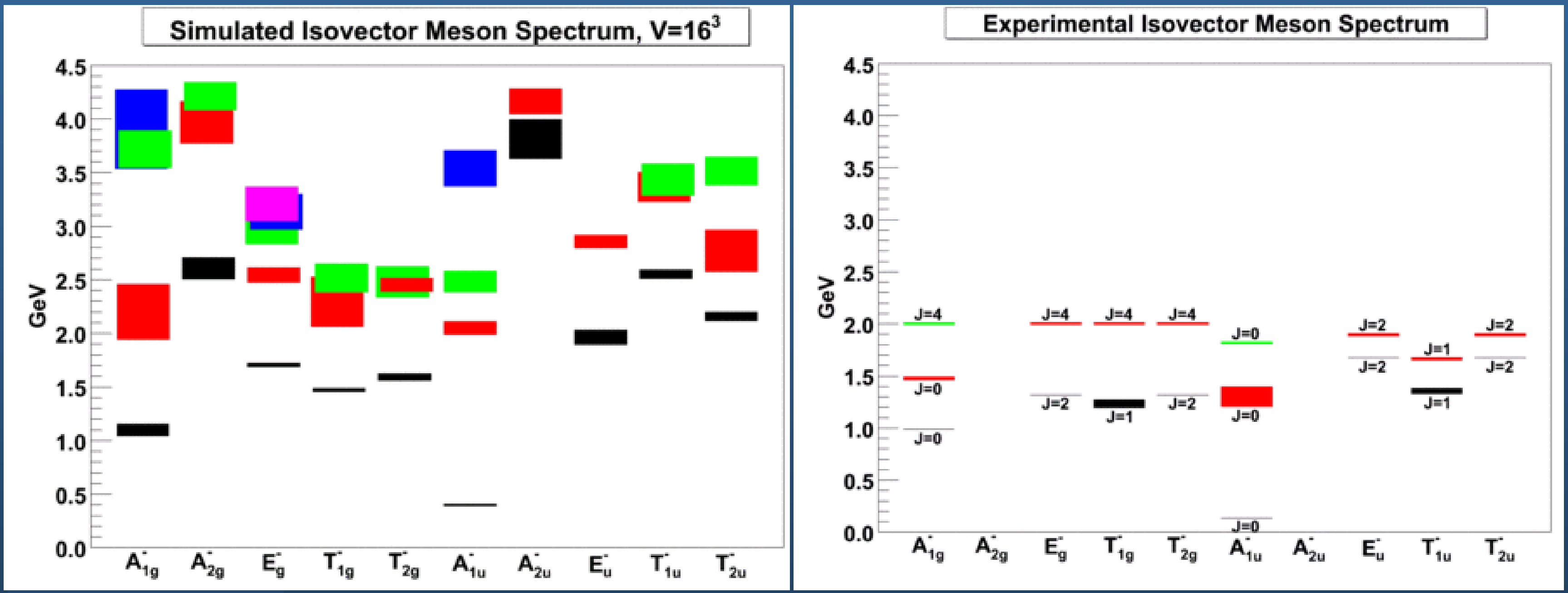
Sigma operator pruning

- N_f=2+1 on $16^3\times128$ lattice, m_π= 380 MeV (100 configs, 32 eigvecs)



Isovector G-parity odd mesons

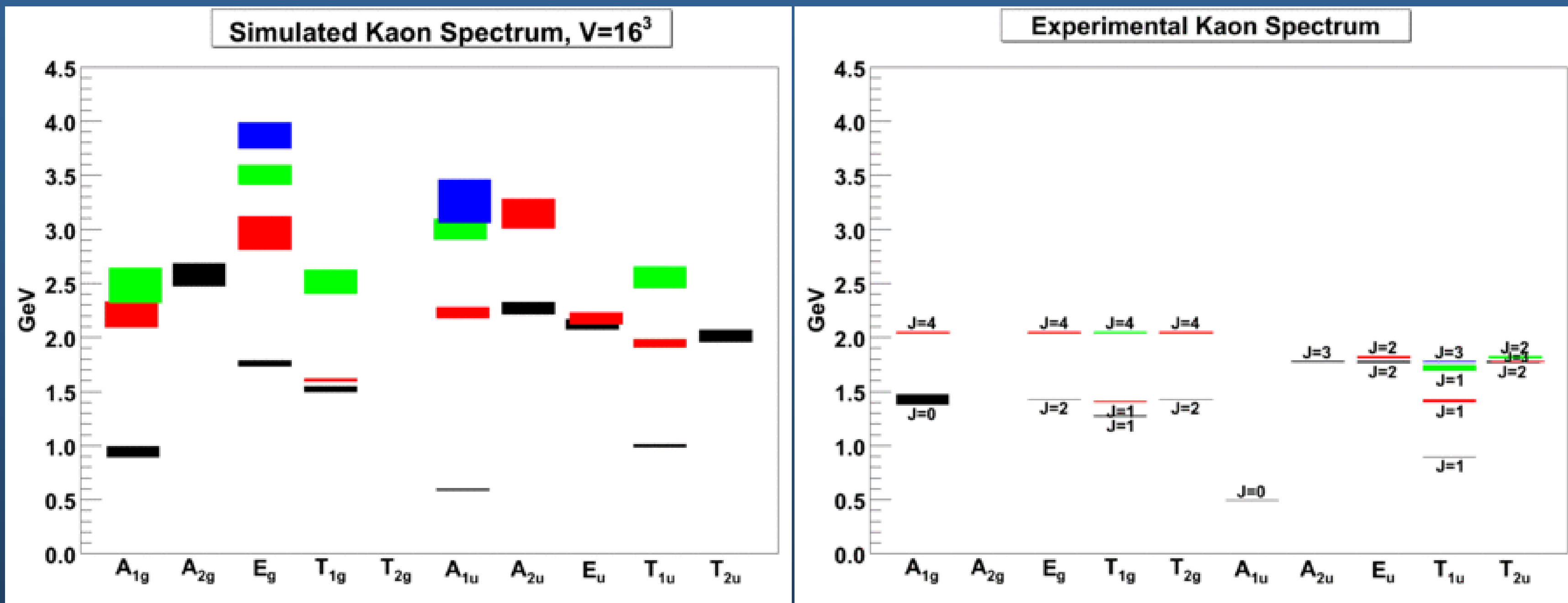
- N_f=2+1 on $16^3 \times 128$ lattice, m_π= 380 MeV (100 configs, 32 eigvecs)



a mesons π mesons

Kaons

- N_f=2+1 on $16^3 \times 128$ lattice, m_π= 380 MeV (100 configs, 32 eigvecs)



Multi-hadron states

- to extract n^{th} level using correlator matrix method, must first extract all levels $0,1,\ldots,n-1$ below it
- as quark mass gets lighter, more and more multi-hadron states lie below the resonance energies of interest
- need multi-hadron operators to reliably extract energies of the multi-hadron states
  - need the quark propagators from all sites on one time slice to all sites on another time slice

Spatial summations

- baryon at rest is operator of form

$$B(\vec{p}=0,t)=\frac{1}{V}\sum_{\vec{x}}\varphi_B(\vec{x},t)$$

- baryon correlator has a double spatial sum

$$\left\langle 0\middle|\overline{B}(\vec{p}=0,t)\ B(\vec{p}=0,0)\middle|0\right\rangle=\frac{1}{V^2}\sum_{\vec{x},\vec{y}}\left\langle 0\middle|\overline{\varphi}_B(\vec{x},t)\ \varphi_B(\vec{y},0)\middle|0\right\rangle$$

- computing all elements of propagators exactly not feasible since Dirac matrix *M* is huge $N_{rows}=N_{columns}=N_xN_yN_zN_t\times N_{spin}\times N_{color}$
  - for $32^3\times 128$ lattice, $N_{\text{rows}} > 50$ million
  - compute solution vectors *x* in $Mx=y$ for handful of source vectors *y*
- translational invariance can limit summation over source site to a single site for local operators

$$\left\langle 0\middle|\overline{B}(\vec{p}=0,t)\ B(\vec{p}=0,0)\middle|0\right\rangle=\frac{1}{V}\sum_{\vec{x}}\left\langle 0\middle|\overline{\varphi}_B(\vec{x},t)\ \varphi_B(0,0)\middle|0\right\rangle$$

Slice-to-slice quark propagators

- good baryon-meson operator of total zero momentum has form

$$B(\vec{p},t)M(-\vec{p},t) = \frac{1}{V^2}\sum_{\vec{x},\vec{y}} \varphi_B(\vec{x},t)\varphi_M(\vec{y},t)e^{i\vec{p}\cdot(\vec{x}-\vec{y})}$$

- cannot limit source to single site for multi-hadron operators
- quark propagator elements from all spatial sites to all spatial sites are needed!
  - resort to stochastic estimations

Stochastic estimation

- quark propagator is just inverse of Dirac matrix M
- noise vectors η satisfying $E(\eta_i)=0$ and $E(\eta_i \eta_j^*)=\delta_{ij}$ are useful for stochastic estimates of inverse of a matrix M
- Z_4 noise is used $\{1, i, -1, -i\}$
- define $X(\eta)=M^{-1}\eta$ then

$$E(X_i \eta_j^*) = E\left(\sum_k M_{ik}^{-1} \eta_k \eta_j^*\right) = \sum_k M_{ik}^{-1} E\left(\eta_k \eta_j^*\right) = \sum_k M_{ik}^{-1} \delta_{kj} = M_{ij}^{-1}$$

- if can solve $M X^{(r)} = \eta^{(r)}$ for each of N_R noise vectors $\eta^{(r)}$ then we have a Monte Carlo estimate of all elements of M^{-1}:

$$M_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} X_i^{(r)} \eta_j^{(r)*}$$

- variances in above estimates usually unacceptably large
- introduce variance reduction using source *dilution*

Source dilution for single matrix inverse

- dilution introduces a complete set of projections:

$$P^{(a)}P^{(b)} = \delta^{ab}P^{(a)}, \qquad \sum_a P^{(a)} = 1, \qquad P^{(a)\dagger} = P^{(a)}$$

- observe that

$$M^{-1}_{ij} = M^{-1}_{ik}\delta_{kj} = \sum_a M^{-1}_{ik}P^{(a)}_{kj} = \sum_a M^{-1}_{ik}P^{(a)}_{kk'}\delta_{k'j'}P^{(a)}_{j'j}$$

$$= \sum_a M^{-1}_{ik}P^{(a)}_{kk'}E\left(\eta_{k'}\eta^*_{j'}\right)P^{(a)}_{j'j} = \sum_a M^{-1}_{ik}E\left(P^{(a)}_{kk'}\eta_{k'}\eta^*_{j'}P^{(a)}_{j'j}\right)$$

- define $\eta^{[a]}_k = P^{(a)}_{kk'}\eta_{k'}, \qquad \eta^{[a]*}_j = \eta^*_{j'}P^{(a)}_{j'j}, \qquad X^{[a]}_k = M^{-1}_{kj}\eta^{[a]}_j$

  so that $$M^{-1}_{ij} = \sum_a E\left(X^{[a]}_i\eta^{[a]*}_j\right)$$

- Monte Carlo estimate is now

$$M^{-1}_{ij} \approx \frac{1}{N_R}\sum_{r=1}^{N_R}\sum_a X^{(r)[a]}_i\eta^{(r)[a]*}_j$$

- $\sum_a \eta^{[a]}_i\eta^{[a]*}_j$ has same expected value as $\eta_i\eta^*_j$, but reduced variance (statistical zeros → exact)

Earlier schemes

- Introduce Z_N noise in color, spin, space, time

$$\eta_{a\alpha}\left(\vec{x},t\right)$$

- Time dilution (particularly effective)

$$P^{(B)}_{a\alpha;b\beta}\left(\vec{x},t;\vec{y},t'\right)=\delta_{ab}\delta_{\alpha\beta}\delta\left(\vec{x},\vec{y}\right)\delta_{Bt}\delta_{Bt'},\qquad B=0,1,\ldots,N_t-1$$

- Spin dilution

$$P^{(B)}_{a\alpha;b\beta}\left(\vec{x},t;\vec{y},t'\right)=\delta_{ab}\delta_{B\alpha}\delta_{B\beta}\delta\left(\vec{x},\vec{y}\right)\delta_{tt'},\qquad B=0,1,2,3$$

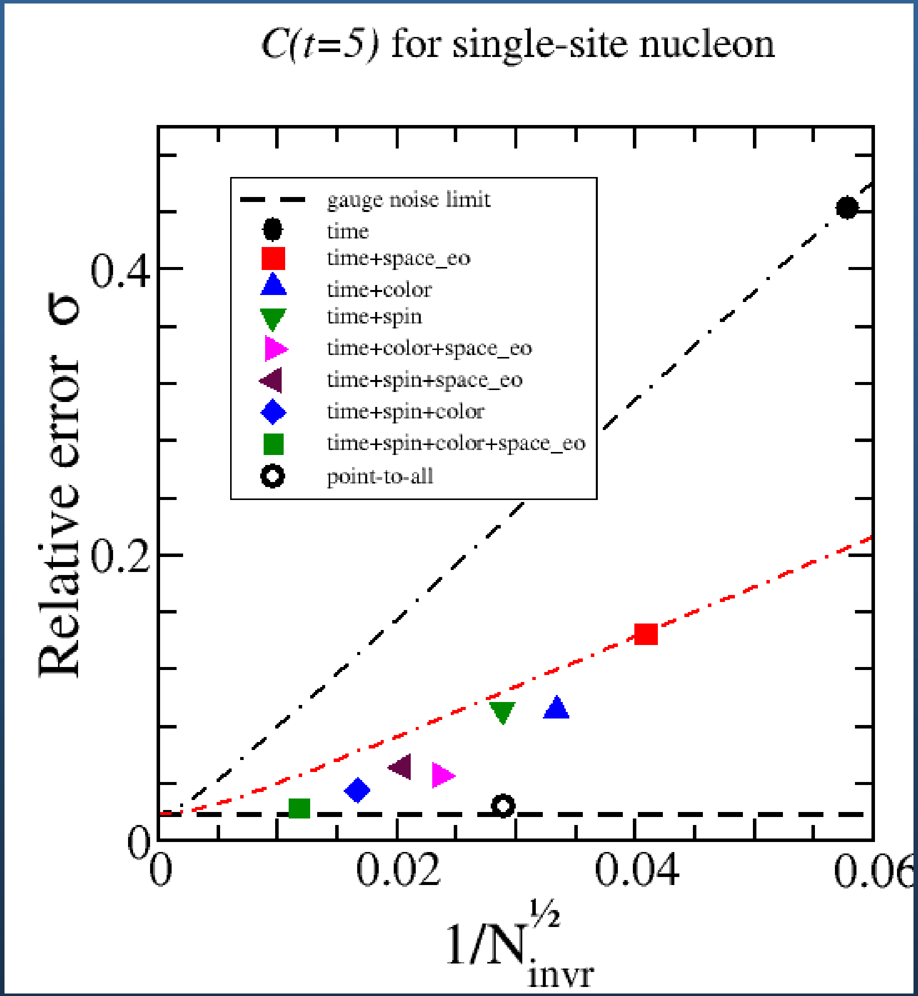
- Color dilution

$$P^{(B)}_{a\alpha;b\beta}\left(\vec{x},t;\vec{y},t'\right)=\delta_{Ba}\delta_{Bb}\delta_{\alpha\beta}\delta\left(\vec{x},\vec{y}\right)\delta_{tt'},\qquad B=0,1,2$$

- Spatial dilutions
  - even-odd

Dilution tests (old method)

- 100 quenched configs, $12^3 \times 48$ anisotropic Wilson lattice



Laplacian Heaviside quark-field smearing

- new quark-field smearing method   PRD80, 054506 (2009)
- judicious choice of quark-field smearing makes exact computations with all-to-all quark propagators possible (on *small* volumes)
- to date, quark field smeared using covariant Laplacian

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

- express in term of eigenvectors/eigenvalues of Laplacian

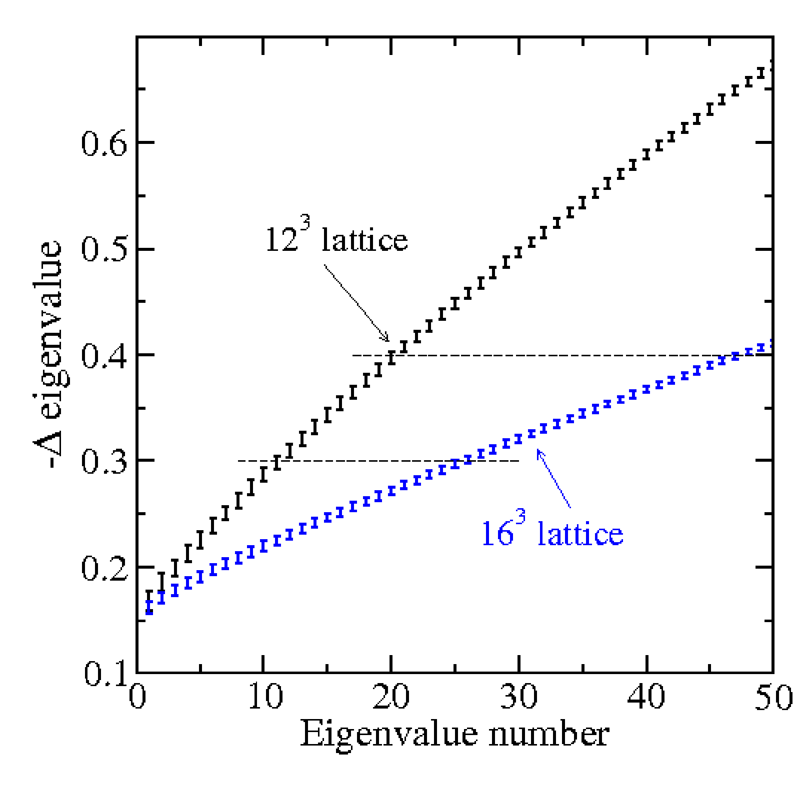
$$\tilde{\psi}(x) = \left(1 + \frac{\sigma_s}{4n_\sigma}\tilde{\Delta}\right)^{n_\sigma} \sum_k |\varphi_k\rangle\langle\varphi_k|\psi(x)$$

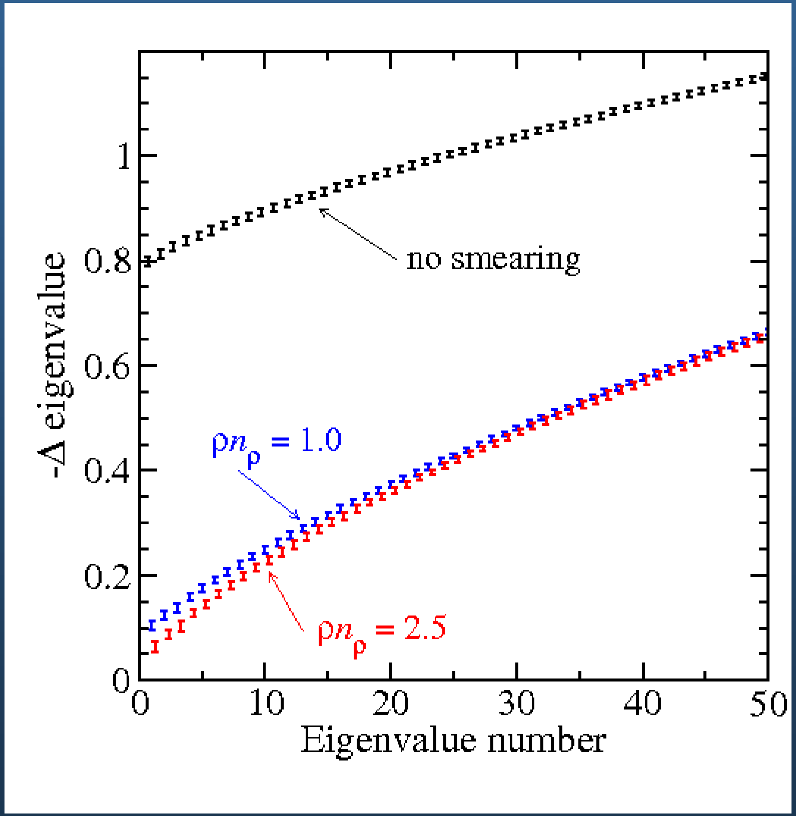
$$= \sum_k \left(1 + \frac{\sigma_s \lambda_k}{4n_\sigma}\right)^{n_\sigma} |\varphi_k\rangle\langle\varphi_k|\psi(x)$$

- truncate sum and set weights to unity → Laplacian Heaviside

Getting to know the Laplacian

- spectrum of the covariant Laplacian
- *left:* dependence on lattice size; *right:* dependence on link smearing





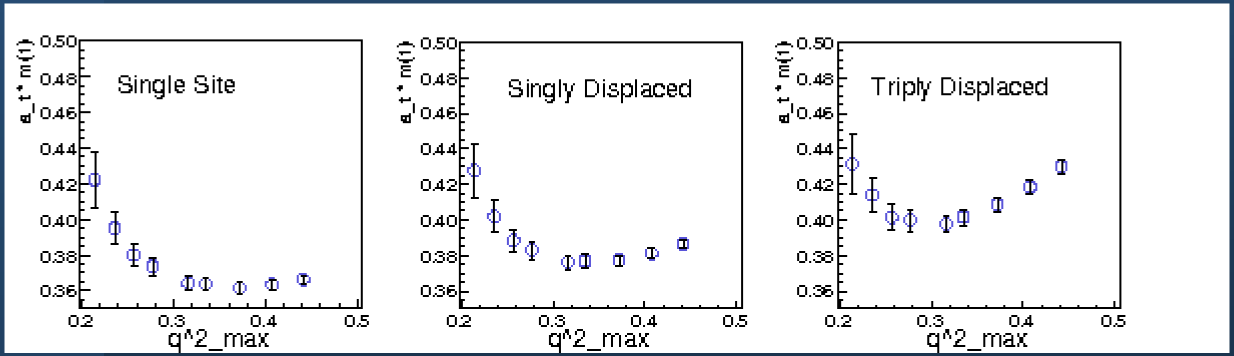
Choosing the smearing cut-off

- Laplacian Heaviside (Laph) quark smearing

$$\tilde{\psi}(x) = \Theta\left(\sigma_s^2 + \tilde{\Delta}\right)\psi(x)$$

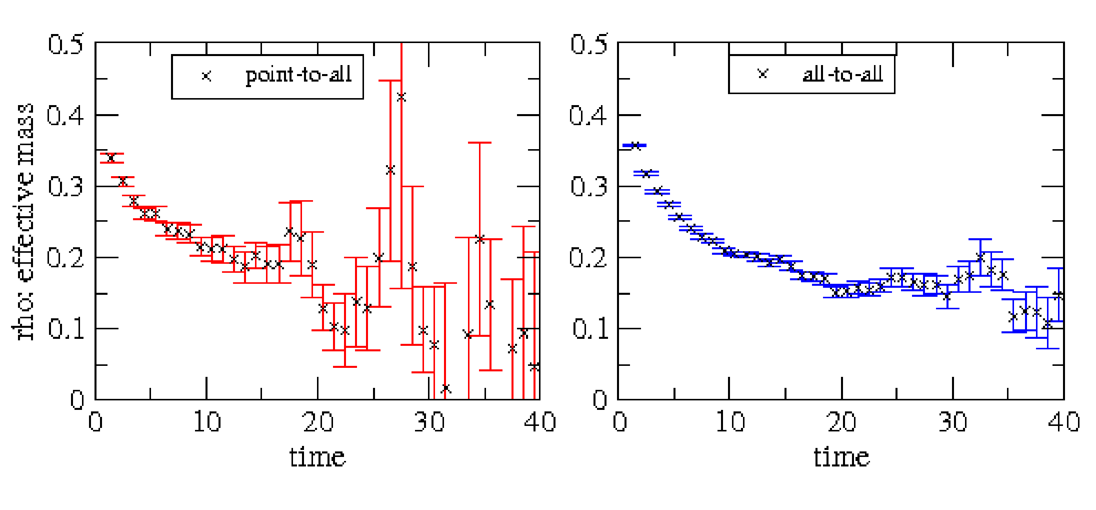
$$\approx \sum_{k=1}^{N_{\max}} |\varphi_k\rangle\langle\varphi_k|\psi(x)$$

- choose smearing cut-off based on minimizing excited-state contamination, keep noise small
  - behavior of nucleon $t=1$ effective masses



Tests of Laplacian Heaviside smearing

- comparison of ρ-meson effective masses using same number of gauge-field configurations



- typically need about 32 modes on 16^3 lattice
- about 128 modes on 24^3 lattice

Stochastic estimation of quark propagators

- new Laph quark smearing method allows exact computation of all-to-all quark propagators on *small* lattices
- *but* number of Laplacian eigenvectors needed becomes prohibitively large on large lattices
  - 128 modes needed on 24^3 lattice
- computational method is rather cumbersome, too
- provides improved variance reduction of stochastic estimation

New stochastic Laph method

- Introduce Z_N noise *in Laph subspace*

$$\rho_{\alpha k}(t) \quad t = \text{time}, \alpha = \text{spin}, k = \text{eigenvector number}$$

- Time dilution (particularly effective)

$$P^{(B)}_{\alpha k;\beta l}\left(t;t'\right) = \delta_{kl}\delta_{\alpha\beta}\delta_{Bt}\delta_{Bt'}, \qquad B = 0,1,\ldots,N_t - 1$$

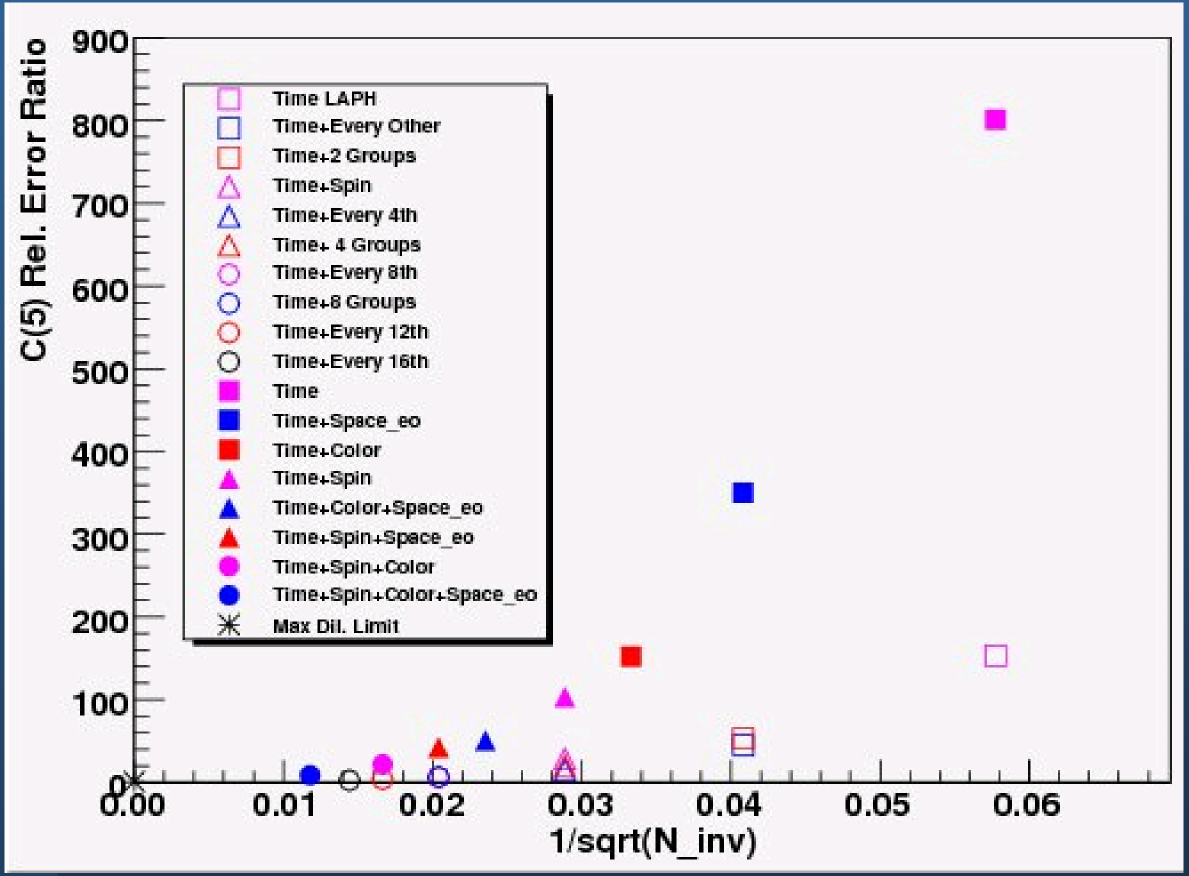
- Spin dilution

$$P^{(B)}_{\alpha k;\beta l}\left(t;t'\right) = \delta_{kl}\delta_{B\alpha}\delta_{B\beta}\delta_{tt'}, \qquad B = 0,1,2,3$$

- Laplacian eigenvector dilution
  - define $P^{(B)}_{\alpha k;\beta l}\left(t;t'\right) = \delta_{Bk}\delta_{Bl}\delta_{\alpha\beta}\delta_{tt'}, \qquad B = 0,1,2,N_{\text{eig}} - 1$
  - group projectors together
    - by blocking
    - as interlaced

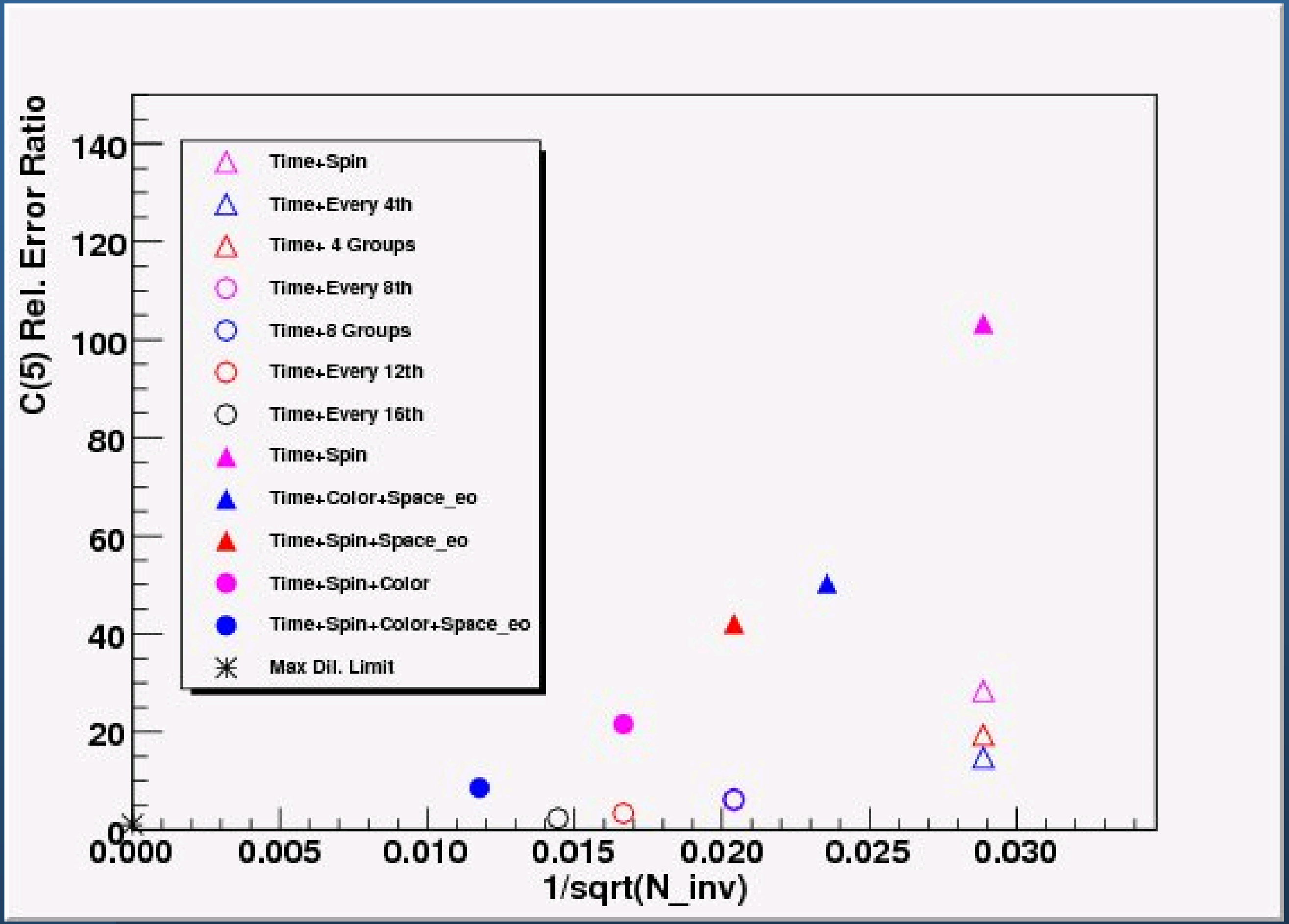
Old stochastic versus new stochastic

- new method (open symbols) has dramatically decreased variance
- test using a triply-displaced-T nucleon operator



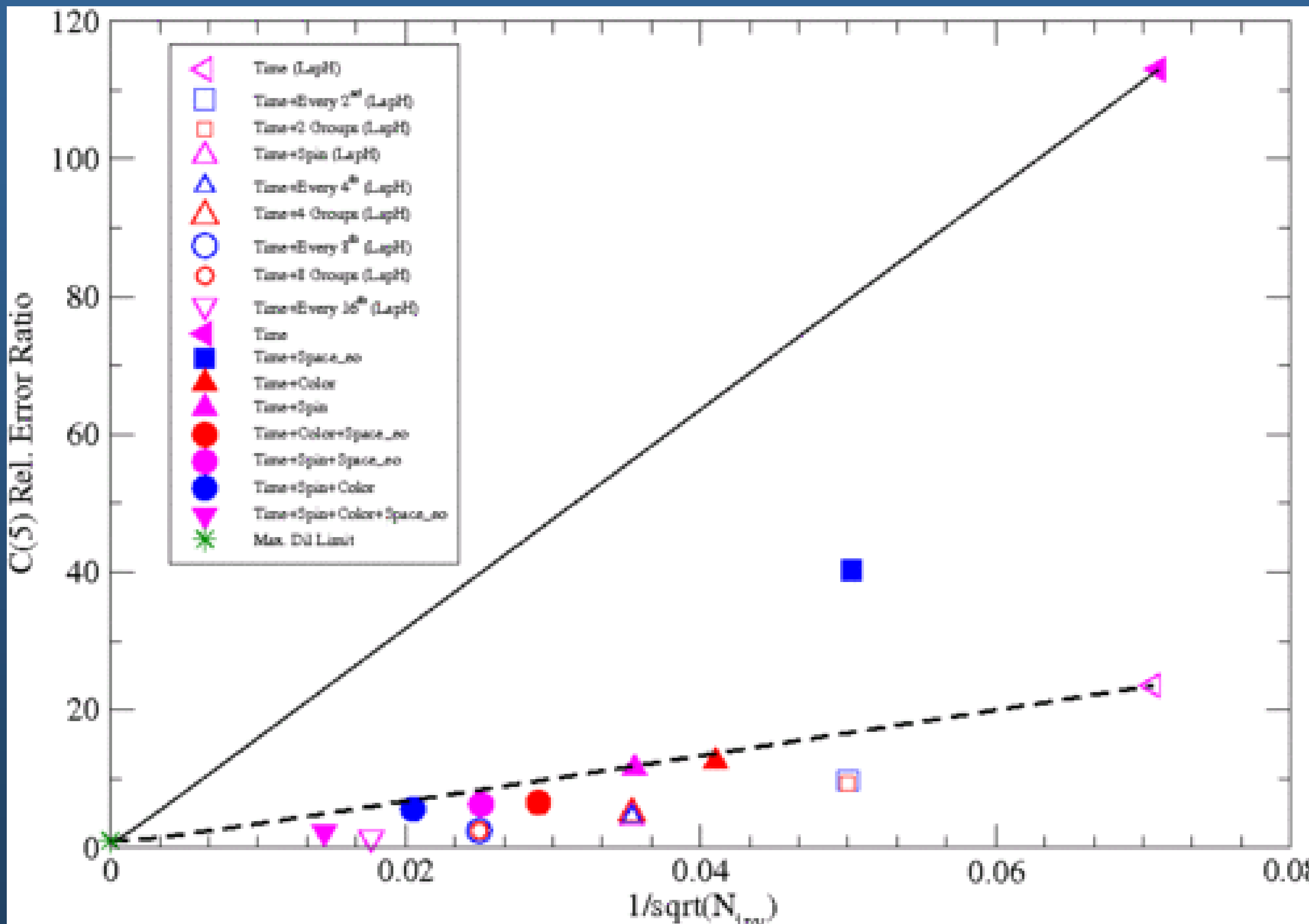
Old stochastic versus new stochastic (zoom in)

- zoom in of triply-displaced-T nucleon plot on last slide



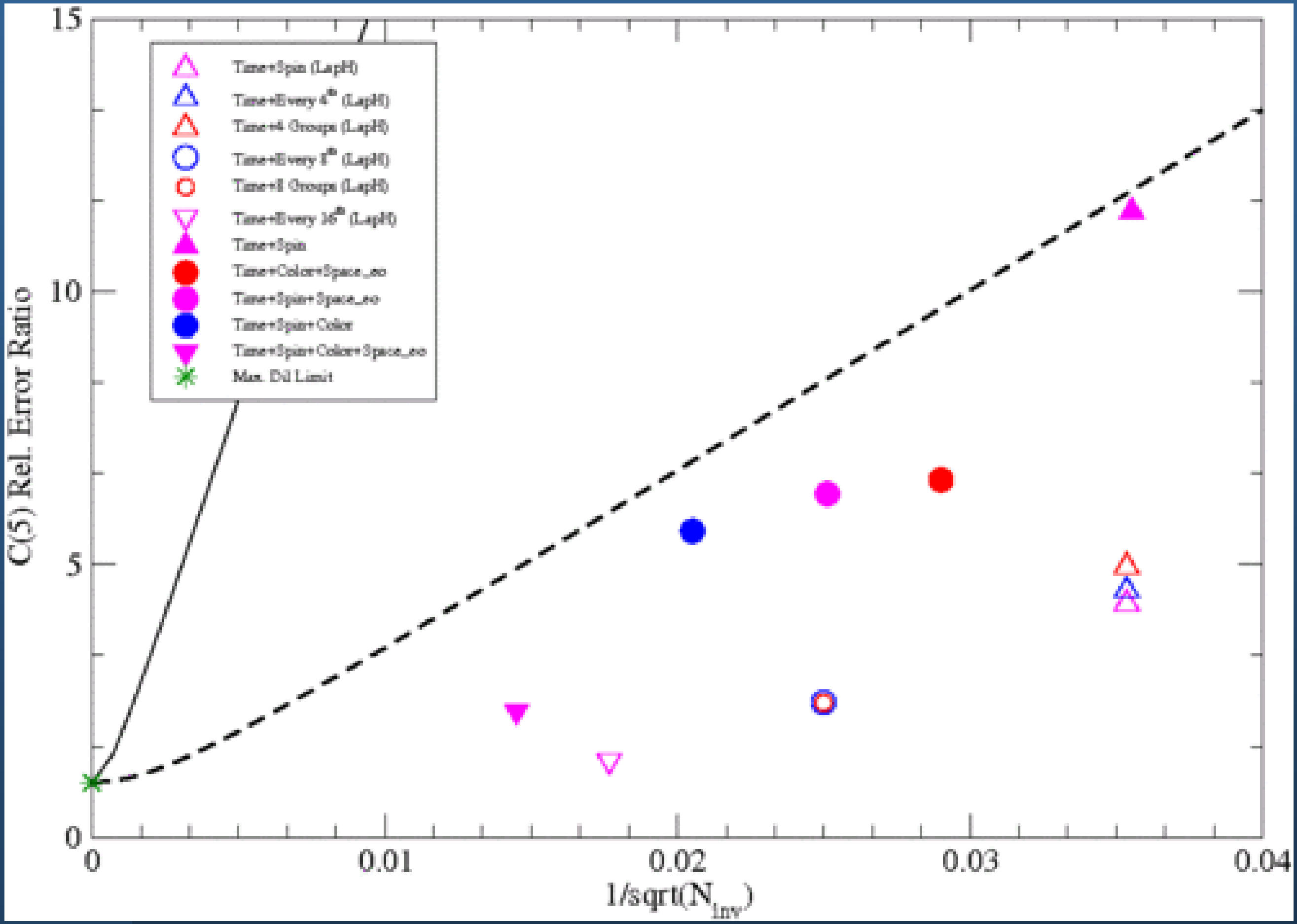
Old stochastic versus new stochastic

- comparison using single-site π operator



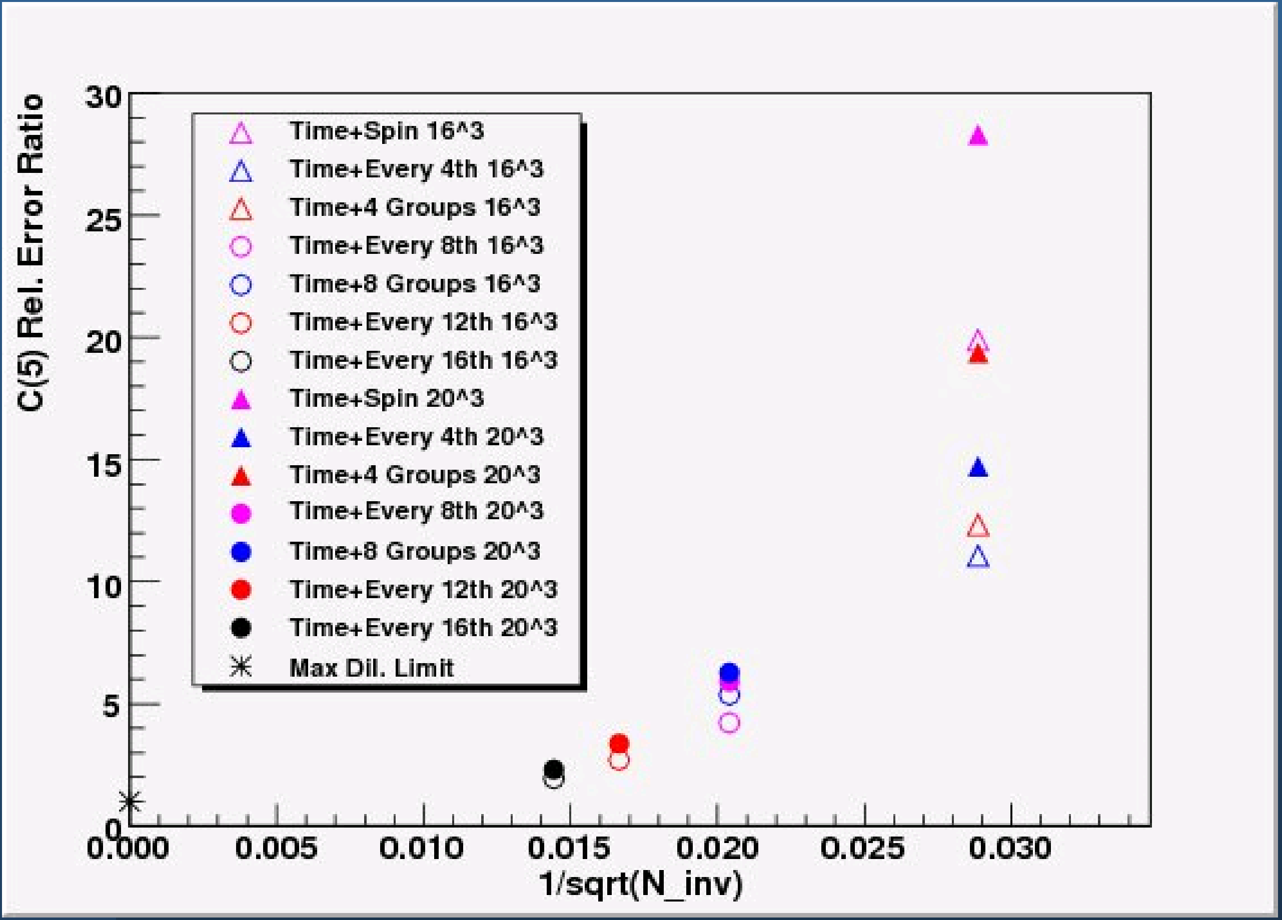
Old stochastic versus new stochastic

- zoom in of π plot on previous slide



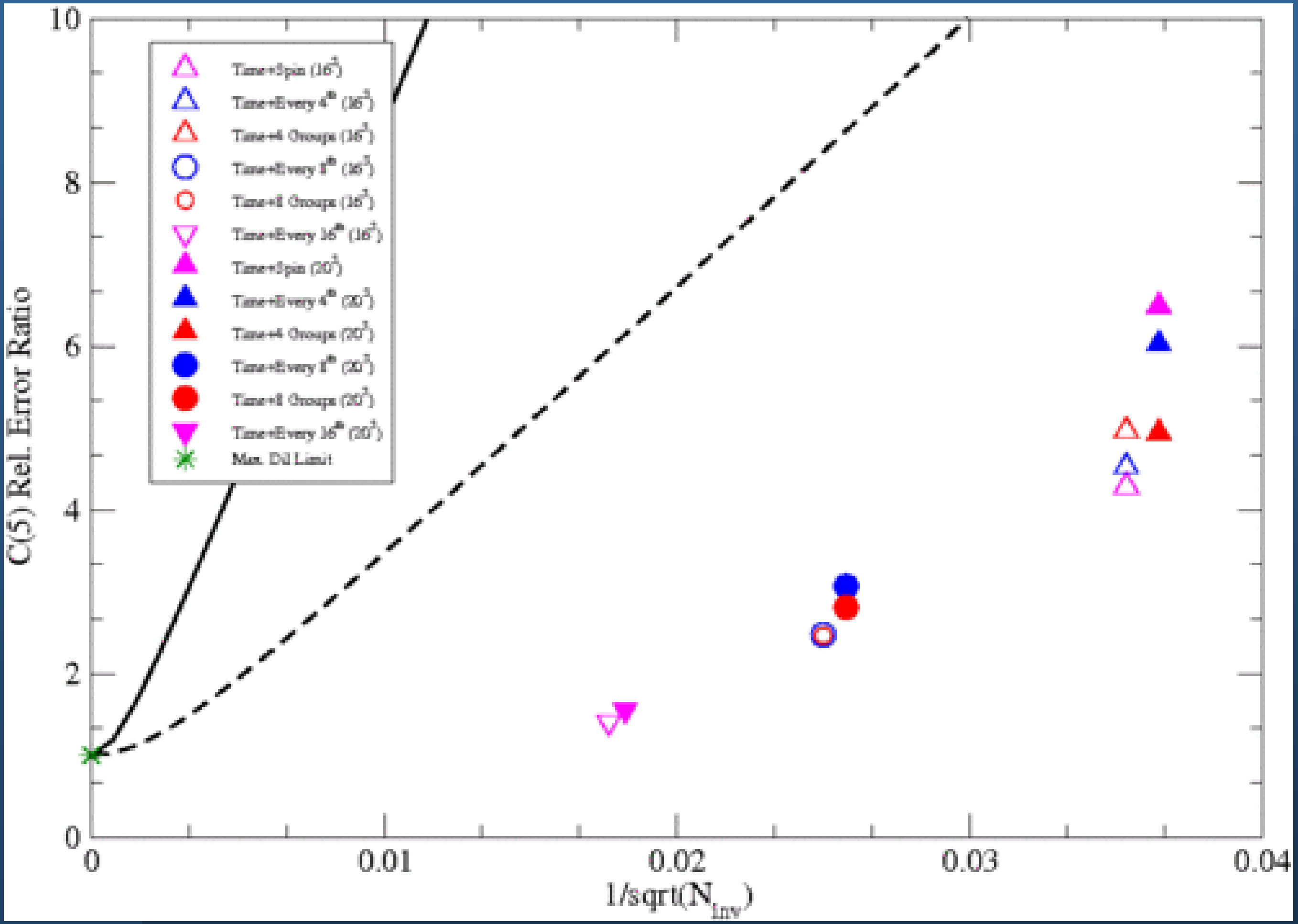
Mild volume dependence

- 16^3 lattice versus 20^3 lattice, both old and new stochastic methods
- test using triply-displaced-T nucleon operator



Mild volume dependence

- zoom in of plot on previous slide



Source-sink factorization

- baryon correlator has form

$$C_{l\bar{l}} = c_{ijk}^{(l)} c_{\bar{i}\bar{j}\bar{k}}^{(\bar{l})*} Q_{i\bar{i}}^{A} Q_{j\bar{j}}^{B} Q_{k\bar{k}}^{C}$$

- stochastic estimates with dilution

$$C_{l\bar{l}} \approx \frac{1}{N_R} \sum_{r} \sum_{d_A d_B d_C} c_{ijk}^{(l)} c_{\bar{i}\bar{j}\bar{k}}^{(\bar{l})*} \left(\varphi_i^{(Ar)[d_A]} \eta_{\bar{i}}^{(Ar)[d_A]*} \right)$$

$$\times \left(\varphi_j^{(Br)[d_B]} \eta_{\bar{j}}^{(Br)[d_B]*} \right) \left(\varphi_k^{(Cr)[d_C]} \eta_{\bar{k}}^{(Cr)[d_C]*} \right)$$

- define

$$\Gamma_l^{(r)[d_A d_B d_C]} = c_{ijk}^{(l)} \varphi_i^{(Ar)[d_A]} \varphi_j^{(Br)[d_B]} \varphi_k^{(Cr)[d_C]}$$

$$\Omega_l^{(r)[d_A d_B d_C]} = c_{ijk}^{(l)} \eta_i^{(Ar)[d_A]} \eta_j^{(Br)[d_B]} \eta_k^{(Cr)[d_C]}$$

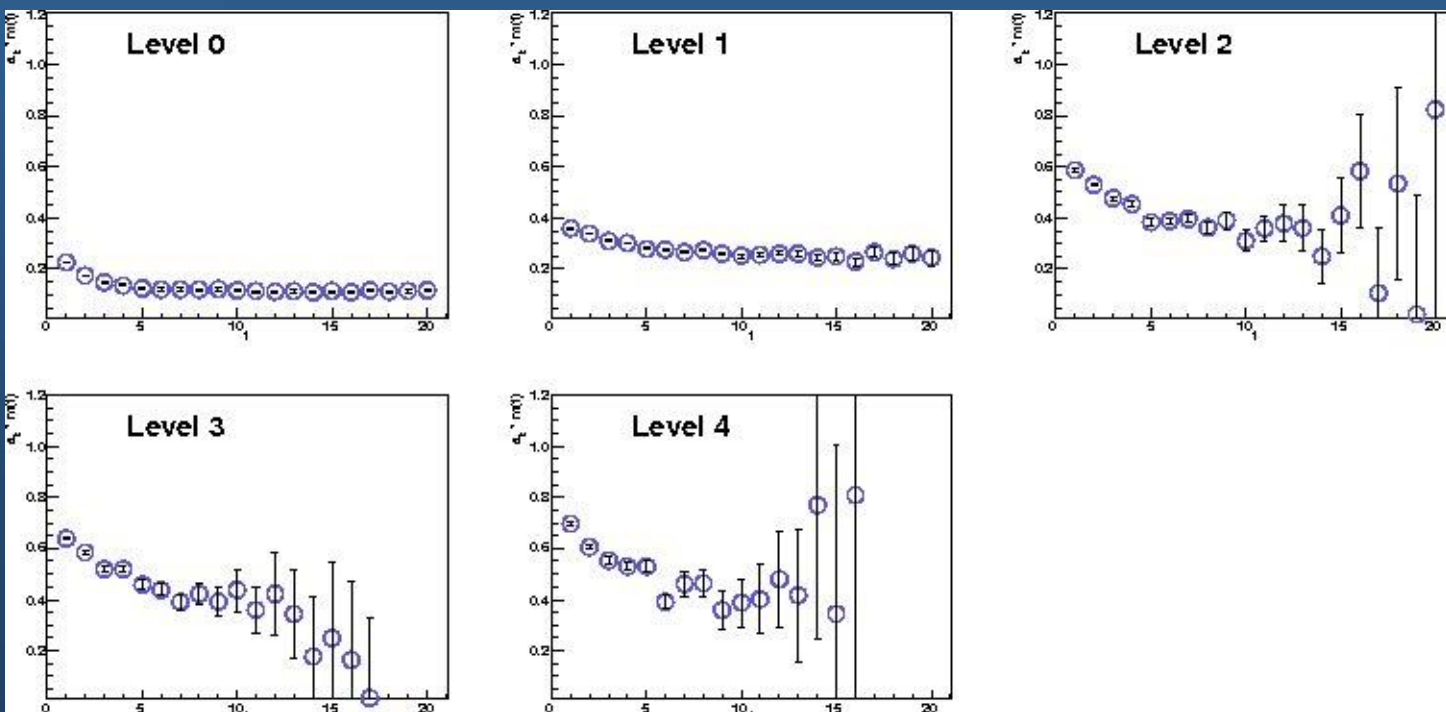
- correlator becomes dot product of source vector with sink vector

$$C_{l\bar{l}} \approx \frac{1}{N_R} \sum_{r} \sum_{d_A d_B d_C} \Gamma_l^{(r)[d_A d_B d_C]} \Omega_{\bar{l}}^{(r)[d_A d_B d_C]*}$$

- store *ABC* permutations to handle Wick orderings

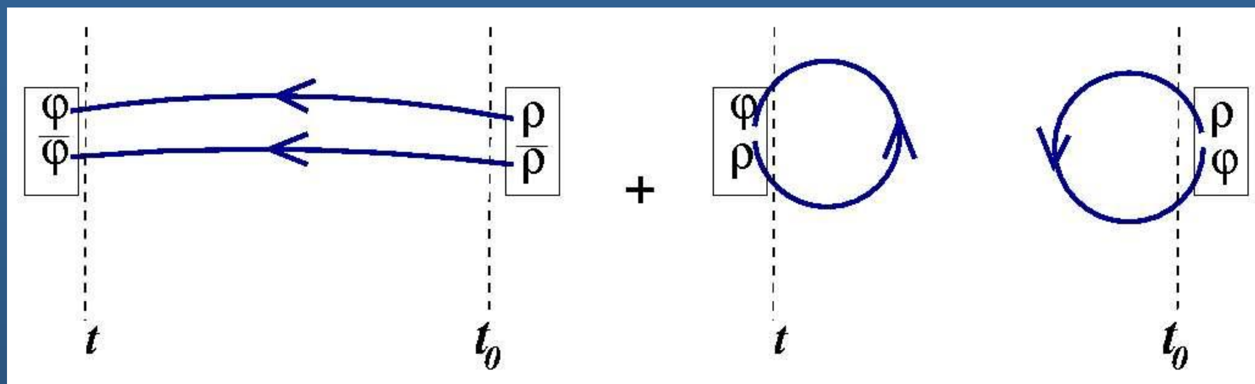
Moving π and *a* mesons

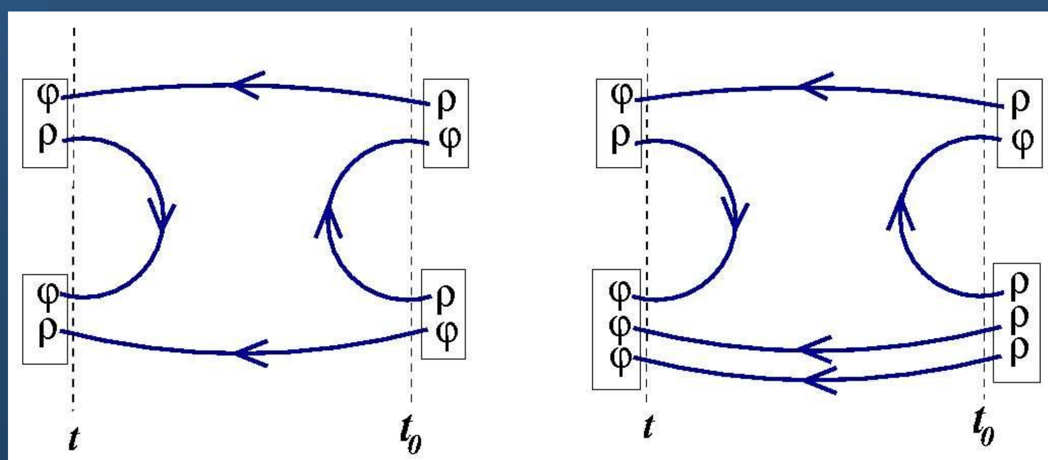
- first step towards including multi-hadron operators:
  - moving single hadrons
  - results below have one unit of on-axis momentum
  - projections onto space group irreps (see J. Foley talk)



Same-time quark lines

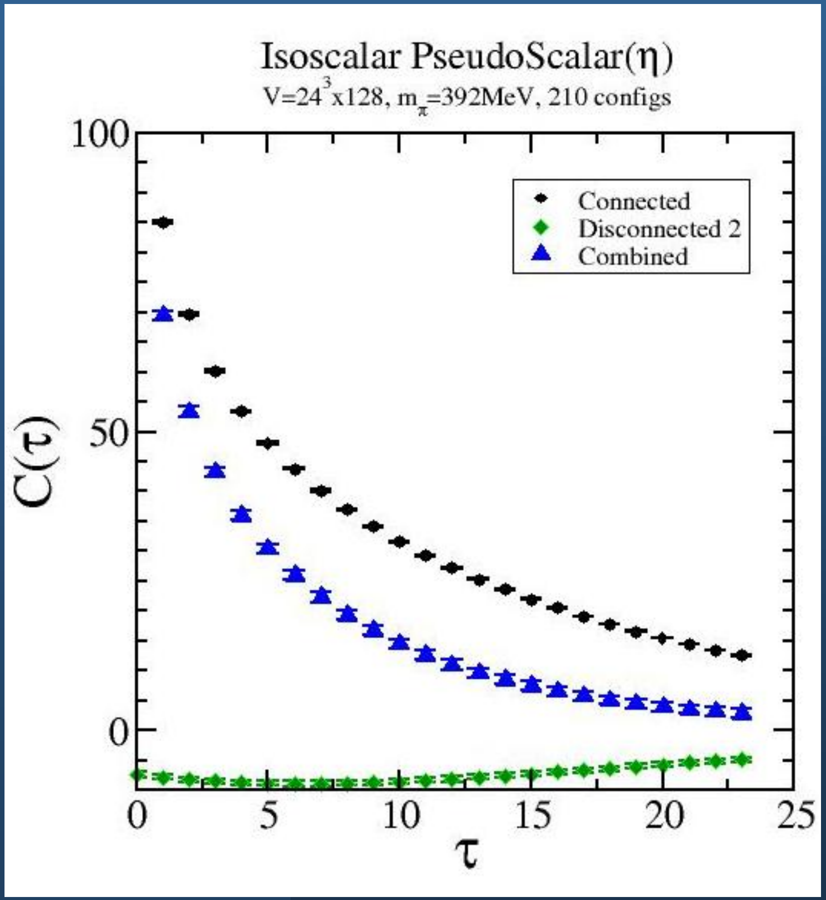
- Last step to finite-box spectra: same time *t*-to-*t* quark lines

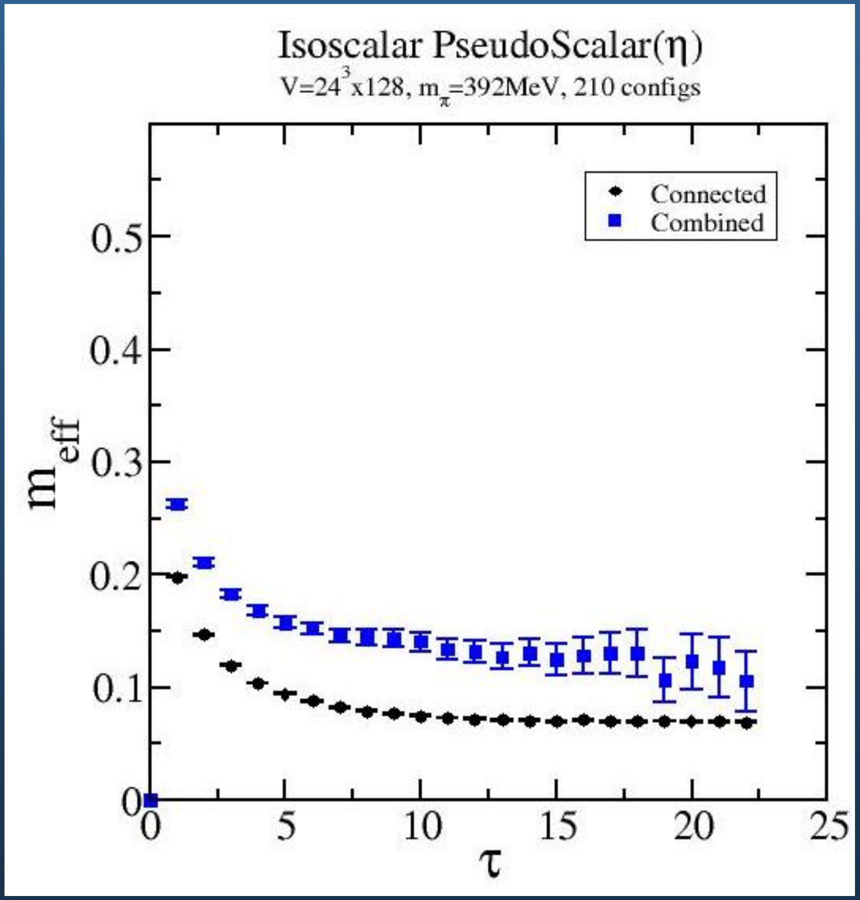




First results with t-to-t diagrams

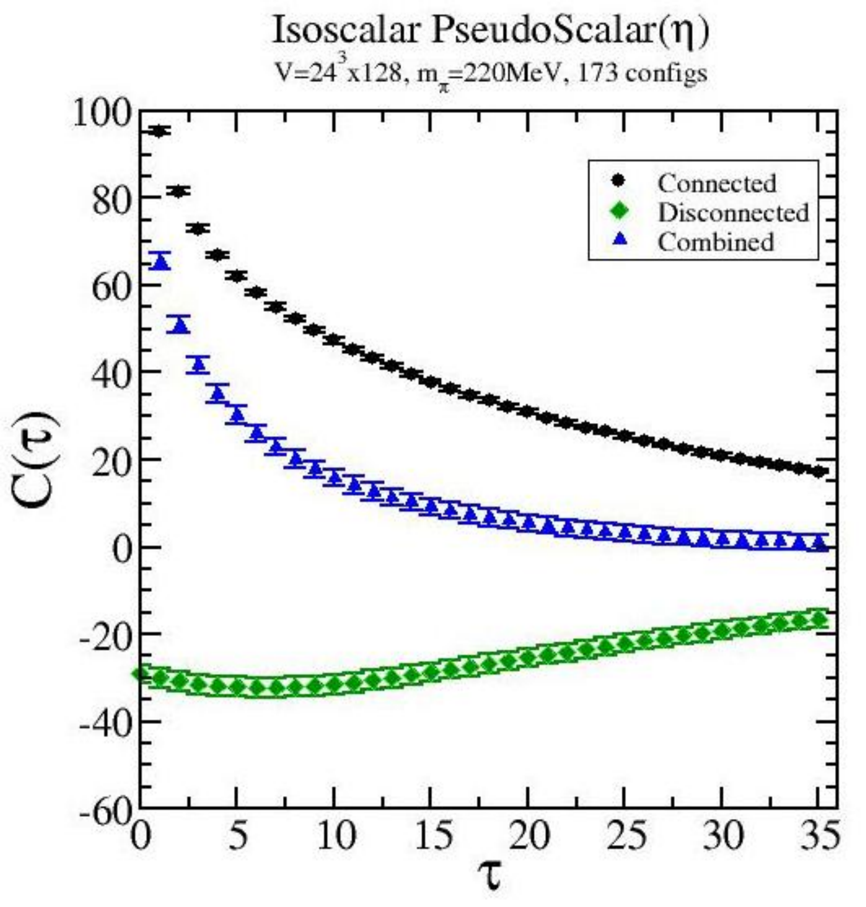
- $24^3 \times 128$ lattice: dilution schemes (TF,SF,LI8) (TI16,SF,LI8)
- 112 eigenvectors, local operators only

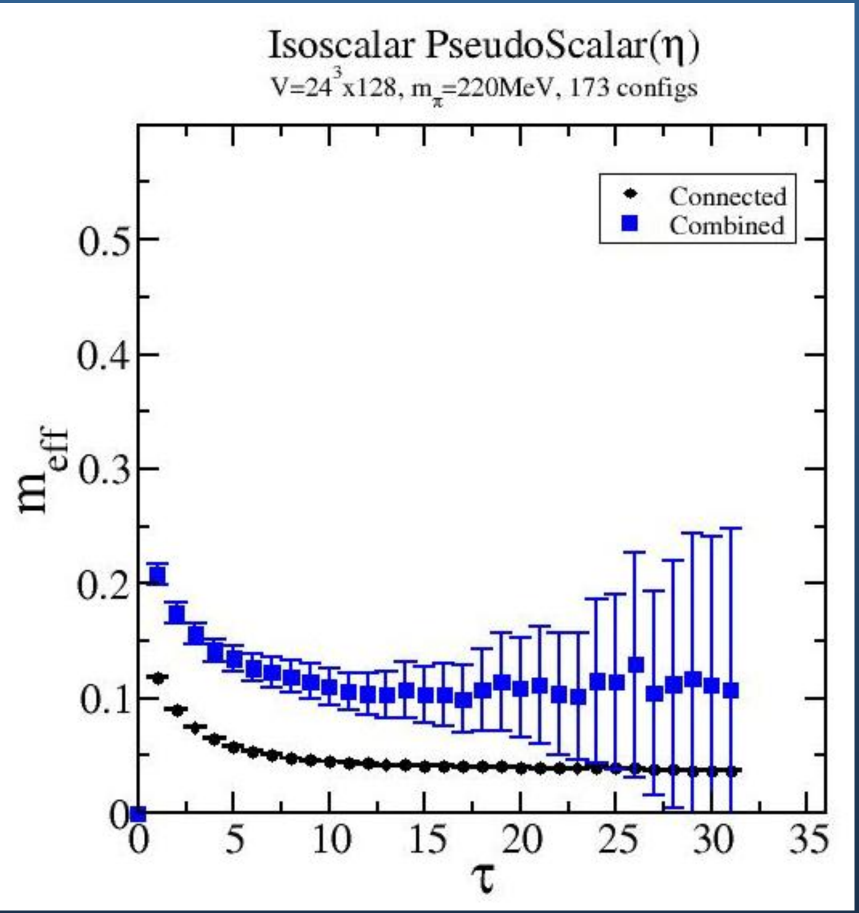




Results at lighter pion mass

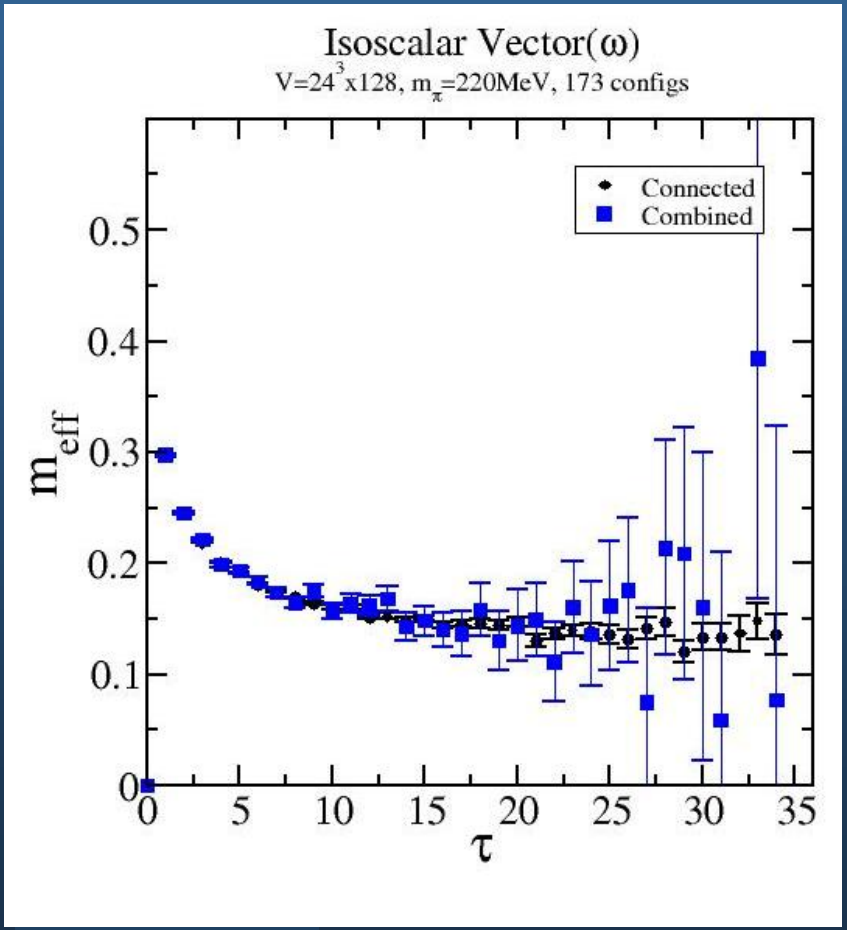
- 24^3x128 lattice: dilution schemes (TF,SF,LI8) (TI16,SF,LI8)
- 112 eigenvectors, local operators only

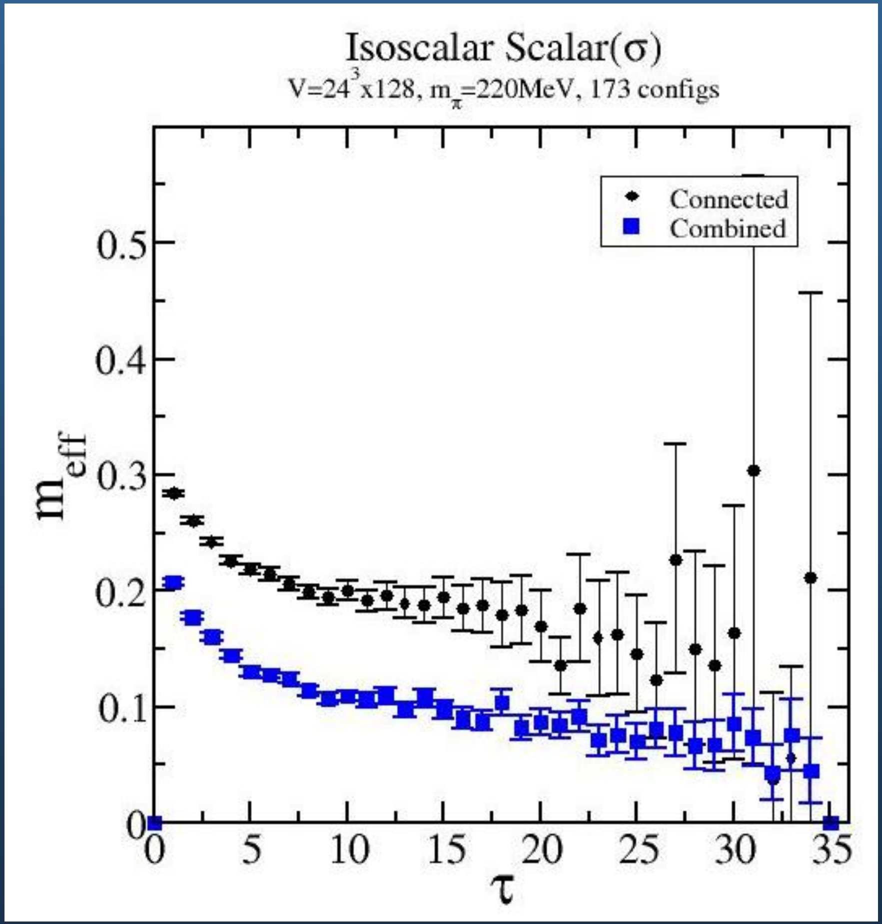




Results at lighter pion mass (cont'd)

- 24^3x128 lattice: dilution schemes (TF,SF,LI8) (TI16,SF,LI8)
- 112 eigenvectors, local operators only





Summary

- goal → to wring out hadron spectrum from QCD Lagrangian using Monte Carlo methods on a space-time lattice
  - stationary state energies in cubic box
- good single hadron operator selected in nearly all baryon and meson channels
- must extract all states lying below a state of interest
  - as pion get lighter, more and more multi-hadron states
- multi-hadron operators → relative momenta
  - need for slice-to-slice quark propagators
- new stochastic Laph method → dramatically reduced variances
- currently running two pion tests