

The Stochastic Feynman-Hellmann Method

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The Feynman-Hellmann method, as implemented by Bouchard et al. [1612.06963], was recently employed successfully to determine the nucleon axial charge. A limitation of the method was the restriction to a single operator and a single momentum during the computation of each "Feynman-Hellmann" propagator. By using stochastic techniques to estimate the all-to-all propagator, we relax this constraint and demonstrate the successful implementation of this new method. We show reproduction of the axial charge on a test ensemble and non-zero momentum transfer points of the axial and vector form factors.

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1. Introduction

The Feynman-Hellmann (FH) method connects matrix elements to variations in the spectrum.

$$\frac{\partial E_n}{\partial \lambda} = \langle n | H_\lambda | n \rangle \quad (1.1)$$

Above, H is some perturbing Hamiltonian: $H = H_0 + \lambda H_\lambda$ and $|n\rangle$ is an eigenstate of H_0 . A few variations of the FH method have been employed in Lattice QCD to compute hadronic matrix elements [1, 2, 3, 4, 5]. As pointed out in Ref. [6], these FH inspired methods are very similar to, or practically the same as those found in older publications [7, 8, 9, 10] and they can be rigorously connected to functional derivatives of the partition function through an application of the FH Theorem.

In the adaptation from [6], a two-point correlation function in the presence of an external field is considered

$$C_\lambda(t) = \langle \lambda | \mathcal{O}(t) \mathcal{O}^\dagger(0) | \lambda \rangle = \frac{1}{\mathcal{Z}_\lambda} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A_\mu e^{-(S+S_\lambda)} \mathcal{O}(t) \mathcal{O}(0) \quad (1.2)$$

$$\mathcal{Z}_\lambda = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A_\mu e^{-(S+S_\lambda)}$$

$$S_\lambda = \lambda \int d^4x j_\mu(x), \quad (1.3)$$

where $j_\mu(x)$ is some current density.

$$\lambda j_\mu(x) = \bar{q}(x) \gamma_\mu \gamma_5 q(x) \quad (1.4)$$

The partial derivative of $C_\lambda(t)$ yields an expression with two terms.

$$\frac{\partial C_\lambda(t)}{\partial \lambda} = - \left[\frac{\partial_\lambda \mathcal{Z}_\lambda}{\mathcal{Z}_\lambda} C_\lambda(t) + \frac{1}{\mathcal{Z}_\lambda} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A_\mu e^{-(S+S_\lambda)} \int d^4x' j(x') \mathcal{O}(t) \mathcal{O}(0) \right] \quad (1.5)$$

The first is the vacuum matrix element, which is zero unless $j(x)$ has vacuum quantum numbers. The second term is an integral over all spacetime of the creation/annihilation operators and current. Setting $\lambda = 0$ reduces \mathcal{Z}_λ to the ordinary partition function in equation 1.5. Therefore, this method is employed in practice on an ensemble sampled with $\lambda = 0$.

$$\left. \frac{\partial C_\lambda(t)}{\partial \lambda} \right|_{\lambda=0} = C_\lambda(t) \int d^4x' \langle \Omega | j(x') | \Omega \rangle - \int dt' \langle \Omega | T [\mathcal{O}(t) J(t') \mathcal{O}(0)] | \Omega \rangle \quad (1.6)$$

Above, $J(t')$ is a time-dependent current given by $J(t') = \int d^3x' j(t', \vec{x}')$. The region for which $0 < t' < t$, the second term is the hadronic matrix element of interest.

In analogy to the effective mass from a standard two-point function, the long-time limit of the partial derivative of the effective mass plateaus to the matrix element of interest.

$$\left. \frac{\partial m_{\text{eff}}(t, \tau)}{\partial \lambda} \right|_{\lambda=0} = \frac{1}{\tau} \left[\frac{-\partial_\lambda C_\lambda(t+\tau)}{C(t+\tau)} - \frac{-\partial_\lambda C_\lambda(t)}{C(t)} \right] \xrightarrow{t \rightarrow \infty} \frac{J_{00}}{2E_0} \quad (1.7)$$

There is a beautiful symmetry between equations 1.1 and 1.7, hence the name, FH method. By studying $J(t')$ in all regions, including where the current is inserted outside of the hadron, a functional fitting form can be derived for which the matrix element of interest is uniquely, linearly temporally-dependent. For a rigorous treatment of this derivation, we refer the reader to [6].

In practice, the derivative of the correlation function is computed by applying a current globally in spacetime to a quark propagator through a matrix product. The resulting object is then treated as a source and used as a right-hand side in solving the Dirac equation.

$$S_\Gamma = \sum_z S(y, z) \Gamma(z) S(z, x) \quad (1.8)$$

We refer to S_Γ as the ‘‘Feynman-Hellman’’ propagator. In order to compute $\partial_\lambda C_\lambda$ the FH propagator intercepts ordinary quark lines in a hadron’s two-point function. This method, as numerically described above, was efficaciously used to calculate the axial coupling to within 1% uncertainty [5].

There are several benefits to using this technique for computing correlation functions. Since the insertion time is summed over, there is only one time variable that may be varied, leading to potentially easier systematics to control. Additionally, for the cost of a single propagator, information from all timeslices is gained. Furthermore, S_Γ is reusable for a variety of different sink interpolators, including different choices of sink smearing and different hadrons altogether.

2. Stochastic Feynman-Hellmann

The FH method has a number of disadvantages compared to the more conventional sequential source approach to computing three-point functions [11, 12]. The current time is summed everywhere on the lattice, including over sites outside of the hadron and at the source/sink, so called contact terms. This yields extra terms that do not appear in other methods. In addition, explicit time dependence of the current is lost. This complicates the analysis for non-zero momentum transfer points, in which transition amplitudes appear due to differing initial and final state energies. Finally, each choice of Γ and momentum injection costs an individual FH propagator, resulting in high computational costs to calculate form factors.

The aim of this work is to remedy two out of the three disadvantages. To achieve this, we employ a stochastic basis, whose vectors obey the property: $\langle \eta(i) \eta^*(j) \rangle = \delta_{ij}$. If we consider one spin/color component of a propagator, the Dirac equation is solved as

$$\begin{aligned} D|\psi\rangle &= |\chi\rangle \\ |\psi\rangle &= D^{-1}|\chi\rangle, \end{aligned}$$

where $|\chi\rangle$ is a spin/color component of the source and $|\psi\rangle$ is of the propagator. A component of the FH propagator is

$$|\phi\rangle = D^{-1} \Gamma e^{iq \cdot x} |\psi\rangle. \quad (2.1)$$

Inserting an outer product of noise vectors factorizes the algorithm, allowing different matrix elements and momentum-transfer points to be computed without requiring additional solves.

$$|\phi'\rangle = \frac{1}{N} \sum_{i=1}^N D^{-1} |\eta_i\rangle \langle \eta_i | \Gamma e^{iq \cdot x} |\psi\rangle \quad (2.2)$$

There are many possible choices for the type of noise basis, such as Gaussian, \mathbb{Z}_2 , \mathbb{Z}_4 , or some kind of dilution pattern. In the context of disconnected diagrams or distillation, the effectiveness

of different types of noise and variance reduction techniques has been studied extensively [13, 14, 15, 16, 17, 18, 19, 20, 21, 22]. For this work we employ fully spin and color diluted hierarchical probing [19].

3. Numerical Results

The stochastic FH method is tested on a Möbius Domain Wall on gradient flowed HISQ mixed action. The lattice spacing, pion mass, and volume of the ensemble are $a = .12$ fm, $m_\pi = 310$ MeV, and $m_\pi L = 4.5$ respectively. Details of the action setup and ensemble can be found in [23]. Figures 1a and 1b show the calculation of g_A and g_V with regular and stochastic FH methods. Figure 2, 3a, and 3b demonstrate the computation of other observables by reusing the same stochastic basis.

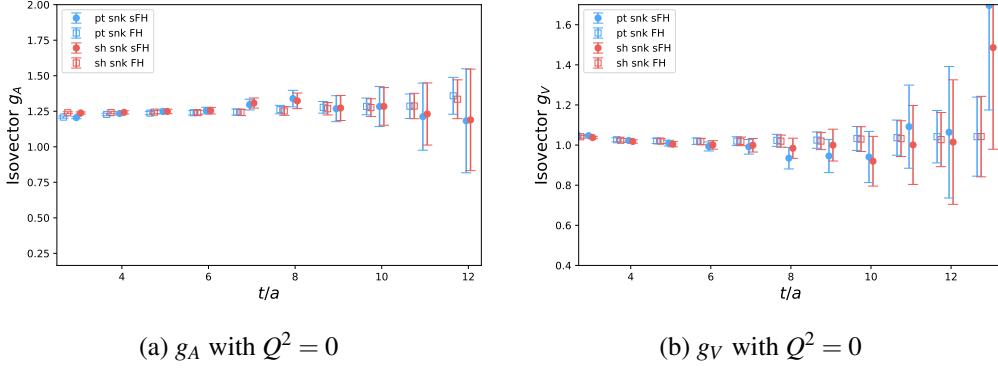


Figure 1: Isovector g_A and g_V with regular FH and stochastic FH (sFH) are plotted. Both methods are at comparable statistics with about 1000 gauge field configurations and 8 smeared sources. Both point (pt) and smeared (sh) sinks are constructed. For the stochastic case, 32 hierarchical probing vectors are used.

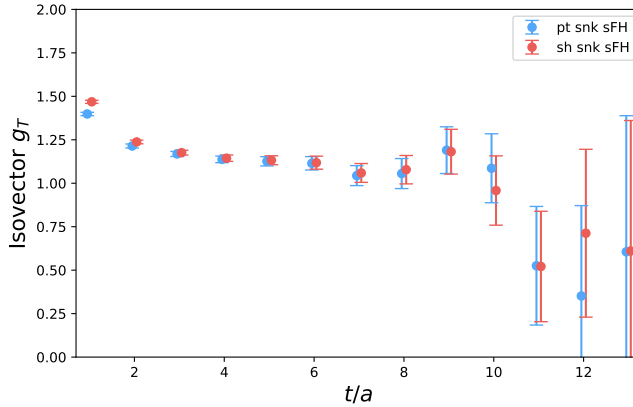


Figure 2: Isovector g_T with the stochastic method is shown. This calculation was done with the same stochastic basis as previous figures, with identical statistics of roughly 1000 configurations and 8 sources.

In these figures, the derivative of the effective mass is plotted by constructing the correlated difference defined in equation 1.7. In the long-time limit, this quantity should plateau to the matrix

element. From Figures 1a and 1b, it's clear that the stochastic basis successfully reproduces the "exact" answer, albeit with larger statistical uncertainty. In the case of Figure 2, there is no exact calculation to compare to, however the signal looks clean and plateaus to a reasonable value of the tensor charge [24].

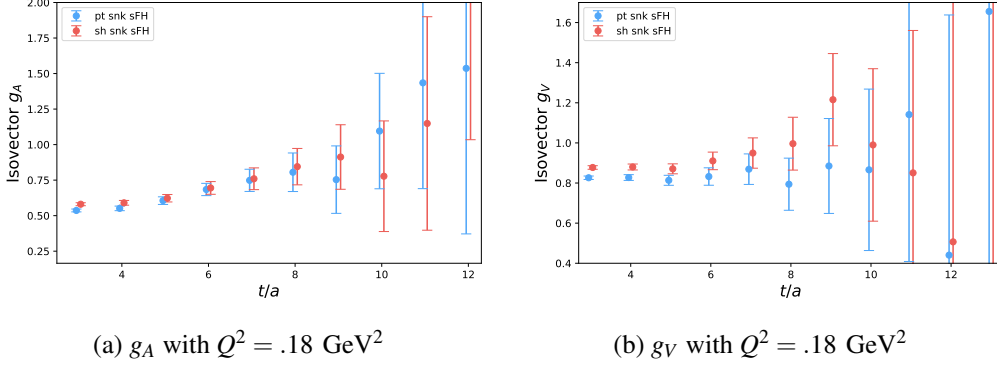


Figure 3: Isovector g_A and g_V with one unit of lattice momentum are shown. This is with approximately 1000 configurations, 8 sources, and 32 hierarchical probing vectors.

Figures 3a and 3b illustrate g_A and g_V with one unit of lattice momentum. This is done by fixing the sink and current with one unit of momentum in the same direction. It should be noted however that with the stochastic FH method, arbitrary momenta may be chosen for both the current insertion and sink. An analysis that takes advantage of different momentum combinations at the current and sink is forthcoming. The statistical uncertainty for non-zero momentum is large; enhancements to the basis are also currently being explored.

4. Conclusion and Outlook

We study an algorithm that computes the FH propagator with a stochastic basis, extending the original FH method to give arbitrary observables and non-zero momentum transfer points in a feasible amount of computing time. This is achieved through a stochastic noise basis. It should be noted that this basis is required to compute disconnected diagrams, therefore amortizing the cost for the connected calculation. Additionally, the current insertion time may be exposed by introducing a delta function in time to the bilinear, thereby recovering the full dependence of the three-point function. Finally, it has been shown in [21, 22] that singular value deflation plays a synergistic role with hierarchical probing in greatly reducing variance. Incorporating deflation into this method is being explored.

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References

- [1] QCDSF/UKQCD, CSSM collaboration, *Feynman-Hellmann approach to the spin structure of hadrons*, *Phys. Rev.* **D90** (2014) 014510 [1405.3019].
- [2] A. J. Chambers et al., *Disconnected contributions to the spin of the nucleon*, *Phys. Rev.* **D92** (2015) 114517 [1508.06856].
- [3] M. J. Savage, P. E. Shanahan, B. C. Tiburzi, M. L. Wagman, F. Winter, S. R. Beane et al., *Proton-Proton Fusion and Tritium β Decay from Lattice Quantum Chromodynamics*, *Phys. Rev. Lett.* **119** (2017) 062002 [1610.04545].
- [4] E. Berkowitz et al., *An accurate calculation of the nucleon axial charge with lattice QCD*, 1704.01114.
- [5] C. C. Chang et al., *A per-cent-level determination of the nucleon axial coupling from quantum chromodynamics*, *Nature* **558** (2018) 91 [1805.12130].
- [6] C. Bouchard, C. C. Chang, T. Kurth, K. Orginos and A. Walker-Loud, *On the Feynman-Hellmann Theorem in Quantum Field Theory and the Calculation of Matrix Elements*, *Phys. Rev.* **D96** (2017) 014504 [1612.06963].
- [7] L. Maiani, G. Martinelli, M. L. Paciello and B. Taglienti, *Scalar Densities and Baryon Mass Differences in Lattice QCD With Wilson Fermions*, *Nucl. Phys.* **B293** (1987) 420.
- [8] S. Gusken, U. Low, K. H. Mutter, R. Sommer, A. Patel and K. Schilling, *Nonsinglet Axial Vector Couplings of the Baryon Octet in Lattice QCD*, *Phys. Lett.* **B227** (1989) 266.
- [9] J. Bulava, M. Donnellan and R. Sommer, *On the computation of hadron-to-hadron transition matrix elements in lattice QCD*, *JHEP* **01** (2012) 140 [1108.3774].
- [10] G. M. de Divitiis, R. Petronzio and N. Tantalo, *On the extraction of zero momentum form factors on the lattice*, *Phys. Lett.* **B718** (2012) 589 [1208.5914].
- [11] B. Bunk, K. Mütter, K. Schilling and N. A. T. O. S. A. Division, *Lattice Gauge Theory: A Challenge in Large-scale Computing*, Basic Life Sciences. Springer Dordrecht, 1986.
- [12] LHPC collaboration, *Nucleon structure from mixed action calculations using 2+1 flavors of asqtad sea and domain wall valence fermions*, *Phys. Rev.* **D82** (2010) 094502 [1001.3620].
- [13] M. F. Hutchinson, *A stochastic estimator of the trace of the influence matrix for Laplacian smoothing splines*, *J. Commun. Statist. Simula.* **19** (1990) 433.
- [14] S.-J. Dong and K.-F. Liu, *Stochastic estimation with Z(2) noise*, *Phys. Lett.* **B328** (1994) 130 [hep-lat/9308015].
- [15] H. Neff, N. Eicker, T. Lippert, J. W. Negele and K. Schilling, *On the low fermionic eigenmode dominance in QCD on the lattice*, *Phys. Rev.* **D64** (2001) 114509 [hep-lat/0106016].
- [16] J. Foley., K. J. Juge, A. O’Cais, M. Peardon, S. Ryan and J.-I. Skullerud, *Practical all-to-all propagators for lattice qcd*, *Comput. Phys. Commun.* **172** (2005) 145 [hep-lat/0505023].

- [17] R. Babich, R. Brower, M. Clark, G. Fleming, J. Osborn and C. Rebbi, *Strange quark contribution to nucleon form factors*, *PoS LAT2007* (2007) 139 [0710.5536].
- [18] C. Morningstar, J. Bulava, J. Foley, K. Juge, D. Lenkner, M. Peardon et al., *Improved stochastic estimation of quark propagation with Laplacian Heaviside smearing in lattice QCD*, *Phys. Rev. D* **83** (2011) [1104.3870v1].
- [19] A. Stathopoulos, J. Laeuchli and K. Orginos, *Hierarchical probing for estimating the trace of the matrix inverse on toroidal lattices*, 1302.4018.
- [20] E. Endress, C. Pena and K. Sivalingam, *Variance reduction with practical all-to-all lattice propagators*, *Comput. Phys. Commun.* **195** (2015) 35 [1402.0831].
- [21] A. S. Gambhir, A. Stathopoulos and K. Orginos, *Deflation as a Method of Variance Reduction for Estimating the Trace of a Matrix Inverse*, 1603.05988.
- [22] A. S. Gambhir, A. Stathopoulos, K. Orginos, B. Yoon, R. Gupta and S. Syritsyn, *Algorithms for Disconnected Diagrams in Lattice QCD*, *PoS LATTICE2016* (2016) 265 [1611.01193].
- [23] E. Berkowitz et al., *Möbius domain-wall fermions on gradient-flowed dynamical HISQ ensembles*, *Phys. Rev.* **D96** (2017) 054513 [1701.07559].
- [24] R. Gupta, Y.-C. Jang, B. Yoon, H.-W. Lin, V. Cirigliano and T. Bhattacharya, *Isvector Charges of the Nucleon from 2+1+1-flavor Lattice QCD*, *Phys. Rev.* **D98** (2018) 034503 [1806.09006].