Extending the Feynman-Hellmann Method to Arbitrary Matrix Elements

Lattice 2018: Michigan State University

Arjun Singh Gambhir with Evan Berkowitz, David Brantley, Chia (Jason) Chang, Kate Clark Thorsten Kurth, Chris Monahan, Amy Nicholson, Enrico Rinaldi, and Pavlos Vranas, André Walker-Loud
Feynman-Hellmann Theorem

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

\[
\frac{\partial E_n}{\partial \lambda} = \langle n | H_{\lambda} | n \rangle
\]

\[
H = H_0 + \lambda H_{\lambda}
\]

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

\[ C_\lambda(t) = \langle \lambda | \mathcal{O}(t) \mathcal{O}^\dagger(0) | \lambda \rangle \]

\[ = \frac{1}{Z_\lambda} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A_\mu e^{-(S + S_\lambda)} \mathcal{O}(t) \mathcal{O}(0) \]

\[ S_\lambda = \lambda \int d^4x j_\mu(x) \]

\[ \lambda j_\mu(x) = \bar{q}(x) \gamma_\mu \gamma_5 q(x) \]
Feynman-Hellmann Theorem

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

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

- Setting $\lambda$ to zero, we obtain

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

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

- 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.

\[ \frac{\partial E_n}{\partial \lambda} = \langle n|H_\lambda|n \rangle \]

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

• 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 $S_{\Gamma}$.

\[ S_{\Gamma} = \sum_{z} S(y, z) \Gamma(z) S(z, x) \]

- $S(z, x)$ 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 $S_{\Gamma}$.
- $S_{\Gamma}$ intercepts normal quarks in a two-point correlation function to give $\partial_{\lambda} C_{\lambda}(t)$.
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 \( \langle \eta(i)\eta^*(j) \rangle = \delta_{ij} \) - “stochastic identity”.
- Factorizes method so different matrix elements and momentum-transfer points are computed without re-inverting.
- \( |\chi> \) is one spin/color component of the source (a vector).
- \( |\psi> \) is the corresponding propagator component.
- \( |\phi> \) is a spin/color component of \( S_\Gamma \).

\[
D|\psi> = |\chi>
\]

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

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

\[
|\phi'> = \frac{1}{N} \sum_{i=1}^{N} D^{-1}|\eta> <\eta|\Gamma e^{iq\cdot x}|\psi>
\]
Many choices of basis and variance reduction techniques have been developed to estimate the all-to-all propagator: $\mathbb{Z}_2/\mathbb{Z}_4$, dilution, eigenvalue deflation, hierarchical probing, singular value deflation, etc.

- PoSLAT2007:139, 2007 (Babich, et al., 2007)
- Phys. Rev. D83 114505 (C. Morningstar et al., 2011)
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:

\[
\begin{align*}
\eta_j &= \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \\
\eta_j &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\end{align*}
\]

\[
\begin{align*}
\eta_j &= \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} \\
\eta_j &= \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}
\end{align*}
\]
Comparison with Exact Method

- Möbius Domain Wall on HISQ
- \( a = 0.12 \, fm \quad m_\pi = 310 \, MeV \quad m_\pi L = 4.5 \)
- \( \sim 1000 \) configurations \( 8 \) sources \( 32 \) "HP Propagators"
Tensor Charge

- Möbius Domain Wall on HISQ
- $a = 0.12 \text{ fm} \quad m_\pi = 310 \text{ MeV} \quad m_\pi L = 4.5$
- ~1000 configurations \quad 8 sources \quad 32 "HP Propagators"
$Q^2 = 0.18 \text{ GeV}^2$

- Möbius Domain Wall on HISQ
- $a = 0.12 \text{ fm}$ $m_\pi = 310 \text{ MeV}$ $m_\pi L = 4.5$
- $\sim 1000$ configurations 8 sources 32 “HP Propagators”
Lalibe Software

- Soon to be public code Lalibe: [https://github.com/callat-qcd/lalibe.git](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).


• 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)
Möbius Domain Wall on HISQ

- $a = 0.12 \; fm$
- $m_\pi = 310 \; MeV$
- $m_\pi L = 4.5$
- ~200 configurations
- 1 source
- 32 “Z4/HP Propagators”
- Left: Z4 noise

Right: HP

[Graphs showing $g_A^{UD}$, $g_V^{UD}$, $g_A^{SUd}$, $g_V^{SUd}$, $g_A^{PUD}$, $g_V^{PUD}$ vs. $t/a$.]