Detailed analysis of excited state systematics in a lattice QCD calculation of ga

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Lattice Quantum Chromodynamics

Discretize QCD in spacetime and put in finite box Non-perturbatively defines both UV and IR cutoff

Observables (mass, form factors) calculated from path integral Euclidean spacetime can be evaluated with Monte Carlo

Hadronic creation operators are unknown Best guesses overlap with a tower of hadronic states

This talk is about understanding this tower of states in the context of the nucleon



Challenges of Baryon Structure for LQCD

Signal-to-Noise ratio as a function of **time**

Signal
$$\langle N\overline{N}\rangle = \sum_{\text{states}} |\langle N|i\rangle|^2 e^{E_i t} \simeq e$$

Noise
$$\sigma(\langle N\overline{N}\rangle) = \sqrt{\langle |N\overline{N}|^2 \rangle} - |\langle N\overline{N}\rangle|^2$$

 $\simeq e^{-3M_{\pi}t/2}$

Signal decays with GeV scale Noise decays with MeV scale

This is further exacerbated for excited states

 $-M_N t$



Possible strategies around this issue

Use large Euclidean time as a filter

How large is enough? Requires exponential amount of MC samples. What happens when there is not quite enough?

Disentangle excited-states at early time

Much more complicated! How to do this reliably?

This talk focuses on latter for the axial-vector correlation function



Data: Post-processed correlation functions

Correlation function from Path integral

$$C_A(t,\tau) = \sum_n |z_n|^2 g_{nn}^A e^{-E_n t}$$
$$+ 2 \sum_{n < m} z_n z_m^{\dagger} g_{nm}^A e^{-(E_n + \Delta_m t)}$$

Ratio correlation function

$$R_A(t,\tau) = C_A(t,\tau)/C_2(t) \to \lim_{t \to \infty} R_A(t,\tau)/C_2(t) \to C_A(t,\tau)/C_2(t)$$

Feynman-Hellmann correlation function

$$\operatorname{FH}_{A}(t) = \left. \frac{\partial E_{\lambda}^{\text{eff}}}{\partial \lambda} \right|_{\lambda=0} = \frac{1}{dt} \left[\frac{\sum_{\tau} C_{A}(t - t))}{C_{2}(t - t)} \right]_{\lambda=0}$$



(nn/2)t



Data: Post-processed correlation functions $R_A(t, \tau)$ FH_A(t)



1) The FH correlator goes to the infinite-time limit much sooner

Why should you believe our infinite-time extrapolation? I show this first... and if you accept it then... How much sooner and why?





Analysis strategies

2-point correlator

3-point correlator at t=[2,14] makes $R_A(t,\tau)$ and $FH_A(t)$

We show 3 ways to fit this dataset





Sensitivity analysis

We are fitting a physics model to data

Data specifications for this work 2-point correlator extracts overlap factor (z_n) and energy (E_n) ~20 data points to constrain 2 parameters per state

3-point correlator extracts matrix elements (g_{nm}) 13 data points to constrain n=m, 1 parameter per state ~50 data points to constraint n!=m, n(n+1)/2 parameters per state

Things to worry about

Underfitting and overfitting Sensitivity of posterior distribution to various hyper parameters number of states, fit region, spectrum model

Sensitivity analysis : fit region and states



Posterior distribution is insensitive to choice... so choice does not matter

13 source-sink separation times allow for proper study enough range to vary t and τ enough data to over-constrain a 7 state fit

Sensitivity analysis : excited state spectrum



The first 5 states inferred from data (because we fit all the curvature in 3pt fcn)

Best fit consistency

The 3 analysis strategies are consistent within 1 standard deviation

Results consistent with publication [Nature 558, 91-94 (2018)]

2) Control systematics by showing no sensitivity to all hyperparameters

Comparison with late time analysis

The best fit late time result is 2 standard deviations in tension 3) Late time data is under sampled (S/N issue) so uncertainty is unreliable

Excited-state contributions

2-point function

$$C_2(t) = C_2^{\rm gs}(t) + C_2^{\rm es}(t)$$

$$C_2^{\text{gs}}(t) = |z_0|^2 e^{-E_0 t}$$
$$C_2^{\text{gs}} = \sum_{n \ge 1} |z_n|^2 e^{-E_n t}$$

Break fit model down to ground state and excited state contributions Have a data driven fit of first 5 states, what are the contributions?

3-point function

$$C_A(t,\tau) = C_A^{\rm gs}(t) + C_A^{\rm sc}(t) + C_A^{\rm tr}(t,\tau)$$

$$C_A^{\rm gs}(t) = |z_0|^2 g_{00}^A e^{-E_0 t}$$

$$C_A^{\rm sc}(t) = \sum_{n \ge 1} |z_n|^2 g_{nn}^A e^{-E_n t}$$

$$C_A^{\rm tr}(t,\tau) = 2 \sum_{n < m} z_n z_m^{\dagger} g_{nm}^A e^{-(E_n + \Delta_{mn}/2)}$$

$$\times \cosh\left[\Delta_{mn}(\tau - t/2)\right]$$

Excited-state contributions

Significant cancellation between 2pt and 3pt sc excited states (red + blue)

$$C_2^{\rm es}(t) = \sum_{n \ge 1} |z_n|^2 e^{-E_n t} \qquad C_A^{\rm sc}(t) = \sum_{n \ge 1} g_{nn}^A |z_n|^2 e^{-E_n t}$$

Result of (partially) conserved currents 4) Excited-state dominated by transition matrix elements (light blue)

Excited-state contributions

4) Excited-state dominated by transition matrix elements (light blue)

Fit and remove the transition excited states (possible with 3pt) Suppress them and fit (possible with FH)

Or just combine both and do a more involved fit

Conclusions

Nucleon observables suffer from S/N issue

Analysis shows transition as dominant excited-state contribution

- 1) Calculation can be done at ~2.5fm for 1% systematic Requires unreasonable amount of statistics or is subject to uncontrollable systematic error
- 2) Fit and remove the transition contributions Standard way of generating correlates makes this possible Need enough source-sink separation time for sensible d.o.f. counting
- 3) Suppress contributions numerically with FH correlation Simpler to analyze and is consistent at the 1% level The cancellation is not exact Unknown how well this works for non-zero momentum transfer

Collaborators

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