Extending the Feynman-Hellmann Method to Arbitrary Matrix Elements

Lattice 2018: Michigan State University

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Feynman-Hellmann Theorem

- The Feynman-Hellman Theorem connects matrix elements to variations in the spectrum.

$$\begin{aligned} \frac{\partial E_n}{\partial \lambda} &= < n|H_\lambda|n > \\ H &= H_0 + \lambda H_\lambda \end{aligned}$$

- Nucl. Phys. B293 (Maina, et al., 1987)
- PLB227 (Güsken et al., 1989)
- JHEP 1201 (Bulava et al., 2012)
- PLB718 (de Divitiis et al., 2012)
- PRD90, PRD92 (Chambers et al., 2014, 2015)
- PRL199 (Savage et al., 2017)
- Phys. Rev. D 96, 014504 (C. Bouchard et al., 2017)

Feynman-Hellmann Theorem

- Consider a two-point correlation function in the presence of an external field

$$
\begin{aligned}
C_\lambda(t) &= < \lambda|\mathcal{O}(t)\mathcal{O}^\dagger(0)|\lambda > \\
&= \frac{1}{\mathcal{Z}_\lambda}\int \mathcal{D}\psi\mathcal{D}\bar{\psi}\mathcal{D}A_\mu e^{-(S+S_\lambda)}\mathcal{O}(t)\mathcal{O}(0) \\
S_\lambda &= \lambda\int d^4x j_\mu(x) \\
\lambda j_\mu(x) &= \bar{q}(x)\gamma_\mu\gamma_5 q(x)
\end{aligned}
$$

Feynman-Hellmann Theorem

- If we differentiate $C_\lambda(t)$ with respect to λ, we find

$$\frac{\partial C_\lambda(t)}{\partial \lambda} = -\left[\frac{\partial_\lambda \mathcal{Z}_\lambda}{\mathcal{Z}_\lambda} C_\lambda(t) + \frac{1}{\mathcal{Z}_\lambda}\int \mathcal{D}\psi\mathcal{D}\bar{\psi}\mathcal{D}A_\mu e^{-(S+S_\lambda)} \int d^4x' j(x')\mathcal{O}(t)\mathcal{O}(0)\right]$$

- Setting λ to zero, we obtain

$$\frac{\partial C_\lambda(t)}{\partial \lambda}|_{\lambda=0} = C_\lambda(t)\int d^4x' < \Omega|j(x')|\Omega > - \int dt' < \Omega|T\left[\mathcal{O}(t)J(t')\mathcal{O}(0)\right]|\Omega >$$

$$J(t') = \int d^3x' \; j(t', \vec{x}')$$

- The first term is a vacuum matrix element and the second term contains the matrix element of interest.

Feynman-Hellmann Theorem

- For a standard two-point correlation function, one constructs an effective mass which plateaus to the ground-state energy.

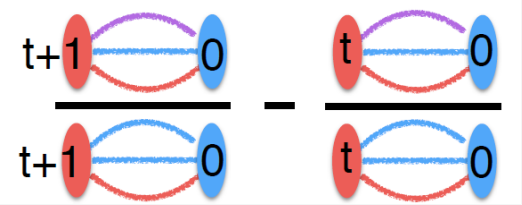
$$m_{eff}(t,\tau) = \frac{1}{\tau}\ln\left[\frac{C(t)}{C(t+\tau)}\right] \xrightarrow[t\to\infty]{} \frac{1}{\tau}\ln e^{E_0\tau}$$

- The lattice manifestation of the Feynman-Hellmann theorem behaves similarly.

$$\frac{\partial E_n}{\partial \lambda} = < n|H_\lambda|n >$$

$$\frac{\partial m_{eff}(t,\tau)}{\partial \lambda}|_{\lambda=0} = \frac{1}{\tau}\left[\frac{-\partial_\lambda C_\lambda(t+\tau)}{C(t+\tau)} - \frac{-\partial_\lambda C_\lambda(t)}{C(t)}\right] \xrightarrow[t\to\infty]{} \frac{J_{00}}{2E_0}$$

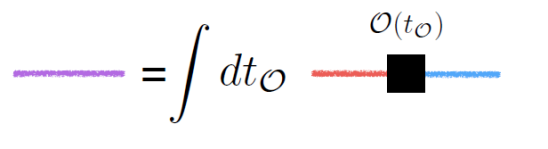
- Since there is a subtraction of two terms, even for currents that couple to the vacuum, disconnected contributions exactly cancel.



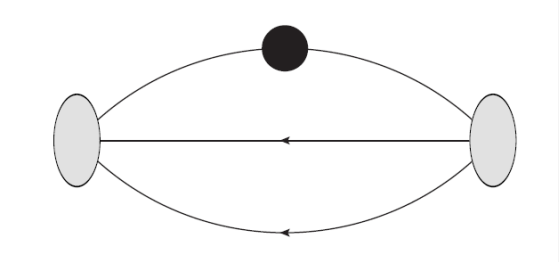
Numerical Implementation

- This is done in practice by computing S_Γ.

$$\mathrm{S}_\Gamma = \sum_z S(y,z)\Gamma(z)S(z,x)$$

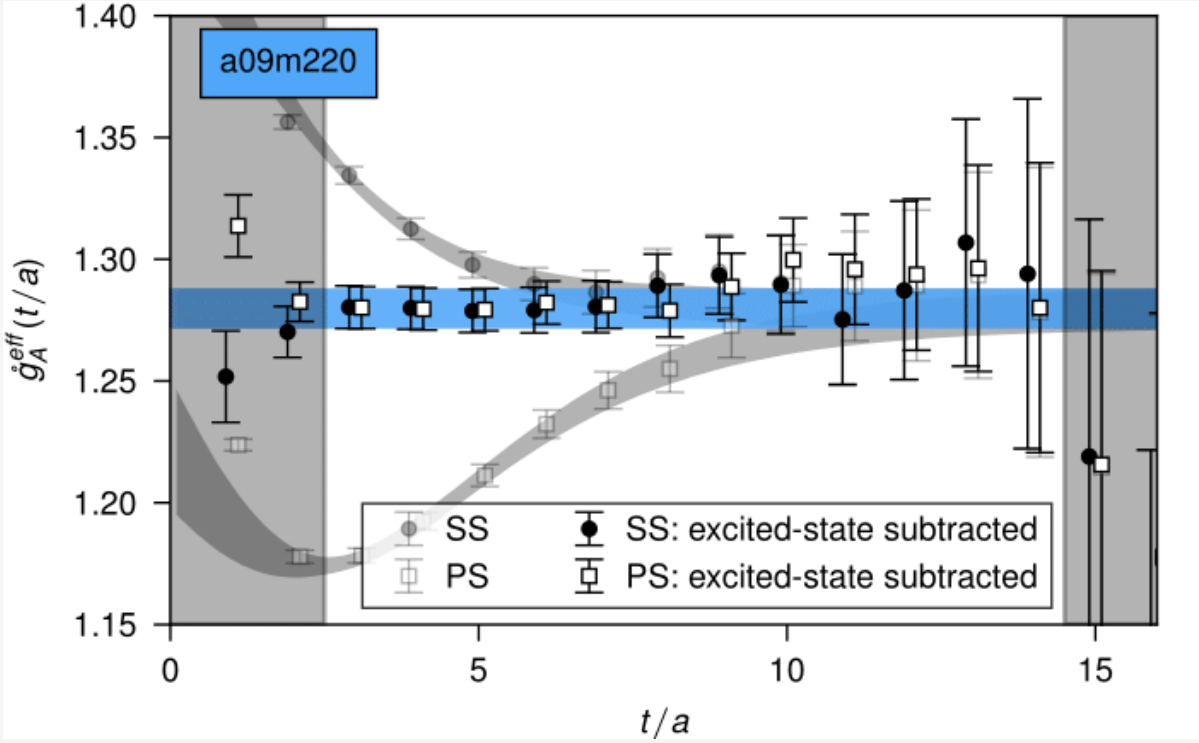


- $S(z,x)$ is the standard propagator.
- $\Gamma(z)$ is the bilinear current-insertion.
- $\Gamma(z)S(z,x)$ acts as a new source, "inverting off" it gives S_Γ.
- S_Γ intercepts normal quarks in a two-point correlation function to give $\partial_\lambda C_\lambda(t)$.



Results from Nature 558, pages 91–94 (2018)

- This method was used to compute the nucleon axial coupling at percent-level.
- Below is the fitted ground-state matrix element from the derivative effective mass.



Strengths/Weaknesses of this Method

- Advantages:
  1. Only one time variable - systematics easy to control.
  2. This method gives all timeslices at the cost of a single source-sink separation.
  3. S_Γ is reusable for any hadronic matrix element.
- Disadvantages:
  1. The current is summed everywhere, including outside of the hadron and at the source/sink (contact regions), this can complicate the analysis.
  2. Lose option to track explicit time dependence of current insertion.
  3. Each Γ operator and momentum-transfer requires a different S_Γ propagator.

Stochastic Feynman-Hellman

- Insert outer product of noise vectors that obey $< \eta(i)\eta^*(j) > = \delta_{ij}$ - "stochastic identity".
- Factorizes method so different matrix elements and momentum-transfer points are computed without re-inverting.
- |χ>is one spin/color component of the source (a vector).
- |ψ>is the corresponding propagator component.

$$D|\psi >= |\chi >$$

$$|\psi >= D^{-1}|\chi >$$

$$|\phi >= D^{-1}\Gamma e^{iq\cdot x}|\psi >$$

$$|\phi' >= \frac{1}{N}\sum_{i=1}^{N} D^{-1}|\eta >< \eta|\Gamma e^{iq\cdot x}|\psi >$$

- |ϕ>is a spin/color component of S_Γ.

What Type of Basis to Use?

- Many choices of basis and variance reduction techniques have been developed to estimate the all-to-all propagator: Z2/Z4, dilution, eigenvalue deflation, hierarchical probing, singular value deflation, etc
- Commun. Statist. Simula., 19 (Hutchinson, 1990)
- Phys. Lett., B328:130–136 (K. F. Liu et al, 1994)
- Phys.Rev.D64:114509,2001 (H. Neff, et al, 2001)
- Comput.Phys.Commun.172:145-162,2005 (Foley, et al, 2005)
- PoSLAT2007:139,2007 (Babich, et al, 2007)
- Phys.Rev. D83 114505 (C. Morningstar et al, 2011)
- SIAM J. Sci. Comput., 35(5), S299–S322 (A. Stathopoulos et al, 2013)
- Comput. Phys. Commun. 195, 35 (Endress et al, 2015)
- SIAM J. Sci. Comput., 39(2), A532 to A558 (A. S. Gambhir et al, 2017)

Hierarchical Probing

- Classical probing (CP) takes advantage of decay in $D_{i,j}^{-1}$ by discovering structure.
- Dilution: probing based on known structure (red black, spin/color, or timeslice).
- Hierarchical probing (HP) uses nested coloring to approximate CP; quadratures may be reused.
- HP basis described by reordered Hadamard matrix for lattices of power 2.
- Simple toy model:
  - $$\begin{matrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{matrix}$$

CP

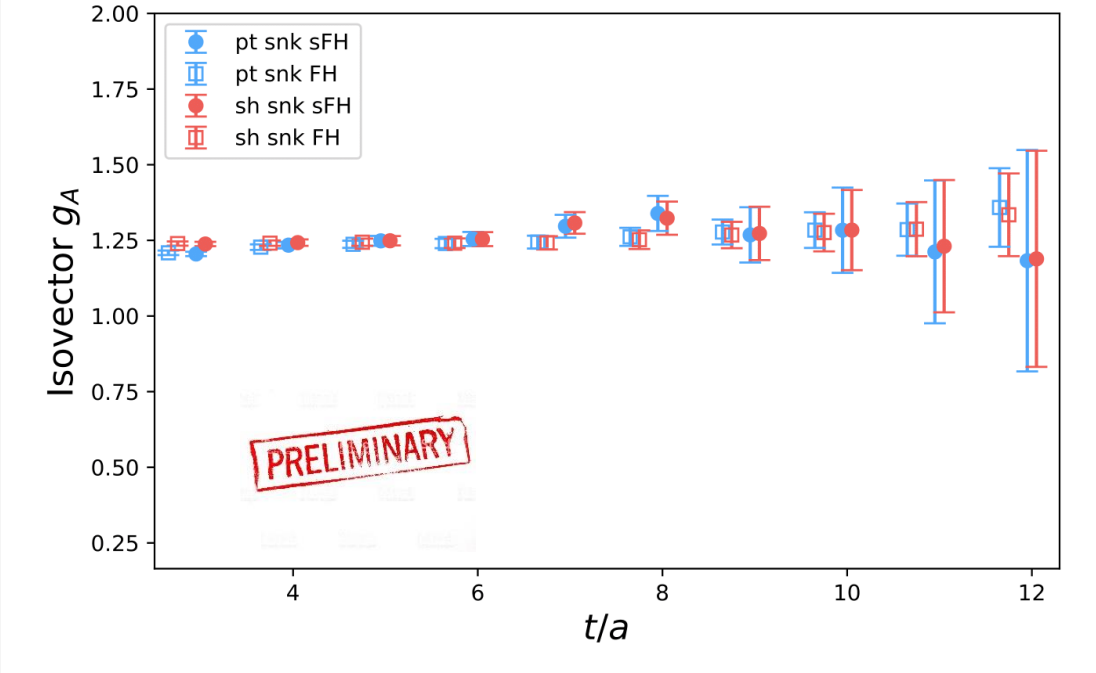
$$\eta_j = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \qquad \eta_j = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

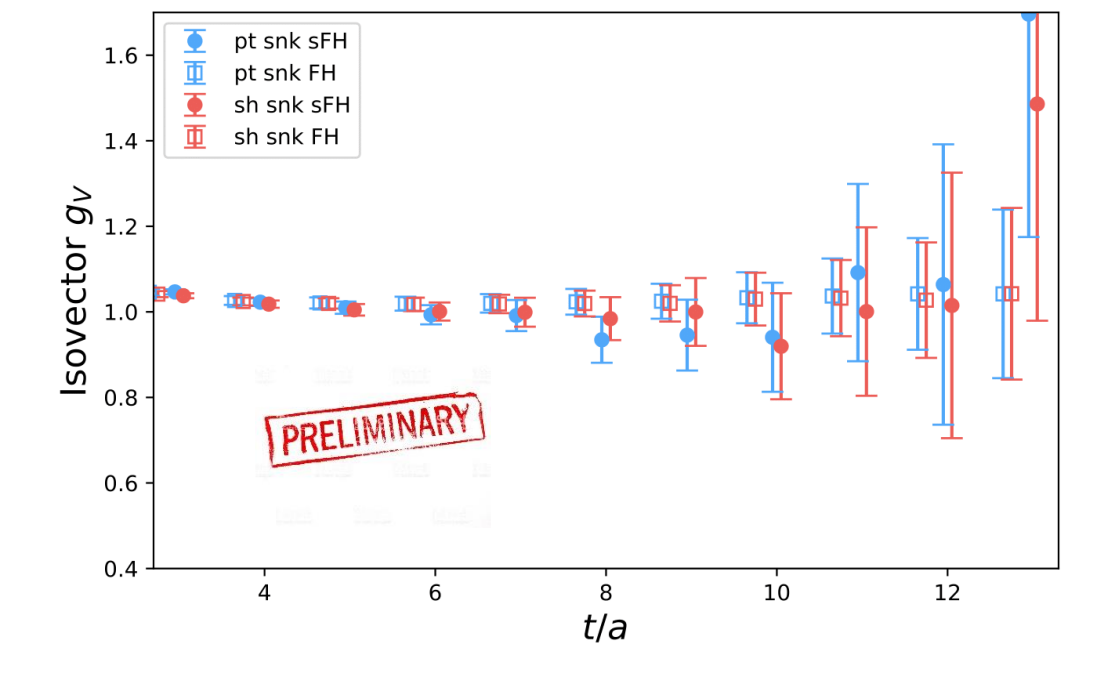
HP

$$\eta_j = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} \qquad \eta_j = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$$

Comparison with Exact Method

- Möbius Domain Wall on HISQ
- $a = .12\ fm$ $m_\pi = 310\ MeV$ $m_\pi L = 4.5$
- ~1000 configurations 8 sources 32 "HP Propagators"





Tensor Charge

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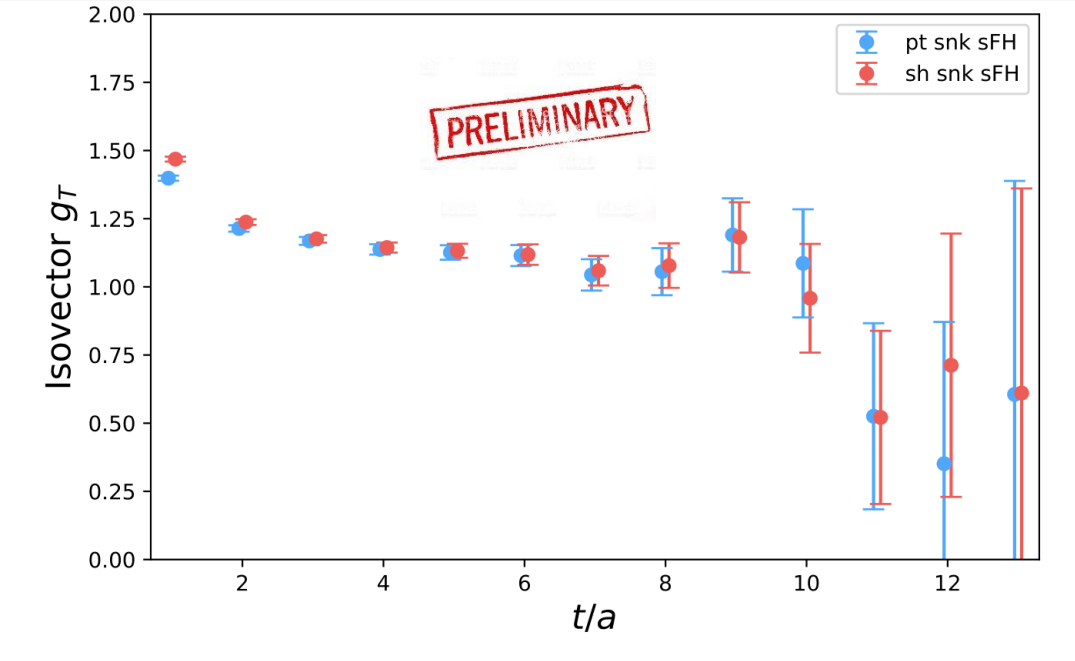

Q^2=.18 GeV^2

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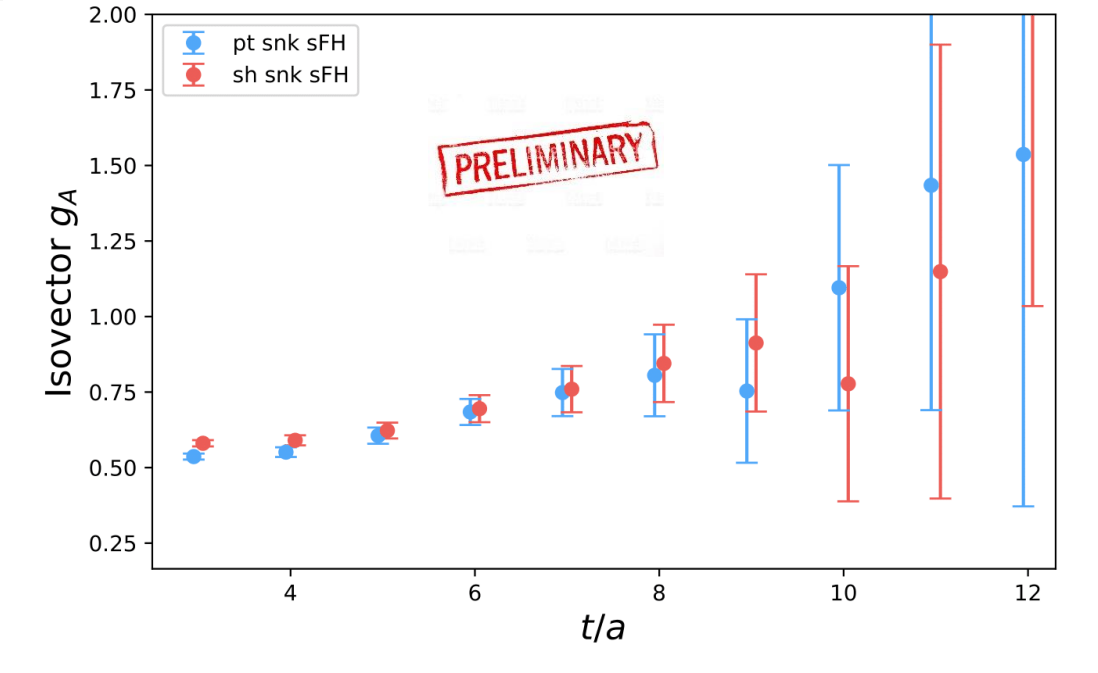
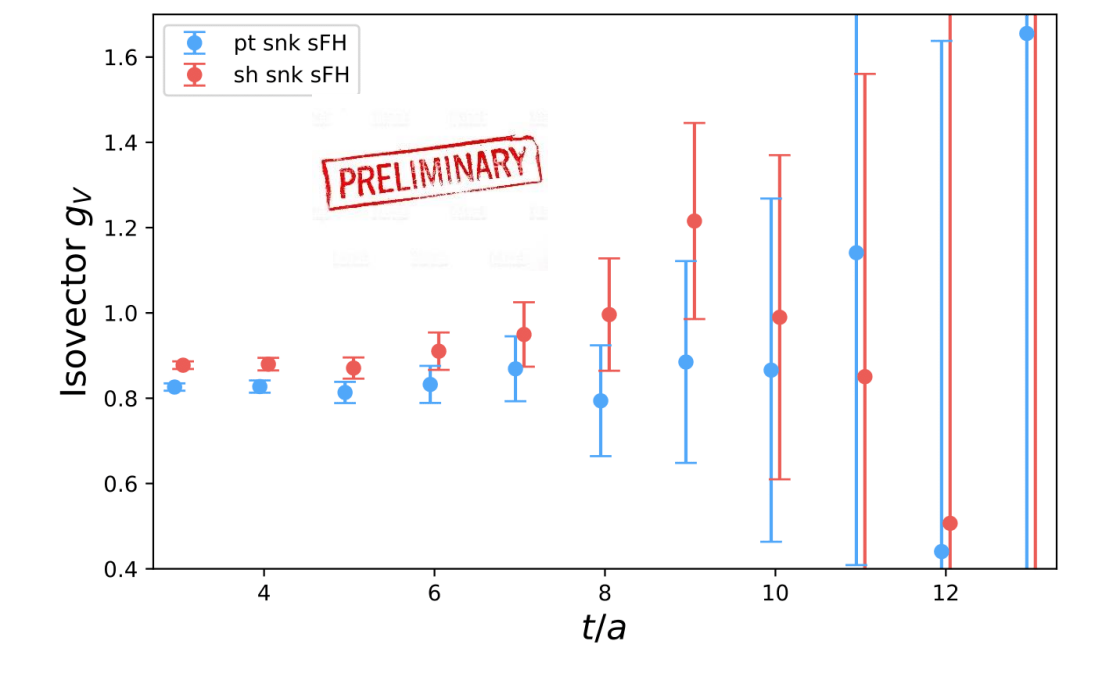
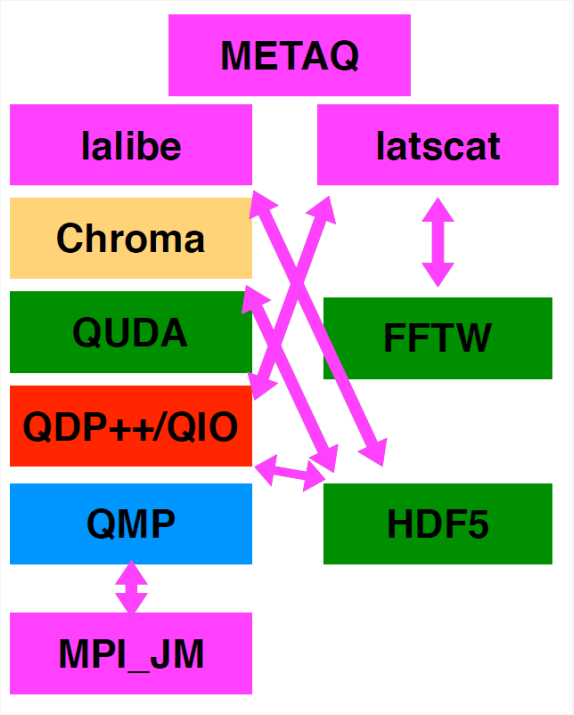




Lalibe Software

- Soon to be public code Lalibe: (https://github.com/callat-qcd/lalibe.git) – currently going through the information management process at LLNL/LBNL.
- Sits on top of the USQCD software stack (links against chroma).
- Exact and stochastic FH routines.
- Baryon contractions and FH contractions, including flavor-changing FH contractions.
- Full parallel HDF5 integration to write out correlators, propagators, and gauge fields from the named object buffer.
- Hierarchical probing
- Will be updated regularly and core contributions (such as HDF5 measurements and QUDA solver interfaces) will be added back to chroma.
- Open Science!!!



Conclusions and Looking Ahead

- Stochastic algorithms allow Feynman-Hellmann technique to be extended to arbitrary matrix elements without need to redo propagator solves.
- Initial results look promising.
- Noise basis can be reused for disconnected diagrams.

- Add deflation to the method to reduce variance (deflation and hierarchical probing are synergistic SIAM J. Sci. Comput., 39(2), A532 to A558, 2017).
- Do full analysis with varying sink momenta and form factors.
- Obtaining the current insertion time dependence is also possible.

Acknowledgements

- This work was supported by an award of computer time by the Lawrence Livermore National Laboratory (LLNL) Multiprogrammatic and Institutional Computing program through a Tier 1 Grand Challenge award.
- This work was performed under the auspices of the U.S. Department of Energy by LLNL under Contract No. DE-AC52-07NA27344 (EB, ER, PV).
- Andreas Stathopoulos - for useful discussions and the bit-arithmetic algorithm that generates the HP vectors (SIAM J. Sci. Comput., 35(5), S299–S322).
- Balint Joo – for generally being helpful with anything chroma related and also interfacing the MDWF QUDA solver that was employed in this work (arXiv:hep-lat/0409003), PoS LATTICE2013, 033.
- MILC Collaboration - for providing the HISQ ensemble used in this work Phys. Rev. D87, 054505, 1212.4768 (A. Bazavov et al. - MILC, 2013) and Phys. Rev. D82, 074501, 1004.0342 (A. Bazavov et al. - MILC, 2010)

Backup

- Möbius Domain Wall on HISQ
- $a = .12\ fm$ $m_\pi = 310\ MeV$ $m_\pi L = 4.5$
- ~200 configurations 1 source 32 "Z4/HP Propagators"
- Left: Z4 noise Right: HP