

# Probing the nucleon and its excitations in Full QCD

Benjamin Owen

Waseem Kamleh, Derek Leinweber, Jack Dragos, M. Selim Mahbub, Ben Menadue &  
James Zanotti

August 1st, 2013

# Outline

- 1 Correlation Matrix Techniques
- 2 Calculation Details
- 3 Cost vs Benefit

# Motivation

- A long standing issue within the lattice community has been the systematically low value for  $g_A$
- A number of systematic effects have been proposed as the cause – many of these were detailed in the Hadron Structure talk at last years Lattice Conference<sup>1</sup>
- The CSSM and others have begun utilising correlation matrix techniques to access excited state properties and transitions<sup>2–7</sup>
- Correlation matrix techniques provide us with a systematic framework to examine excited state effects on the calculation of  $g_A$

<sup>1</sup> *H. W. Lin, PoS LATTICE 2012, 013 (2012)*

<sup>2</sup> *B. J. Owen et al., Phys. Lett. B 723, 217 (2013) [arXiv:1212.4668 [hep-lat]]*

<sup>3</sup> *B. J. Owen et al., PoS LATTICE 2012, 173 (2012)*

<sup>4</sup> *B. J. Menadue et al., PoS LATTICE 2012, 178 (2012)*

<sup>5</sup> *J. Dudek et al., Phys. Rev. D 79, 094504 (2009) [arXiv:0902.2241 [hep-ph]].*

<sup>6</sup> *J. Bulava et al., JHEP 1201, 140 (2012) [arXiv:1108.3774 [hep-lat]]*

<sup>7</sup> *T. Maureret al., arXiv:1202.2834 [hep-lat] (2012)*

# CM Analysis

- A systematic framework for generating ideal operators for Hamiltonian Eigenstates
- Require a basis of operators:  $\{\chi_i\}; i \in [1, N]$
- Calculate set of cross-correlation functions

$$\begin{aligned} \mathcal{G}_{ij}(t, \vec{p}; \Gamma) &= \sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}} \text{tr}(\Gamma \langle \Omega | \chi_i(x) \bar{\chi}_j(0) | \Omega \rangle) \\ &= \sum_{\alpha=0}^{N-1} e^{-E_\alpha(\vec{p})t} Z_i^\alpha(\vec{p}) \bar{Z}_j^\alpha(\vec{p}) \text{tr} \left( \frac{\Gamma(\not{p} + m_\alpha)}{2E_\alpha(\vec{p})} \right) \end{aligned}$$

where  $Z_i^\alpha, \bar{Z}_j^\alpha$  are the couplings of sink operator ( $\chi_i$ ) and source operator ( $\bar{\chi}_j$ ) for the state  $\alpha$

## CM Analysis (cont)

- Desire  $N$  linearly independent sink ( $\phi_\alpha$ ) and source ( $\bar{\phi}_\alpha$ ) operators
- Ideally, we want these operators to satisfy

$$\langle \Omega | \phi^\beta | m_\alpha, p, s \rangle = \delta_{\alpha\beta} \mathcal{Z}^\alpha(\vec{p}) \sqrt{\frac{m_\alpha}{E_\alpha(\vec{p})}} u(p, s)$$

- use our basis of operators to construct these new operators

$$\left. \begin{aligned} \bar{\phi}_\alpha(x, \vec{p}) &= \sum_{i=1}^N u_i^\alpha(\vec{p}) \bar{\chi}_i(x) \\ \phi_\alpha(x, \vec{p}) &= \sum_{i=1}^N v_i^\alpha(\vec{p}) \chi_i(x) \end{aligned} \right\} \text{optimal coupling to state } |m_\alpha, p, s\rangle$$

## CM Analysis (cont)

- Using the above definitions, it is easy to show that the desired values for  $u_i^\alpha$ ,  $v_i^\alpha$  are the components of the eigenvectors for the following eigenvector equations

### CM Eigenvalue Equation

$$[\mathcal{G}^{-1}(t_0, \vec{p}; \Gamma) \mathcal{G}(t_0 + \Delta t, \vec{p}; \Gamma)]_{ij} u_j^\alpha(\vec{p}) = \lambda^\alpha u_j^\alpha(\vec{p}) \quad (1a)$$

$$v_i^\alpha(\vec{p}) [\mathcal{G}(t_0 + \Delta t, \vec{p}; \Gamma) \mathcal{G}^{-1}(t_0, \vec{p}; \Gamma)]_{ij} = \lambda^\alpha v_i^\alpha(\vec{p}) \quad (1b)$$

where  $\lambda^\alpha = e^{-E_\alpha(\vec{p})\Delta t}$ .

- Using  $v_i^\alpha(\vec{p})$ ,  $u_j^\alpha(\vec{p})$  we are able to project out the correlation function for the state  $|m_\alpha, p, s\rangle$

$$\mathcal{G}_\alpha(t, \vec{p}; \Gamma) = v_i^\alpha(\vec{p}) \mathcal{G}_{ij}(t, \vec{p}; \Gamma) u_j^\alpha(\vec{p})$$

# Our operator basis

- For the best results, one needs a basis of operators which are significantly independent to ensure that their overlap with energy eigenstates is different.
- Smearing alters the overlap of an operator with the eigenstates
- In this work we will use Gauge Invariant Gaussian smearing as a method to increase the number of available operators

# Gauge Invariant Gaussian smearing

- Gauge invariant smeared sources are constructed via an iterative process evaluated on point source  $\psi_0(x)$ ,

$$\psi_i(x) = \sum_{x'} F(x, x') \psi_{i-1}(x')$$

where

$$F(x, x') = (1 - \alpha) \delta_{x', x} + \frac{\alpha}{6} \sum_{\mu=1}^3 [U_\mu(x) \delta_{x', x+\hat{\mu}} + U_\mu^\dagger(x - \hat{\mu}) \delta_{x', x-\hat{\mu}}].$$

- Thus we smeared source with  $n$  sweeps of smearing is

$$\psi_n(x) = \sum_{x'} F^n(x, x') \psi_0(x')$$

# Smearing Parameters

In this work we have used four levels of smearing with smearing fraction  $\alpha = 0.7$ . This choice was determined<sup>1</sup> to best span the operator space resulting in the best projection of energy eigenstates.

Below we list the corresponding rms-radii for these sources.

**Table :** The rms radii for the various levels of smearing considered in this work.

Sweeps of smearing	rms radius (fm)
16	0.216
35	0.319
100	0.539
200	0.778

<sup>1</sup>*M. S. Mahbub et al., Phys. Lett. B. 707, (2012) 389*

## CM Analysis for 3pt-functions

- As we have for two-point case, we calculate the set of three-point cross-correlation functions,

$$G_{ij}(\vec{p}', \vec{p}; t_2, t_1; \Gamma') = \sum_{\vec{x}_1, \vec{x}_2} e^{-i\vec{p}' \cdot \vec{x}_2} e^{+i(\vec{p}' - \vec{p}) \cdot \vec{x}_1} \text{tr} \left( \Gamma' \langle \Omega | \chi_i(x_2) \mathcal{O}(x_1) \bar{\chi}_j(0) | \Omega \rangle \right),$$

where  $\mathcal{O}(x)$  is the current operator to be inserted.

- This we can expand in an analogous manner to give couplings, exponential factors and the desired matrix element,

$$G_{ij}(\vec{p}', \vec{p}; t_2, t_1; \Gamma') = \sum_{\alpha, \beta} e^{-E_\beta(\vec{p}')(t_2 - t_1)} e^{-E_\alpha(\vec{p})t_1} Z_i^\beta(\vec{p}') \bar{Z}_j^\alpha(\vec{p}) \sqrt{\frac{m_\alpha m_\beta}{E_\alpha(\vec{p}) E_\beta(\vec{p}')}} \text{tr} \left( \Gamma' \sum_{s', s} u(p', s') \langle \beta, p', s' | \mathcal{O}(0) | \alpha, p, s \rangle \bar{u}(p, s) \right).$$

## CM Analysis for 3pt-functions (cont)

- The eigenvectors derived from the two-point analysis can be used to project out the three-point function
- The key is to ensure that the eigenvector corresponds to the momentum to be projected at the source / sink

$$G^\alpha(\vec{p}', \vec{p}; t_2, t_1; \Gamma') = v_i^\alpha(\vec{p}') G_{ij}(\vec{p}', \vec{p}; t_2, t_1; \Gamma') u_j^\alpha(\vec{p}).$$

- With the desired state now isolated, one simply uses the projected correlation functions in the ratio to extract the matrix element.
- In this work we have used the following ratio,

$$R^\alpha(\vec{p}', \vec{p}; \Gamma', \Gamma) = \sqrt{\frac{G^\alpha(\vec{p}', \vec{p}; t_2, t_1; \Gamma') G^\alpha(\vec{p}, \vec{p}'; t_2, t_1; \Gamma')}{G^\alpha(\vec{p}, t_2; \Gamma) G^\alpha(\vec{p}', t_2; \Gamma)}}.$$

# Accessing the Nucleon Axial Charge

- Probe the nucleon via the axial current.

This vertex can be expressed as,

$$\langle p(p', s') | A_\mu^{u-d} | p(p, s) \rangle = \left( \frac{m^2}{E_{p'} E_p} \right)^{1/2} \bar{u}(p', s') \left[ \gamma_\mu \gamma_5 G_A(Q^2) + \gamma_5 \frac{q_\mu}{2m} G_P(Q^2) \right] u(p, s),$$

where  $A_\mu^{u-d} = \bar{u} \gamma_\mu \gamma_5 u - \bar{d} \gamma_\mu \gamma_5 d$ .

- Selecting the nucleon rest frame, we extract correlation matrix improved value for  $g_A$  from the following ratio

$$g_A^{CM} = \frac{v_i^0(\vec{0}) \mathcal{G}_{ij}(\vec{0}, \vec{0}; t_2, t_1; \Gamma_3) u_j^0(\vec{0})}{v_i^0(\vec{0}) \mathcal{G}_{ij}(\vec{0}, t; \Gamma_4) u_j^0(\vec{0})}.$$

# Configuration Details

- For this calculation we are working with the PACS-CS (2+1)-flavour Full QCD ensembles<sup>1</sup> made available through the ILDG
- These are  $32^3 \times 64$  lattices with  $\beta = 1.9$ , corresponding to a physical lattice spacing of 0.0907(13) fm
- Iwasaki gauge action and pre-conditioned Wilson-Clover quark action
- There are five light quark-masses resulting in pion masses that range from 622 MeV through to 156 MeV
- Here we focus on the second lightest mass with  $m_\pi^2 = 290$  MeV over 200 gauge field configurations

<sup>1</sup>*S. Aoki et al., Phys. Rev. D* **79**, 034503 (2009)

# Simulation Parameters

- The variational parameters  $t_0 = 18$  and  $\Delta t = 2$  were used having been shown<sup>1</sup> to give the best balance between systematic and statistical uncertainties
- For this calculation, we choose to use fixed current SST method where we use a naive axial current inserted at  $t_C = 21$  relative to the source at  $t_0 = 16$
- The current renormalization parameter  $Z_A = 0.781(20)$  and was determined<sup>2</sup> non-perturbatively using a Schrödinger functional scheme

<sup>1</sup>*M. S. Mahbub et al., Phys. Lett. B. 707, (2012) 389*

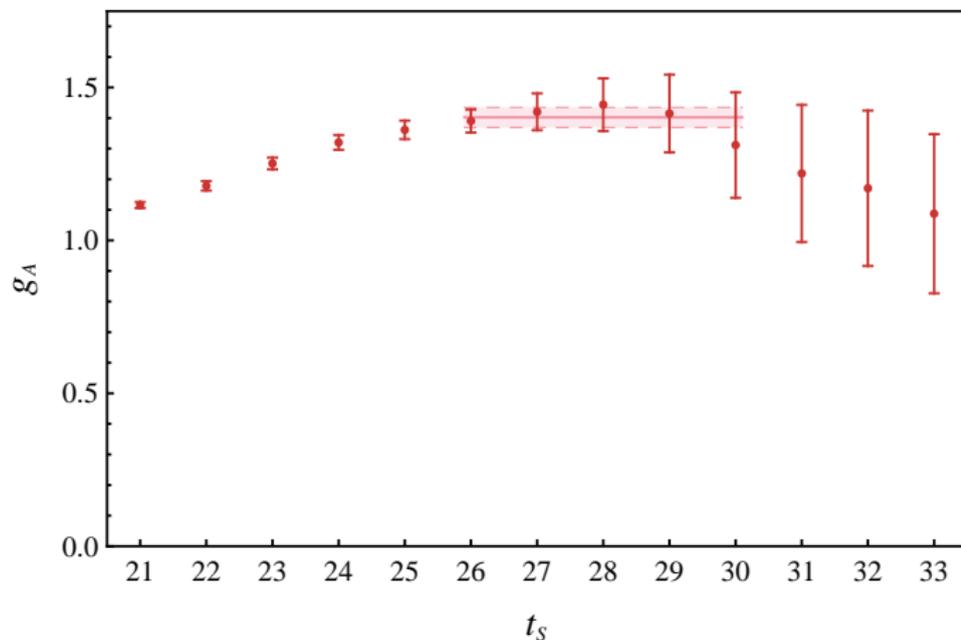
<sup>2</sup>*S. Aoki et al., JHEP. 1008 (2010) 101*

## Comparison between methods

- We shall compare standard single correlation function method with our correlation matrix improved method.
- Red dataset will be smeared source to point sink
- Purple dataset will be smeared source to smeared sink
- Blue dataset will be correlation matrix method
- The fits have been chosen by criterion that the  $\chi_{\text{dof}}^2$  obtained via a covariance matrix analysis be as close to 1 as possible

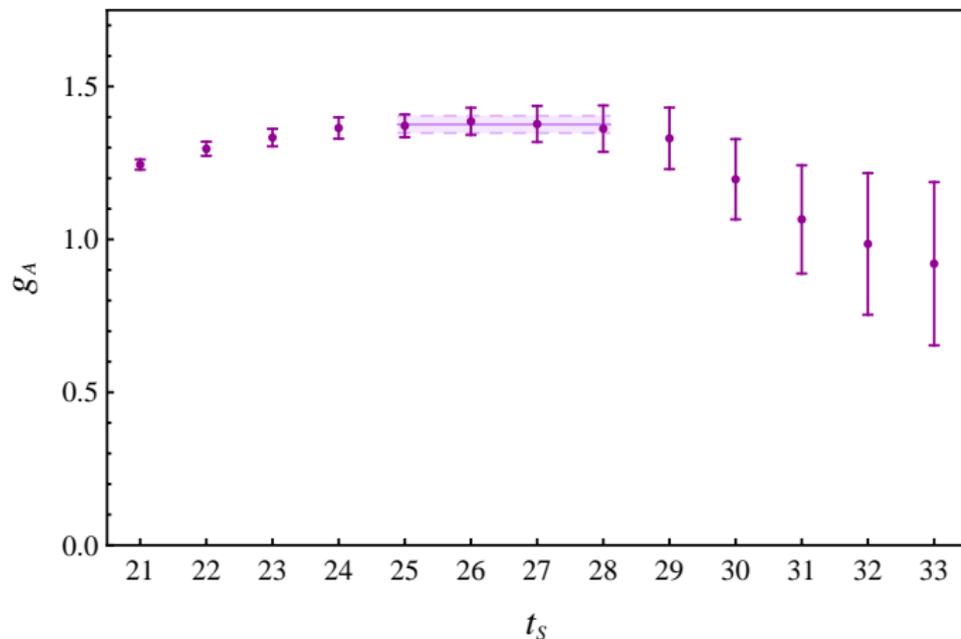
## Standard method: smeared source to point sink

- Search for plateau following current at  $t_C = 21$
- Clear presence of excited state effects from times 21 to 25
- Based on the  $\chi^2_{\text{dof}}$ , earliest possible fit-window is at  $t_S = 26$



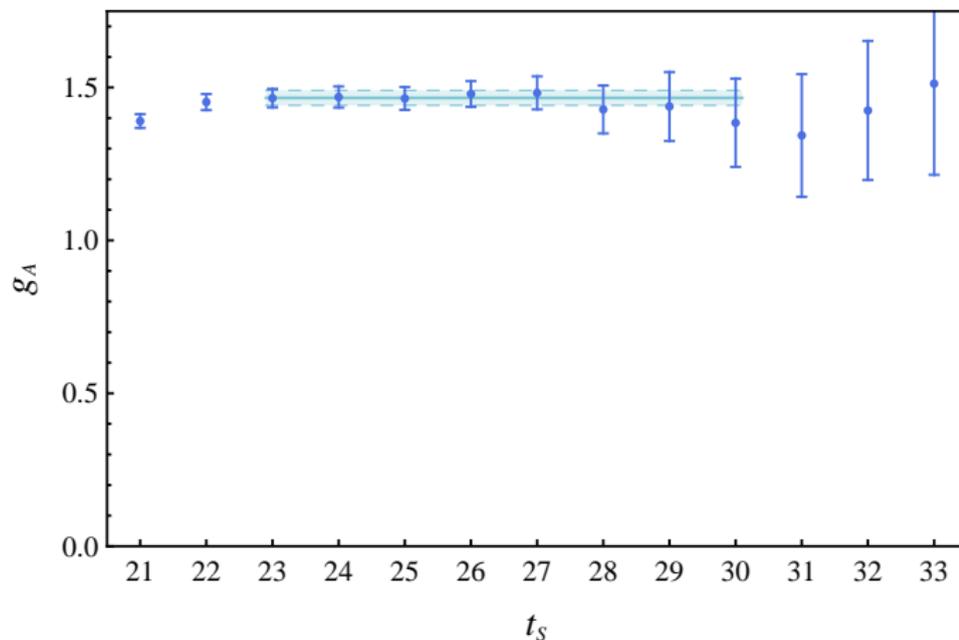
## Standard method: smeared source to smeared sink

- Diminished excited state effects, but still present
- Earliest possible fit-window is now at  $t_S = 25$

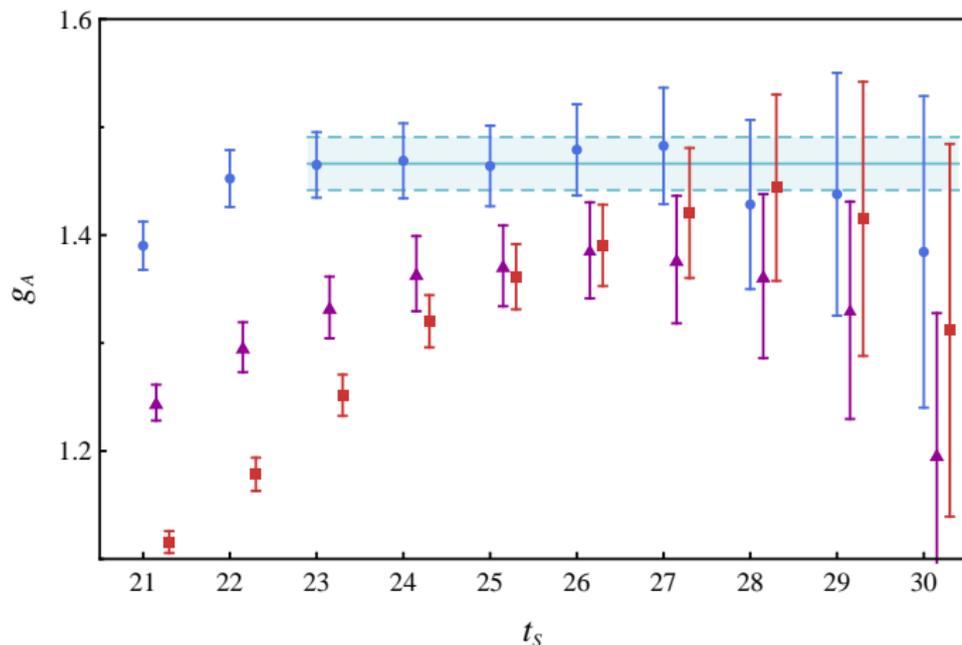


## Variational method

- Excited state effects limited to a single time-slice after the current
- Early onset of ground state dominance provides smaller statistical uncertainties



## Overlay of previous three plots



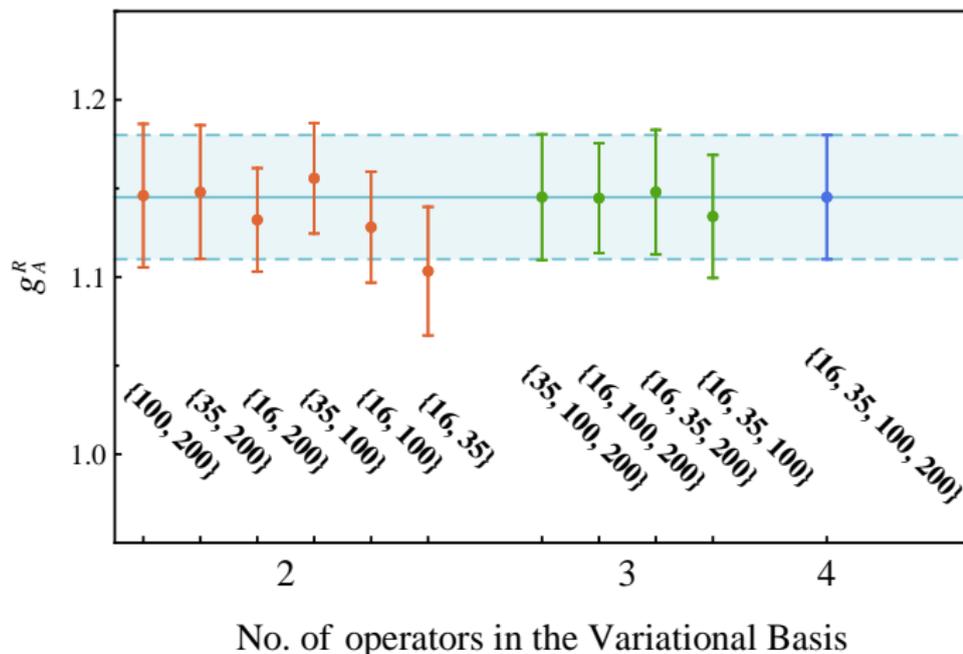
- Note that the smeared-smeared approach has no overlap with the fit for the correlation matrix approach
- Failure to obtain ground state dominance by  $t_C = 21$  leads to incorrect plateau values in the standard method

# Fine tuning

- In practice one could tune their smearing to give the best overlap with the ground state
- This can be an expensive exercise in itself and this tuning is unique to a single state at a particular quark mass
- Using variational approach as we have here automatically gives optimal overlap without the need for tedious fine tuning
- In practice, if one wants to control excited state contaminations, the only robust solution is to remove, not suppress these contributions

## Examining the operator basis

- The larger the variational basis the more excited states are removed
- Here we have considered all subsets of our variational basis to consider how small one can make the operator basis



# Cost vs Benefit

- A concern with a correlation matrix approach is the associated cost
- In our implementation (fixed current SST), we require  $2n$  inversions per configuration where  $n$  is the number of smearings
  - ▶ A total of 8 inversions per configuration were used herein
  - ▶ The minimal method requires 2 inversions per configuration
  - ▶ Using a fixed sink SST inversion would require an inversion for each source-sink smearing combination resulting in  $n^2 + n$  inversions per configurations
- At large Euclidean times, the standard approach is consistent with the correlation matrix approach, albeit with larger errors
- It is worth considering what the required increase in statistical sample would be for the standard method to produce similar errors

## Cost vs Benefit (cont)

- Consider the ratio

$$\frac{N_{\text{required}}}{N_{\text{current}}} = \left( \frac{(\Delta g_A)_{\text{current}}}{(\Delta g_A)_{\text{desired}}} \right)^2 = \left( \frac{(\Delta g_A)_{\text{sm-sm}}}{(\Delta g_A)_{\text{CM}}} \right)^2 .$$

- As the leading error dominates the error on the fit, we will use this as being indicative of the uncertainty in  $g_A$
- For the variational method
  - ▶ Ground dominance of the two-point function occurs at  $t = 21$
  - ▶ Ground dominance of the three-point function occurs two time slices after the current
  - ▶ At  $t_S = 21 + 2 = 23$  we have  $(\Delta g_A)_{\text{CM}} = 0.030$
- For the standard method using smeared source and smeared sink
  - ▶ Ground dominance of the two-point function occurs at  $t = 23$
  - ▶ Ground dominance of the three-point function (from Fig. 2) occurs six time slices after the current
  - ▶ At  $t_S = 23 + 6 = 29$  we have  $(\Delta g_A)_{\text{sm-sm}} = 0.101$

## Cost vs Benefit (cont)

- Using these values we get

$$\frac{N_{\text{required}}}{N_{\text{current}}} = \left( \frac{0.101}{0.030} \right)^2 \simeq 11.3.$$

a factor of 11 increase in statistics!

- If one were solely interested in properties of a single state, ie. ground state, then one could use the optimised sources generated via the two-point correlation matrix as input for the SST inversion
- This reduces the cost from  $2n$  (fixed current) or  $n^2 + n$  (fixed sink) down to  $n + 1$  for either case
- Based on Fig. 5, a basis of 3 (well chosen) operators is enough to isolate the ground state – this gives a total cost of 4 inversions per configuration
- Thus for a factor of two increase in cost, we effectively obtain an order of magnitude improvement in the statistics

# Concluding Remarks

- As the variational approach enables one to:
  - ▶ rapidly isolate the ground state following the source enabling an earlier current insertion, and
  - ▶ rapidly isolate the ground state again after inserting the current enabling an earlier Euclidean time fit,
- The associated reduction in the error bar from this process outweighs the increased cost in constructing the matrix of cross-correlators
- In practice, if one wants to control excited state contaminations, the only robust solution is to remove, not suppress these contributions
- The variational approach offers improved access to observables and will be instrumental in the era of precision matrix element determinations