Hadron Spin Structure from Lattice QCD using the Feynman-Hellmann Theorem

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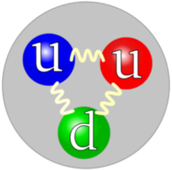
Motivation

The proton

- $Q = +e$, $S = \frac{1}{2}$



Where do these quantum numbers come from?

Understand as bound state of 3 quarks

u quarks

- $Q = +\frac{2}{3}e$, $S = \frac{1}{2}$

d quark

- $Q = -\frac{1}{3}e$, $S = \frac{1}{2}$

Charge is sum of quark charges

- Maybe S_z is as well?

Spin-up proton $\implies$ 2 quarks spin-up, 1 spin-down

Does the quarks' spin account for 100% of the proton's spin?

Spin Decomposition

[EMC] Ashman et al., 1988

- Quark spin contribution 1(12)(24)%

[COMPASS] Alexakhin et al., 2007

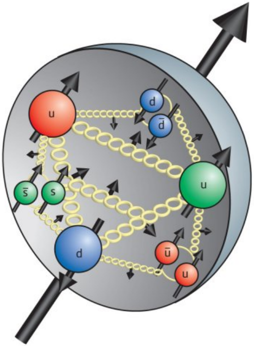
- Quark spin contribution 33(3)(5)%

Ji, 1997

- Can gauge-invariantly decompose the total spin of the proton

$$\frac{1}{2} = \frac{1}{2}\Delta\Sigma + L_q + J_g\,, \qquad \Delta\Sigma = \sum_q \Delta q$$

Similarly for other hadrons



How can we calculate spin fractions using lattice QCD?

Lattice QCD

Want to calculate

$$\langle \mathcal{O} \rangle$$

Path-integral formalism gives

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A\, \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, \mathcal{O}[A, \bar{\psi}, \psi]\, e^{-S[A,\bar{\psi},\psi]}$$

Grassmanian integration of quark fields leaves

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}A\, \overline{\mathcal{O}}[A]\, \det[D(A)]\, e^{-S_g[A]}}{\int \mathcal{D}A\, \det[D(A)]\, e^{-S_g[A]}}$$

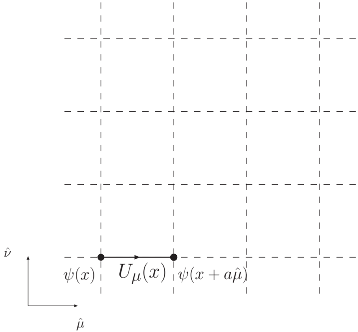
Quark fields in $\mathcal{O}$ Wick-contracted $\rightarrow$ Quark propagators

Discretise expression and estimate via importance sampling

Lattice QCD

Gauge field $\rightarrow$ link variables

$$A \rightarrow U$$



Generate gauge fields with weighting

$$\det[D(U)]\, e^{-S_g[U]}$$

Weighted integral $\rightarrow$ unweighted sum

$$\langle \mathcal{O} \rangle \approx \frac{1}{N} \sum_{i=1}^{N} \overline{\mathcal{O}}[U_{(i)}]$$

Calculate propagators in $\overline{\mathcal{O}}$ by inverting Dirac matrix

$$S^{ab}_{\alpha\beta}(x,y) = \left[D^{ab}_{\alpha\beta}(x,y) \right]^{-1}$$

Lattice QCD

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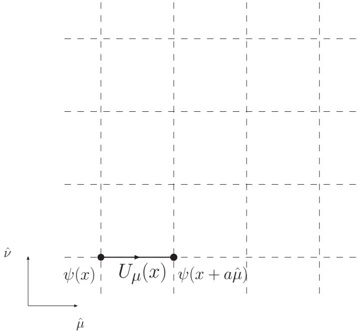

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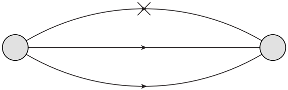
Quark Spin Contribution

Quark spin contribution and quark axial charges

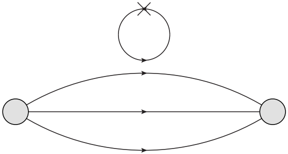
$$\Delta\Sigma = \sum_q \Delta q \qquad \Delta q\, s_\mu = \frac{1}{2M} \langle H \,|\bar{q} i \gamma_5 \gamma_\mu q|\, H \rangle$$

Connected contribution



- Straightforward
- 3-pt. function methods

Disconnected contribution



- Exact calculation unfeasible
  - Too many inversions!
- Use stochastic techniques

Previous Results

A quick search on arXiv.org...

Connected contributions

- 20+ papers since 2005

Disconnected contributions

- $\sim$ 5 papers since 1995

There is a need for a simpler way access to disconnected contributions.

The Feynman-Hellmann Theorem

Suppose the action of our theory depends on some parameter λ,

$$S \to S(\lambda) \, .$$

Then for any hadron state H,

$$\frac{\partial E_H(\lambda)}{\partial \lambda} = \frac{1}{2E_H(\lambda)} \left\langle H \left| \frac{\partial S(\lambda)}{\partial \lambda} \right| H \right\rangle_\lambda \, .$$

The Feynman-Hellmann Method

Want to calculate matrix element

$$\langle H | \mathcal{O} | H \rangle$$

Modify action such that

$$S \rightarrow S + \lambda \int \mathrm{d}^4 x \, \mathcal{O}$$

Feynman-Hellmann Theorem gives

$$\left. \frac{\partial E_H(\lambda)}{\partial \lambda} \right|_{\lambda=0} = \frac{1}{2E_H} \langle H | \mathcal{O} | H \rangle$$

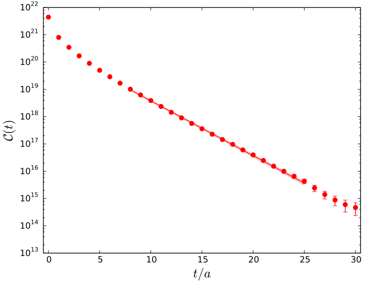
Calculation of matrix element $\equiv$ Hadron spectroscopy!

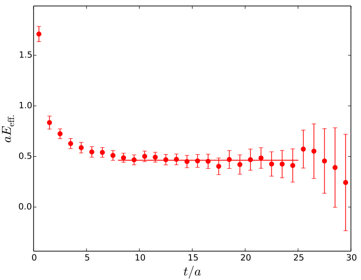
Fourier project correlation function to zero momentum

$$\mathcal{C}(t) = \int \mathrm{d}^3x \, \langle \Omega \,|\mathcal{O}(\vec{x}, t)\bar{\mathcal{O}}(0)|\, \Omega \rangle \xrightarrow{\text{large } t} \frac{e^{-Et}}{2E}|A|^2$$

Define effective mass

$$E_{\text{eff.}}(t + \frac{a}{2}) = \frac{1}{a} \ln \left[\frac{\mathcal{C}(t)}{\mathcal{C}(t+a)} \right] \xrightarrow{\text{large } t} E$$





Quark Spin Contribution

Modify action to include axial operator term

$$S \to S + \lambda \int \mathrm{d}^4 x \, \bar{q} i \gamma_5 \gamma_3 q$$

Feynman-Hellmann Theorem gives

$$\left.\frac{\partial E(\lambda)}{\partial \lambda}\right|_{\lambda=0} = \frac{1}{2M} \langle H | \bar{q} i \gamma_5 \gamma_3 q | H \rangle = \Delta q s_3$$

If hadron polarised in z-direction

$$\Delta q = \left.\frac{\partial E(\lambda)}{\partial \lambda}\right|_{\lambda=0}$$

Reversing polarisation $\equiv$ Changing sign of λ

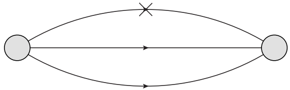
We can double our sampled parameters by measuring energies of both polarisations.

Quark Spin Contribution

Where do we modify the action in a simulation?

When calculating propagators

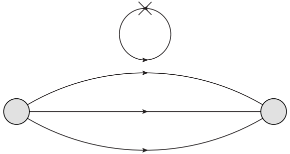
$$S^{ab}_{\alpha\beta}(x,y) = \left[D^{ab}_{\alpha\beta}(x,y)\right]^{-1}$$



- Connected contribution
- Simple to implement
- Use existing ensembles

During gauge-field generation

$$\det[D(U)]\, e^{-S_g[U]}$$



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- Require new lattice trajectories

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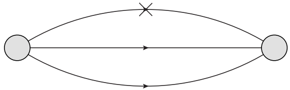

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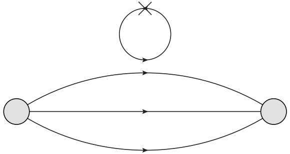

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Simulation Details

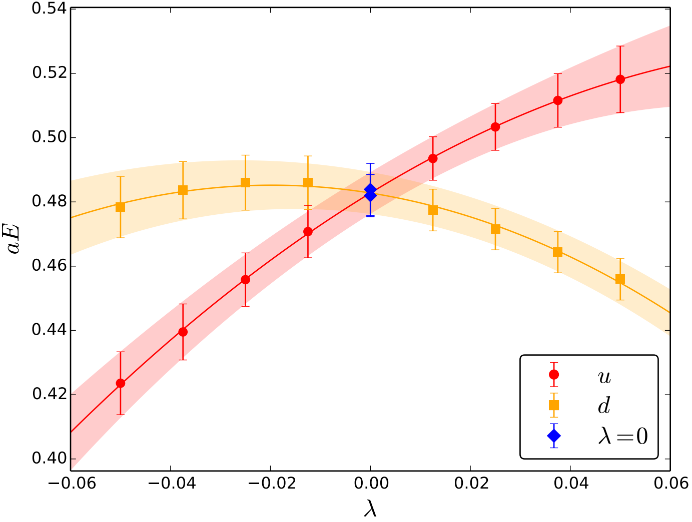
Software

- BQCD for gauge-field generation
- Chroma library for simulations

Two lattice ensembles

- 2+1 quark flavours (isospin-symmetric limit)
- Lattice volume $L^3 \times T = 32^3 \times 64$
- Lattice spacing $a = 0.074(2)$ fm
- At SU(3) symmetric point and away
  - Singlet quark mass constant
- π masses of $\sim$ 470 MeV and 360 MeV
- 350 measurements

Proton Energy



Quark Spin Contributions

Results from Feynman-Hellmann method (unrenormalised)

$$\Delta u^{\text{latt.}}_{\text{conn.}} = 0.94(13)$$
$$\Delta d^{\text{latt.}}_{\text{conn.}} = -0.25(10)$$

[QCDSF] Cooke et al., 2013, 3-pt. function method

$$\Delta u^{\text{latt.}}_{\text{conn.}} = 0.966(17)$$
$$\Delta d^{\text{latt.}}_{\text{conn.}} = -0.2768(57)$$

- Agree within error, standard method more precise
- Same ensemble, 350 vs. 1500 measurements

But we can do better!

Correlator Ratios

Correlation function (now a function of λ)

$$\mathcal{C}(t,\lambda) \overset{\text{large } t}{=} \frac{e^{-E(\lambda)t}}{2E(\lambda)}|A(\lambda)|^2$$

Take ratio

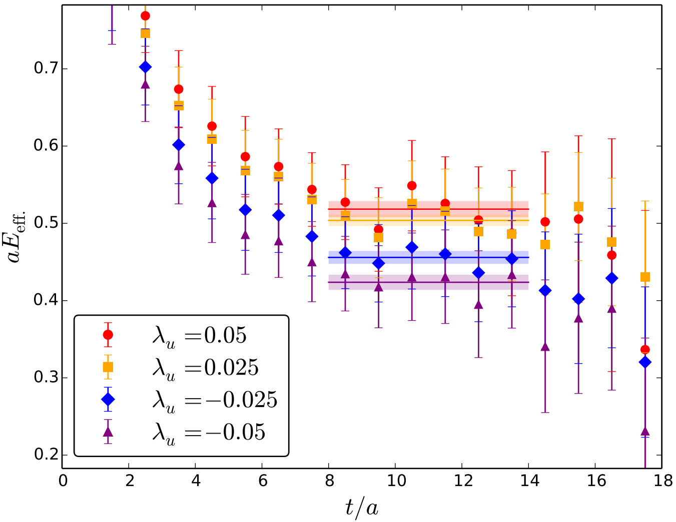
$$\frac{\mathcal{C}(t,\lambda)}{\mathcal{C}(t,0)} \overset{\text{large } t}{\propto} e^{-[E(\lambda)-E(0)]t}$$

We can measure energy shifts directly.

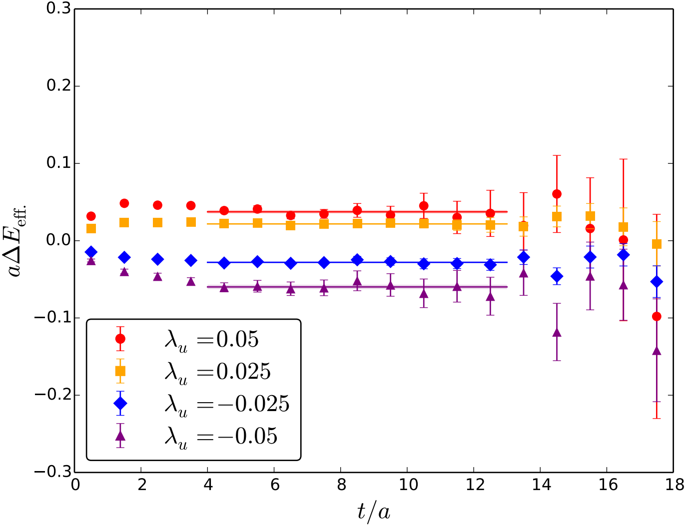
Measurements at different λ highly correlated

- Fluctuations in correlation functions cancel

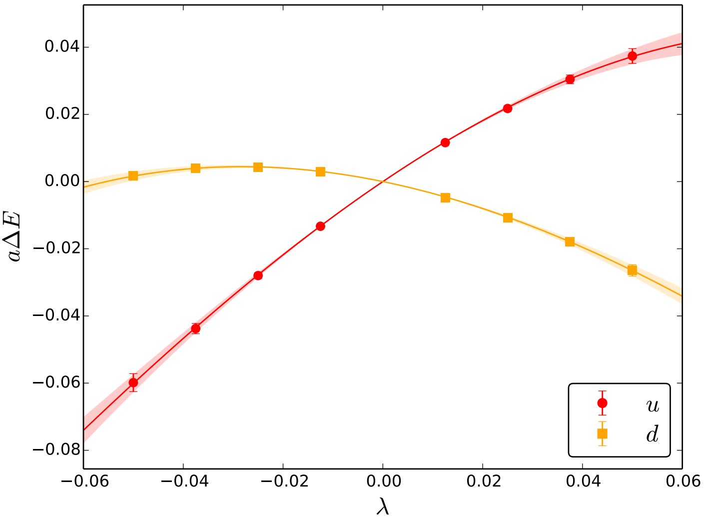
Proton Effective Mass Plot - Before...



Proton Effective Mass Plot - After...



Proton Energy Shifts



Quark Axial Charges - Improved

Improved results

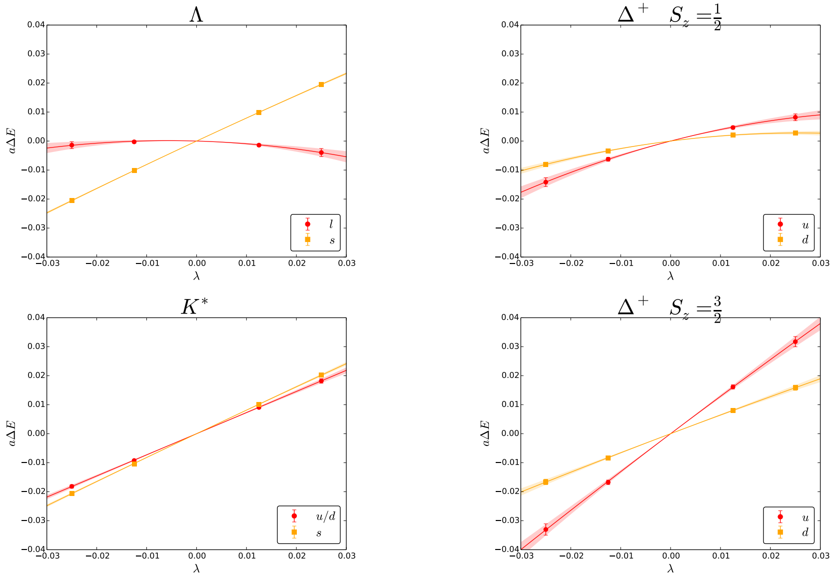
$$\Delta u^{\text{latt.}}_{\text{conn.}} = 1.004(16)$$
$$\Delta d^{\text{latt.}}_{\text{conn.}} = -0.306(10)$$

[QCDSF] Cooke et al., 2013, 3-pt. function method

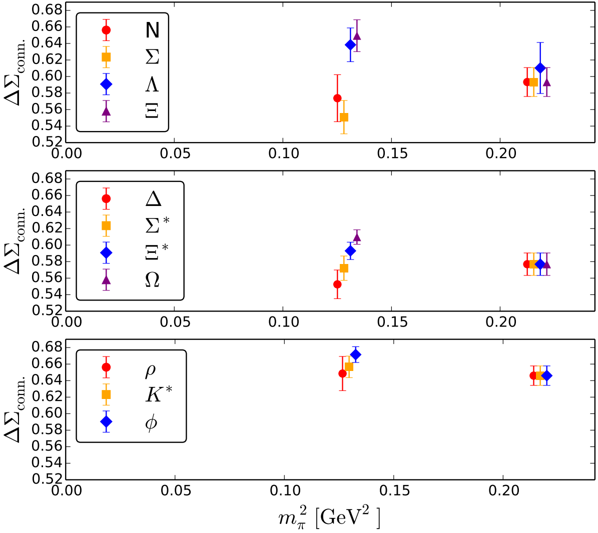
$$\Delta u^{\text{latt.}}_{\text{conn.}} = 0.966(17)$$
$$\Delta d^{\text{latt.}}_{\text{conn.}} = -0.2768(57)$$

- Agree within error, comparable precision
- Same ensemble, 350 vs. 1500 measurements
- Possible excited-state contamination with 3-pt. function method

More Hadrons



Baryon Octet/Decuplet & Vector Mesons



Feynman-Hellmann Method - Advantages/Disadvantages

Advantages

- Simple to implement
- Reduced excited-state contamination
- Comparable/better precision to existing methods
- Excellent for studying a single operator in many hadrons
- Straightforward access to disconnected quantities

Disadvantages

- Different inversions for each operator
- Disconnected quantities require new lattice trajectories
  - For each operator and λ
  - Plenty of computational time

Future Work

Connected spin contributions at lighter quark masses

- Chiral extrapolation

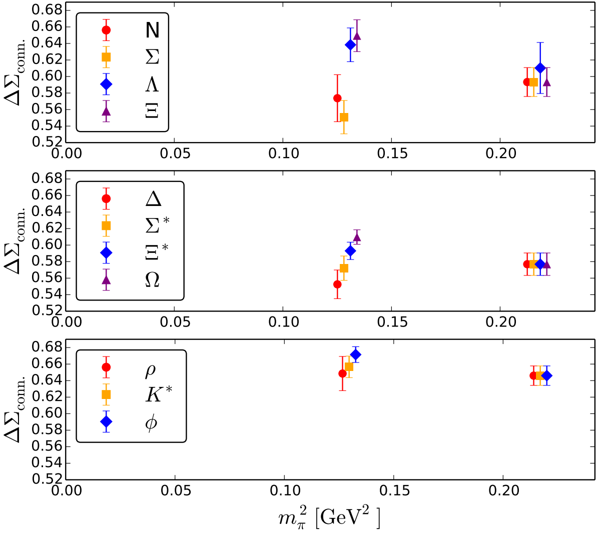
Disconnected spin contributions

- Currently generating new lattice trajectories

σ_{12} operator

- New ensembles already generated, analysis required

Baryon Octet/Decuplet & Vector Mesons



Backup slides

Optimisation

How many values of λ can we get away with?

- Reduce computational time
- Important for generating new lattice trajectories

λ_1	λ_2	$\Delta u_{\text{conn.}}$	$\Delta d_{\text{conn.}}$
0.0125	0.0250	0.995(18)	-0.301(11)
0.0125	0.0375	0.990(23)	-0.293(13)
0.0125	0.0500	0.974(30)	-0.283(16)
0.0250	0.0375	0.991(22)	-0.294(12)
0.0250	0.0500	0.977(29)	-0.285(15)
0.0500	0.0750	0.978(28)	-0.285(15)

- Two minimum for goodness of fit estimate
- Smaller $\lambda \implies$ smaller errors
- Avoid effects of higher-order terms in λ

Proton Energy Shifts - Residual