Quasi-degenerate baryon energy states, the Feynman–Hellmann theorem and transition matrix elements

M. Batelaan, K. U. Can, R. Horsley, Y. Nakamura, H. Perlt, P. E. L. Rakow, G. Schierholz, H. Stüben, R. D. Young, J. M. Zanotti

– QCDSF-UKQCD–CSSM Collaboration –

Adelaide – Edinburgh – RIKEN (Kobe) – Leipzig – Liverpool – DESY (Hamburg) – Hamburg

Lattice 2022, Bonn, Germany

[Monday 08/08/22 14:00, HS6]

Feynman–Hellmann (FH) papers:

- 'A Lattice Study of the Glue in the Nucleon'
  arXiv:1205.6410 (PLB)
- 'A Feynman-Hellmann approach to the spin structure of hadrons'
  arXiv:1405.3019 (PRD)
- 'A novel approach to nonperturbative renormalization of singlet and nonsinglet lattice operators'
  arXiv:1410.3078 (PLB)
- 'Disconnected contributions to the spin of the nucleon'
  arXiv:1508.06856 (PRD)
- 'Electromagnetic form factors at large momenta from lattice QCD'
  arXiv:1702.01513 (PRD)
- 'Nucleon structure functions from lattice operator product expansion'
  arXiv:1703.01153 (PRL)
- 'Lattice QCD evaluation of the Compton amplitude employing the Feynman-Hellmann theorem'
  arXiv:2007.01523 (PRD)
- 'Generalized parton distributions from the off-forward Compton amplitude in lattice QCD'
  arXiv:2110.11532 (PRD)

+ Various (Lattice) conferences

Other related FH talks:

- **Mischa Batelaan** — Monday 8/8/21 14:20 HS6
  Calculation of hyperon transition form factors from two-point functions using the Feynman–Hellmann method
- **Rose Smail** — Tuesday 9/8/21 14:40 HS3
  Constraining beyond the standard model nucleon isovector charges
- **Utku Can** — Wednesday 10/8/21 8:50 HS2 (plenary)
  The Compton amplitude and Nucleon structure functions
- **Alec Hannaford-Gunn** — Wednesday 10/8/21 18:10 HS2
  A lattice QCD calculation of the off-forward Compton amplitude and generalised parton distributions
- **James Zanotti** — Friday 12/8/21 16:40 HS2
  The momentum sum rule via the Feynman–Hellmann theorem

Motivation:

Need computation of non-perturbative quantities:

$$\langle H' | O | H \rangle$$

General structure

- $H \sim \overline{\psi}\psi$ (meson) or $H \sim \psi\psi\psi$ (baryon)
- $O \sim \overline{\psi}\gamma\psi \sim J$ or $O \sim FF$ or even more complicated $O \sim JJ$

This talk:

Generalisation of Feynman–Hellmann approach to determination of (nucleon) matrix elements from degenerate energy states to near-degenerate or ‘quasi-degenerate’ energy states

- This talk: explanation of the above statement / theory
- Numerical results, following talk: Mischa Batelaan

Contents

- Feynman–Hellmann approach via transfer matrix to computation of 2-pt correlation functions
  - Quasi-degenerate states
  - Dyson expansion
  - Reduction to a Generalised EigenVector Problem (GEVP)
- Examples
  - N scattering: flavour diagonal matrix elements
  - Decay/transition matrix elements, eg $\Sigma \to N$
  - Sketches of avoided energy levels
- Inclusion of spin
- Conclusions

Feynman–Hellmann (FH) — some Mathematical Details

Hamiltonian formalism: regard Euclidean time (at least) as continuous

Consider the 2-point nucleon correlation function

$$C_{\lambda\, B'B}(t;\vec{p},\vec{q}) = {}_{\lambda}\langle 0| \underbrace{\hat{\tilde{B}}'(0;\vec{p}\,')}_{\text{Sink: mom op}} \hat{S}(\vec{q})^t \underbrace{\hat{\bar{B}}(0,\vec{0})}_{\text{Source: spatial}} |0\rangle_{\lambda}$$

where $\hat{S}$ is the $\vec{q}$-dependent transfer matrix

$$\hat{S}(\vec{q}) = e^{-\hat{H}(\vec{q})}$$

and in the presence of a perturbation $[\lambda_\alpha = |\lambda_\alpha| e^{i\phi_\alpha}]$

$$\hat{H}(\vec{q}) = \hat{H}_0 - \sum_{\alpha} \lambda_\alpha \hat{\tilde{\mathcal{O}}}_\alpha(\vec{q})$$

where [At leading order can drop α index]

$$\hat{\tilde{\mathcal{O}}}(\vec{q}) = \int_{\vec{x}} \left(\hat{O}(\vec{x}) e^{i\vec{q}\cdot\vec{x}} + \hat{O}^\dagger(\vec{x}) e^{-i\vec{q}\cdot\vec{x}} \right)$$

Physical situation (quasi-degenerate energies):

- Quasi-degenerate states:

$$\hat{H}_0 |B_r(\vec{p}_r)\rangle = E_{B_r}(\vec{p}_r)|B_r(\vec{p}_r)\rangle \quad r = 1, \ldots, d_S$$

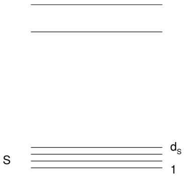
where

$$E_{B_r}(\vec{p}_r) = \bar{E}(\vec{p}, \vec{q}) + \epsilon_r(\vec{p}, \vec{q})$$

- Well separated from higher energy states:

$$\hat{H}_0 |X(\vec{p}_X)\rangle = E_X(\vec{p}_X)|X(\vec{p}_X)\rangle \quad E_X \gg \bar{E}$$

- Quasi-degenerate states taken as lowest energy states



Now insert two complete sets of unperturbed states $\quad |X\rangle \to \frac{|X\rangle}{\sqrt{\langle X|X\rangle}}\,,\ |0\rangle \to |0\rangle$

$$\sum\!\!\!\!\!\!\!\int_{X(\vec{p}_X)} |X(\vec{p}_X))\rangle\,\langle X(\vec{p}_X)|$$

$$\equiv \quad \sum_r \underbrace{|B_r(\vec{p}_r)\rangle\langle B_r(\vec{p}_r)|}_{\text{of interest}} + \sum\!\!\!\!\!\!\!\int_{E_X \gg \bar{E}} \underbrace{|X(\vec{p}_X))\rangle\,\langle X(\vec{p}_X)|}_{\text{higher states}} = \hat{1}$$

before and after $\hat{S}^t$ to give

$$C_{\lambda\, B'B}(t;\vec{p},\vec{q}) =$$

$$\sum\!\!\!\!\!\!\!\int_{X(\vec{p}_X)} \sum\!\!\!\!\!\!\!\int_{Y(\vec{p}_Y)} {}_\lambda\langle 0|\hat{\bar{B}}'(\vec{p}')|X(\vec{p}_X)\rangle\, \underbrace{\langle X(\vec{p}_X)|\hat{S}_\lambda(\vec{q})^t|Y(\vec{p}_Y)\rangle}_{\text{need}} \langle Y(\vec{p}_Y)|\hat{\bar{B}}(\vec{0})|0\rangle_\lambda$$

Time dependent perturbation theory via the Dyson Series

Dyson expansion – iterate identity

$$e^{-(\hat{H}_0-\lambda_\alpha \hat{\hat{\mathcal{O}}}_\alpha)t} = e^{-\hat{H}_0 t} + \lambda_\alpha \int_0^t dt'\, e^{-\hat{H}_0(t-t')}\, \hat{\hat{\mathcal{O}}}_\alpha\, e^{-(\hat{H}_0-\cancel{\lambda_\beta \hat{\hat{\mathcal{O}}}_\beta})t'}$$

- $O(\lambda^2)$ gives Compton like amplitudes $\sim \langle \dots | O_\alpha O_\beta | \dots \rangle$ – not considered here
- Consider 4 possible pieces separately:

$$\langle B_r | e^{-(\hat{H}_0-\lambda\hat{\hat{\mathcal{O}}})t} | B_s \rangle = e^{-\bar{E}t}\left(\delta_{rs} + tD_{rs} + O(2)\right)$$

$$\langle B_r | e^{-(\hat{H}_0-\lambda\hat{\hat{\mathcal{O}}})t} | Y \rangle = e^{-\bar{E}t}\left(\lambda \frac{\langle B_r|\hat{\hat{\mathcal{O}}}|Y\rangle}{E_Y - E_{B_r}} + O(2)\right) + \text{more damped}$$

$$\dots = \dots$$

- $D_{rs}(\vec{p}, \vec{q})$:

$$D_{rs}(\vec{p}, \vec{q}) = -\epsilon_r \delta_{rs} + \lambda \langle B_r(\vec{p}_r) | \hat{\hat{\mathcal{O}}}(\vec{q}) | B_s(\vec{p}_s) \rangle$$

As $d_S \times d_S$ dimensional Hermitian matrix:

$$D_{rs} = \sum_{i=1}^{d_S} \mu^{(i)} e_r^{(i)} e_s^{(i)\,*} \qquad \mu, e_r \text{ eigenvalues/eigenvectors}$$

This gives finally:

$$C_{\lambda\, B'B}(t;\vec{p},\vec{q}) = \sum_{i=1}^{d_S} A^{(i)}_{\lambda\, B'B}(\vec{p},\vec{q})\, e^{-E^{(i)}_{\lambda}(\vec{p},\vec{q})t} + \text{more damped} + \ldots$$

Perturbed energies:

$$E^{(i)}_{\lambda}(\vec{p},\vec{q}) = \bar{E}(\vec{p},\vec{q}) - \mu^{(i)}(\vec{p},\vec{q})\,, \quad i = 1,\ldots,d_S$$

with

$$A^{(i)}_{\lambda\, B'B}(\vec{p},\vec{q}) = \sum_{rs}\left({}_{\lambda}\langle 0|\hat{\tilde{B}}'(\vec{p}\,')|B_r(\vec{p}_r)\rangle_{\lambda}\, e^{(i)}_r \right)\left(e^{(i)*}_s\, {}_{\lambda}\langle B_s(\vec{p}_s)|\hat{\tilde{B}}(\vec{0})|0\rangle_{\lambda} \right)$$

$$|B_s(\vec{p}_s)\rangle_{\lambda} = |B_s(\vec{p}_s)\rangle + \lambda \sum\!\!\!\!\!\!\!\int_{E_Y \gg \bar{E}} |Y(\vec{p}_Y)\rangle\, \frac{\langle Y(\vec{p}_Y)|\hat{\tilde{\mathcal{O}}}(\vec{q})|B_s(\vec{p}_s)\rangle}{E_Y - E_{B_s}}$$

[So a factorisation where unwanted $|Y\rangle$ states have been absorbed into time indept renormalisation of wavefunction]

Finally set

$$B' \sim B_r(\vec{p}_r) \qquad B \sim B_s$$

giving

$$C_{\lambda\, rs}(t) = \sum_{i=1}^{d_S} v_r^{(i)}\, \bar{u}_s^{(i)}\, e^{-E_\lambda^{(i)} t}$$

where

$$v_r^{(i)} = Z_r e_r^{(i)} \qquad \bar{u}_s^{(i)} = \bar{Z}_s e_s^{(i)*}$$

[Z_r, $\bar{Z}_s$ are wavefunctions]

- So problem is now reduced to a GEVP to determine eigenvalues $E_\lambda^{(i)}$
- GEVP eigenvectors should follow pattern of $\vec{e}^{(i)}$

Relation between momenta

- For the matrix elements have

$$[\hat{O}(\vec{x}) = e^{-i\hat{\vec{p}}\cdot\vec{x}}\,\hat{O}(\vec{0})\,e^{i\hat{\vec{p}}\cdot\vec{x}}]$$

$$\langle B(\vec{p}_r)|\hat{\tilde{\mathcal{O}}}(\vec{q})|B(\vec{p}_s)\rangle$$
$$= \quad \langle B_r(\vec{p}_r)|\hat{O}(\vec{0})|B_s(\vec{p}_s)\rangle\,\delta_{\vec{p}_r,\vec{p}_s+\vec{q}} + \langle B(\vec{p}_r)|\hat{O}^\dagger(\vec{0})|B(\vec{p}_s)\rangle\,\delta_{\vec{p}_r,\vec{p}_s-\vec{q}}$$

- So matrix elements step up or down in $\vec{q} \neq \vec{0}$

$$\vec{p}_r = \vec{p}_s + \vec{q} \quad \text{or} \quad \vec{p}_r = \vec{p}_s - \vec{q}$$

[Momentum conservation]

- Diagonal matrix elements vanish
  So quasi-degenerate states have to mix
  [ie must consider degenerate perturbation theory]
- Each step up or down corresponds to another order in λ (Dyson expansion)
  So (eg) $O(\lambda^2)$ gives Compton like amplitudes $\sim \langle \ldots | O_\alpha O_\beta | \ldots \rangle$
  Step up step down now possible: $\vec{p} \to \vec{p} \pm \vec{q} \to \vec{p}$ relevant for DIS

Quasi–degenerate baryon energy states I

- Flavour diagonal matrix elements – N scattering

$$O(\vec{x}) \sim (\bar{u}\gamma u)(\vec{x}) - (\bar{d}\gamma d)(\vec{x})$$

- d_S = 2-dimensional space: $r,\, s = 1,\, 2$

$$\underbrace{|B_1(\vec{p}_1)\rangle = |N(\vec{p})\rangle}_{E_{B_1}(\vec{p}_1)\equiv E_N(\vec{p})=\bar{E}+\epsilon_1} \qquad \underbrace{|B_2(\vec{p}_2)\rangle = |N(\vec{p}+\vec{q})\rangle}_{E_{B_2}(\vec{p}_2)\equiv E_N(\vec{p}+\vec{q})=\bar{E}+\epsilon_2}$$

$$\langle B_r(\vec{p}_r)|\hat{\tilde{\mathcal{O}}}(\vec{q})|B_s(\vec{p}_s)\rangle = \begin{pmatrix} 0 & a^* \\ a & 0 \end{pmatrix}_{rs}$$

where

$$a = \langle B_2(\vec{p}_2)|\hat{O}(\vec{0})|B_1(\vec{p}_1)\rangle \equiv \langle N(\vec{p}+\vec{q})|\hat{O}(\vec{0})|N(\vec{p})\rangle$$

Quasi–degenerate baryon energy states II

- Flavour transition matrix elements – (eg) $\Sigma(sdd) \to N(udd)$ decay

$$O(\vec{x}) \sim (\bar{u}\gamma s)(\vec{x})$$

- d_S = 2-dimensional space: $r, s = 1, 2$

$$\underbrace{|B_1(\vec{p}_1)\rangle = |\Sigma(\vec{p})\rangle}_{E_{B_1}(\vec{p}_1)\equiv E_\Sigma(\vec{p})=\bar{E}+\epsilon_1} \qquad \underbrace{|B_2(\vec{p}_2)\rangle = |N(\vec{p}+\vec{q})\rangle}_{E_{B_2}(\vec{p}_2)\equiv E_N(\vec{p}+\vec{q})=\bar{E}+\epsilon_2}$$

$$\langle B_r(\vec{p}_r)|\hat{\tilde{\mathcal{O}}}(\vec{q})|B_s(\vec{p}_s)\rangle = \begin{pmatrix} 0 & a^* \\ a & 0 \end{pmatrix}_{rs}$$

where

$$a = \langle B_2(\vec{p}_2)|\hat{O}(\vec{0})|B_1(\vec{p}_1)\rangle \equiv \langle N(\vec{p}+\vec{q})|\hat{O}(\vec{0})|\Sigma(\vec{p})\rangle$$

- ie similar structure to N scattering case

Diagonalising $D_{rs}(\vec{p},\vec{q})$:

$$D_{rs}(\vec{p},\vec{q}) = -\epsilon_r \delta_{rs} + \lambda \langle B_r(\vec{p}_r)|\hat{\tilde{\mathcal{O}}}(\vec{q})|B_s(\vec{p}_s)\rangle = \begin{pmatrix} -\epsilon_1 & a^* \\ a & -\epsilon_2 \end{pmatrix}_{rs}$$

1) Eigenvalues $\mu_\pm$:

[quadratic equation]

Giving energies

$$\begin{aligned} E_\lambda^{(\pm)}(\vec{p},\vec{q}) &= \bar{E} - \mu_\pm \\ &= \frac{1}{2}(E_N(\vec{p}+\vec{q}) + E_{N/\Sigma}(\vec{p})) \mp \frac{1}{2}\Delta E_\lambda(\vec{p},\vec{q}) \end{aligned}$$

with

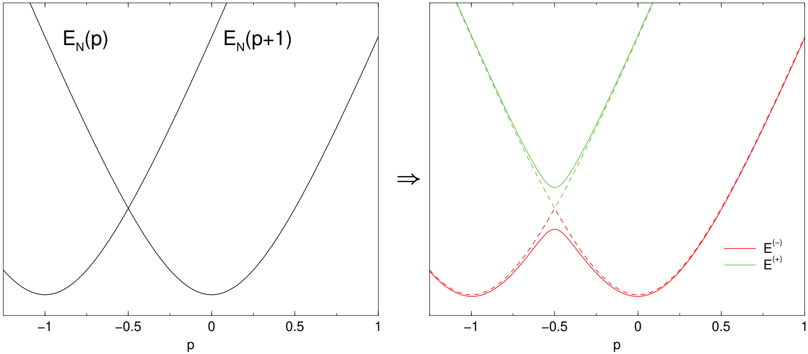
$$\Delta E_\lambda = E_\lambda^{(-)} - E_\lambda^{(+)}$$

and

$$\Delta E_\lambda(\vec{p},\vec{q}) = \sqrt{(E_N(\vec{p}+\vec{q}) - E_{N/\Sigma}(\vec{p}))^2 + 4\lambda^2 \underbrace{\left|\langle N(\vec{p}+\vec{q})|\hat{O}(\vec{0})|N/\Sigma(\vec{p})\rangle\right|^2}_{|a|^2}}$$

Degenerate energy states – N scattering

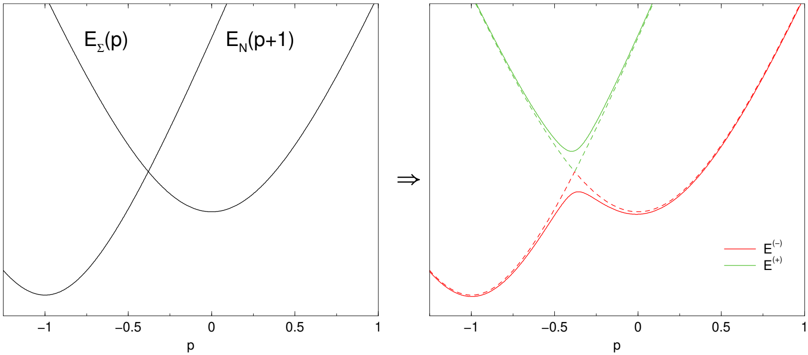
eg 1-dimensional (exaggerated) sketch: $[\lambda^2 |a|^2 = \text{const.},\ q = 1]$



- Free case ⇒ Interacting case: avoided energy levels
- Sketch curves based on previously derived formulae: $E^{(+)}$, $E^{(-)}$
- Degeneracy: $E_N(p) = E_N(p+q)$ at $p = -q/2$
  [Similarly when $E_N(p) = E_N(p-q)$ at $p = q/2$]

Quasi–degenerate energy states – $\Sigma \to N$ decay

eg 1-dimensional (exaggerated) sketch: $[\lambda^2|a|^2 = \text{const.},\ q = 1]$



- Free case ⇒ Interacting case: avoided energy levels
- Sketch based on previous formulae

Diagonalising $D_{rs}(\vec{p},\vec{q})$:

$$D_{rs}(\vec{p},\vec{q}) = -\epsilon_r \delta_{rs} + \lambda \langle B_r(\vec{p}_r)|\hat{\tilde{\mathcal{O}}}(\vec{q})|B_s(\vec{p}_s)\rangle = \begin{pmatrix} -\epsilon_1 & a^* \\ a & -\epsilon_2 \end{pmatrix}_{rs}$$

2) Eigenvectors $e_r^{(\pm)}$:

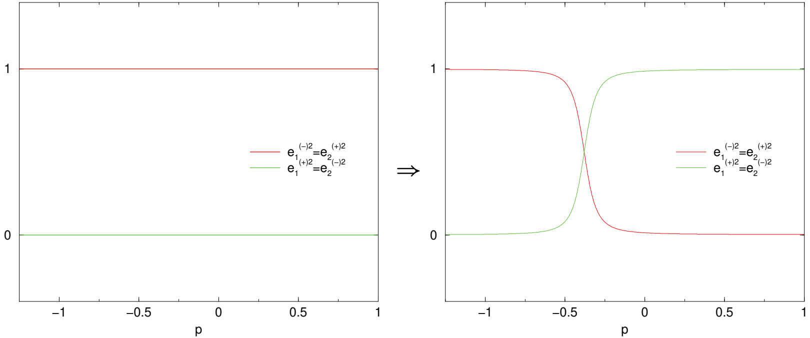
$$e_r^{(\pm)} = N^{(\pm)}(a) \begin{pmatrix} \lambda|a| \\ \gamma_\pm e^{i\theta_a} \end{pmatrix}_r$$

- $\gamma_\pm = \frac{1}{2}(E_{N/\Sigma} - E_N) \pm \frac{1}{2}\Delta E$
- $N^{(\pm)}(a)$ normalisation factor
- θ_a phase of a: $a = |a|e^{i\theta_a}$, ie phase of matrix element contained in eigenvectors
- Components related: $e_2^{(-)} = -e_1^{(+)}e^{i\theta_a}$ and $e_2^{(+)} = e_1^{(-)}e^{i\theta_a}$

Quasi–degenerate eigenvectors – $\Sigma \to N$ decay

$$\vec{e}^{(\pm)} = \begin{pmatrix} e_1^{(\pm)} \\ e_2^{(\pm)} \end{pmatrix}$$

eg 1-dimensional sketch: $[\lambda^2|a|^2 = \text{const.},\ \theta_a = 0,\ q = 1]$



- Free case ⇒ Interacting case: change of state
- Sketch based on previous formulae

Incorporating the spin index

- $|B_r(\vec{p}_r)\rangle \to |B_r(\vec{p}_r, \sigma_r)\rangle$, $\sigma_r = \pm 1$ spin index
- D matrix doubled in size: $\sigma_r r = +1, -1, \ldots + d_S, -d_S$ ie $2d_S \times 2d_S$
- Energy states corresponding to $|B_r(\vec{p}_r, \sigma_r)\rangle$, $\sigma = \pm$ are degenerate [Kramers degeneracy] so still have d_S eigenvalues: $E_\lambda^{(i)}$
- Explicit form factor decomposition of matrix element shows that different spin components of matrix elements related to each other
- Upshot for previous examples $[\eta = \pm]$

$$\langle B_r(\vec{p}_r, \sigma_r)|\hat{\tilde{\mathcal{O}}}(\vec{q})|B_s(\vec{p}_s, \sigma_s)\rangle = \begin{pmatrix} 0 & a^* \\ a & 0 \end{pmatrix}_{\sigma_r r, \sigma_s s} \qquad a \to \begin{pmatrix} a_{++} & a_{+-} \\ -\eta a_{+-}^* & \eta a_{++}^* \end{pmatrix}$$

- Giving

$$\Delta E_\lambda(\vec{p}, \vec{q}) = \sqrt{(E_N(\vec{p}+\vec{q}) - E_{N/\Sigma}(\vec{p}))^2 + 4\lambda^2 \left|\det a\right|^2}$$

where

$$\left|\det a\right|^2 = \underbrace{\left|\langle N(\vec{p}+\vec{q},+)|\hat{O}(\vec{0})|N/\Sigma(\vec{p},+)\rangle\right|^2}_{|a_{++}|^2} + \underbrace{\left|\langle N(\vec{p}+\vec{q},+)|\hat{O}(\vec{0})|N/\Sigma(\vec{p},-)\rangle\right|^2}_{|a_{+-}|^2}$$

Conclusions

- FH approach is a viable alternative to conventional method of 3-pt correlation functions for computing matrix elements
- FH approach only requires 2-pt correlation functions
- FH approach now generalised to decays
- With quasi-degenerate theory, don't need to tune for degenerate energies as before – in principle can re-use propagators for other decay/transition processes
- Example of method for $\Sigma \to N$ decay for $\langle N|\bar{u}\gamma_4 s|\Sigma\rangle$ in next talk