Excited States and Precision Calculations of Hadron Structure

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Systematic Uncertainties

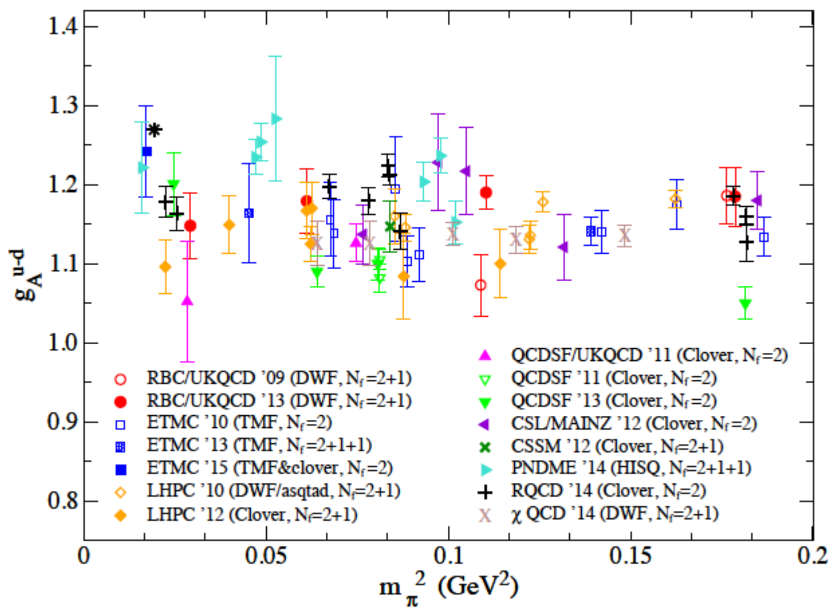
- Non-zero lattice spacing and continuum limit $a \rightarrow 0$
- Finite volume $V \rightarrow \infty$
- $m_\pi \rightarrow m_\pi^{phys}$
- Number of quark flavors
- *Isolating ground states*

- Nucleon Charges
- Nucleon Charge Radius

Precision Calculations of Nucleon Charges

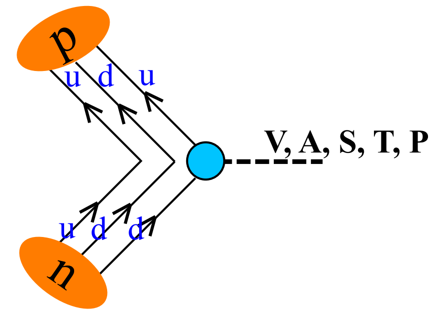
Hadron Structure

M Constantinou, arXiv:1511.00214



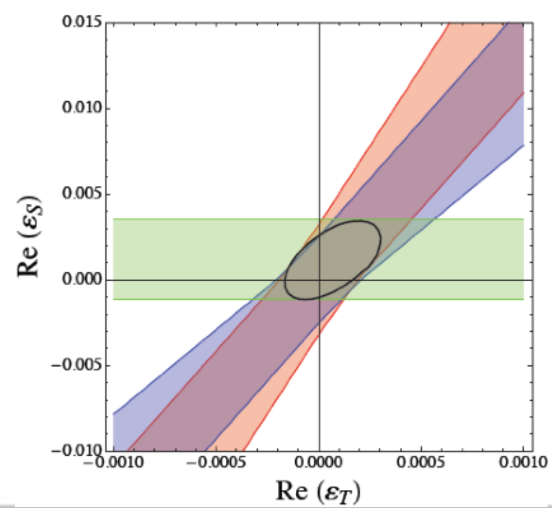
- Governs beta-decay rate
- Important for proton-proton fusion rate in solar models
- Benchmark for lattice QCD calculations of hadron structure

e.g. novel interactions probed in ultra-cold neutron decay



$$H_{eff} \supset G_F\left[\varepsilon_S\, \bar{u}d \times \bar{e}(1-\gamma_5)\nu_e + \varepsilon_T\, \bar{u}\sigma_{\mu\nu}d \times \bar{e}\sigma^{\mu\nu}(1-\gamma_5)\nu_e\right]$$

$$g_S = Z_S \langle p|\bar{u}d|n\rangle \quad g_T = Z_T \langle p|\bar{u}\,\sigma_{\mu\nu}\, d|n\rangle$$



R Gupta, 2014

Calculation of Physics Observables

Our paradigm: nucleon mass $$C(t) = \sum_{\vec{x}} \langle N(\vec{x}, t)\bar{N}(0)\rangle = \sum_n \mid A_n \mid^2 e^{-E_n t}$$

Noise: $$C_{\sigma^2}(t) = \sum_{\vec{x}} \langle \bar{N}N(\vec{x}, t)\bar{N}N(0)\rangle \longrightarrow e^{-3m_\pi t}$$

whence $$\boxed{C(t)/\sqrt{C_{\sigma^2}(t)} \simeq e^{-(m_N - 3m_\pi/2)t}}$$

Use local nucleon interpolating operators $[uC\gamma_5(1 \pm \gamma_4)d]u$

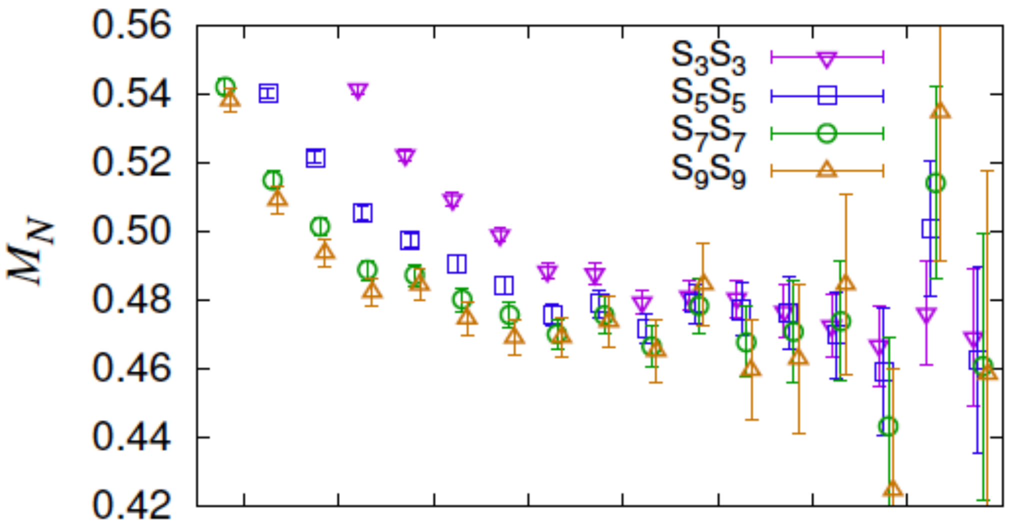
Replace quark field by spatially extended (smeared) quark field

$$\psi \longrightarrow (1 - \sigma^2\nabla^2/4N)^N \psi$$

Excited States: Smearing Radii

Yoon et al., Phys. Rev. D 93, 114506 (2016)

ID	Method	Analysis	Smearing Parameters	$t_{\rm sep}$	LP	HP
R1	AMA	2-state	$\{5, 60\}$	10,12,14,16,18	96	3
R2	LP	VAR	$\{3, 22\}$, $\{5, 60\}$, $\{7, 118\}$	12	96	
R3	AMA	VAR	$\{5, 46\}$, $\{7, 91\}$, $\{9, 150\}$	12	96	3
R4	AMA	2-state	$\{9, 150\}$	10,12,14,16,18	96	3



$$m_{\rm eff} = \ln C(t)/C(t+1) \to E_0$$

Variational Method

Subleading terms → *Excited* states

Construct matrix of correlators: *different smearing radii*

$$C_{ij}(t) = \sum_{\vec{x}} \langle N_i(\vec{x},t)\bar{N}_j(0)\rangle = \sum_n A_n^i A_n^{j\dagger} e^{-E_n t}$$

Delineate contributions using *variational method*: solve

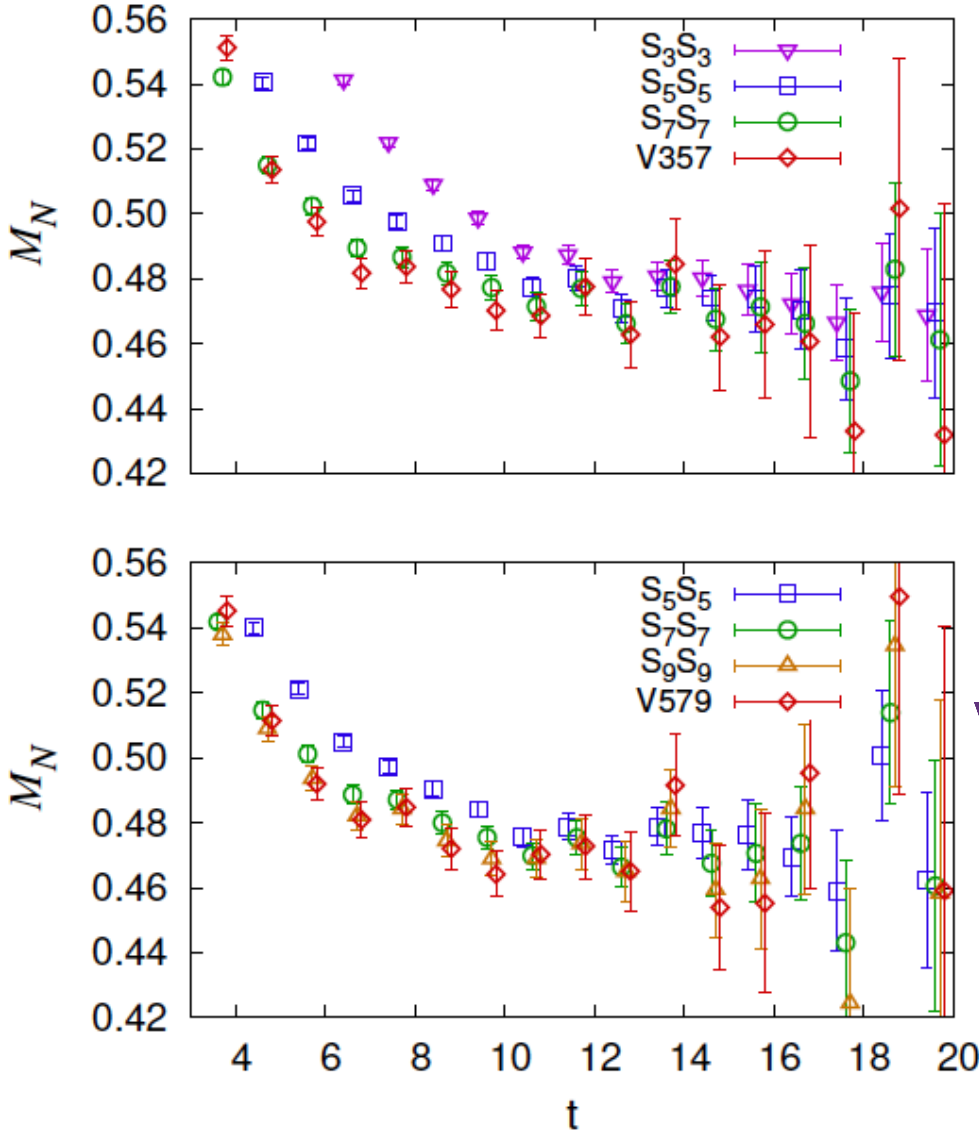
$$C(t)v^{(N)}(t,t_0) = \lambda_N(t,t_0)C(t_0)v^{(N)}(t,t_0).$$

$$\lambda_N(t,t_0) \to e^{-E_N(t-t_0)}(1+\mathcal{O}(e^{-\Delta E(t-t_0)}))$$

Eigenvectors, with metric $C(t_0)$, are orthonormal and project onto the respective states

$$v^{(N')\dagger}C(t_0)v^{(N)} = \delta_{N,N'}$$

Nucleon Mass - II



$$m_{\text{eff}} = \ln C(t)/C(t+1) \to E_0$$

Variational method: single-state domination nearer source

increase signal-to-noise

} Fixed Smearing

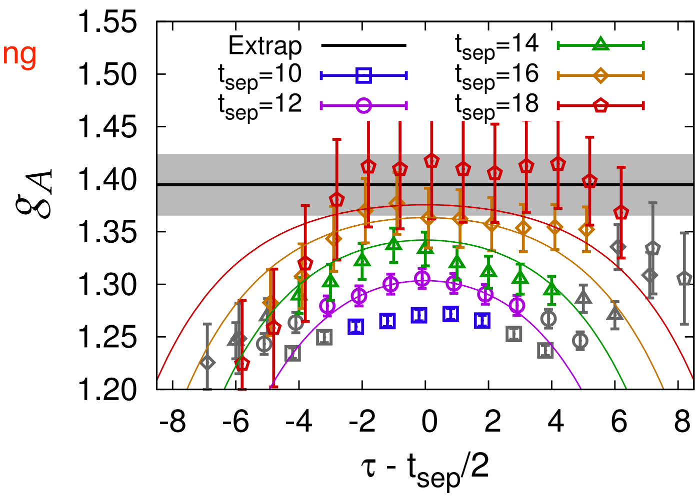
Variational

Variational Method

Fixed source smearing

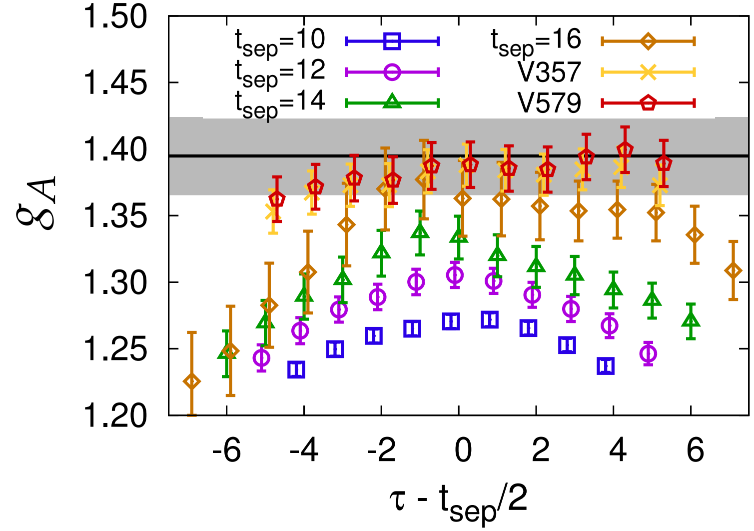
$$C_\Gamma^{3\text{pt}}(t_{\text{sep}},\tau) = \sum_{\vec{x},\vec{y}} \langle N(\vec{x},t_{\text{sep}})\Gamma(\vec{y},\tau)\bar{N}(0,0)\rangle$$

$$= |A_0|^2 \langle 0|\Gamma|0\rangle e^{-M_0 t_{\text{sep}}} + |A_1|^2 \langle 1|\Gamma|1\rangle e^{-M_1 t_{\text{sep}}} + A_0 A_1^* \langle 0|\Gamma|1\rangle e^{-M_0\tau} e^{-M_1(t_{\text{sep}}-\tau)} \ldots$$

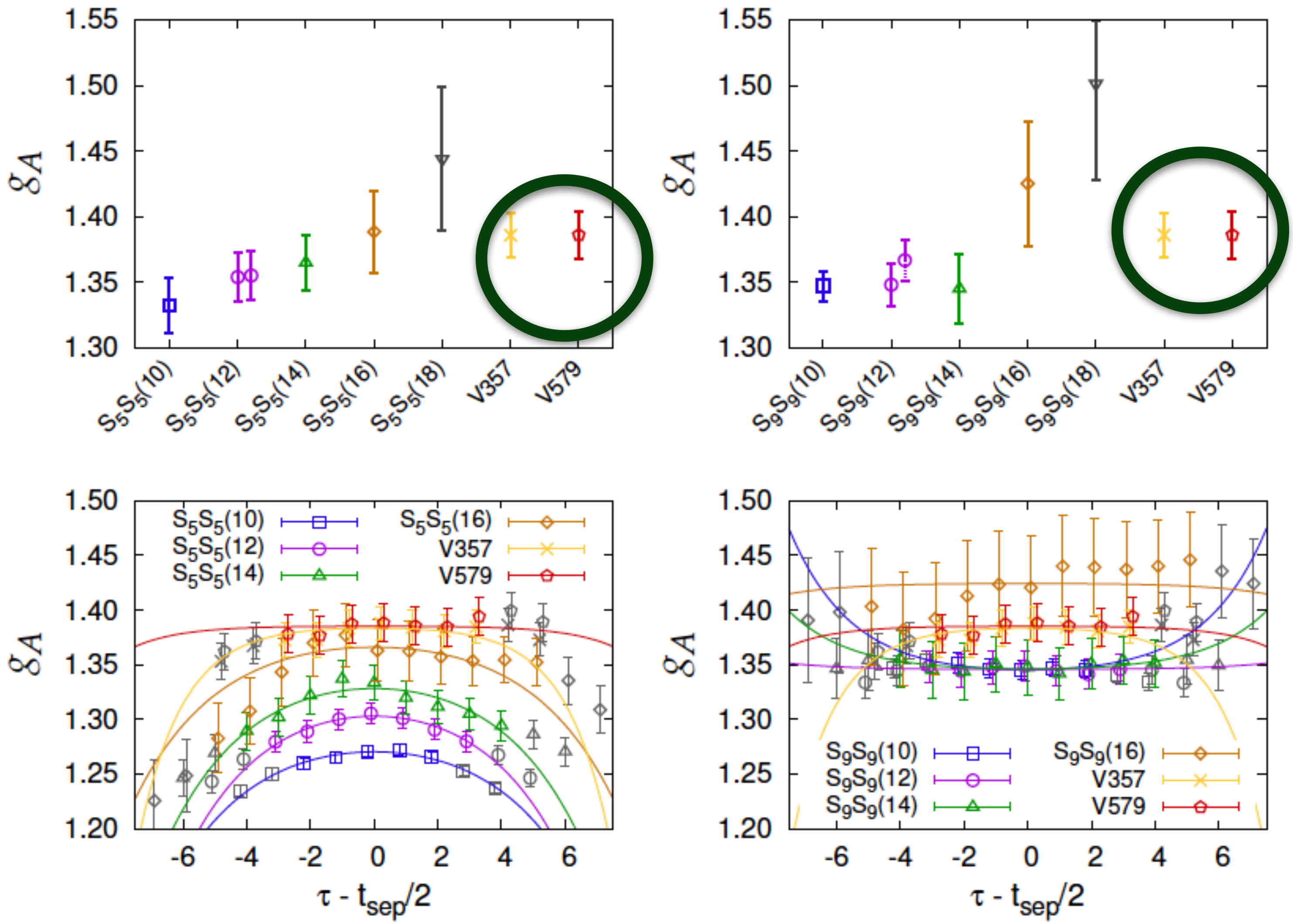


Grey Band : $t_{\text{sep}} \to \infty$

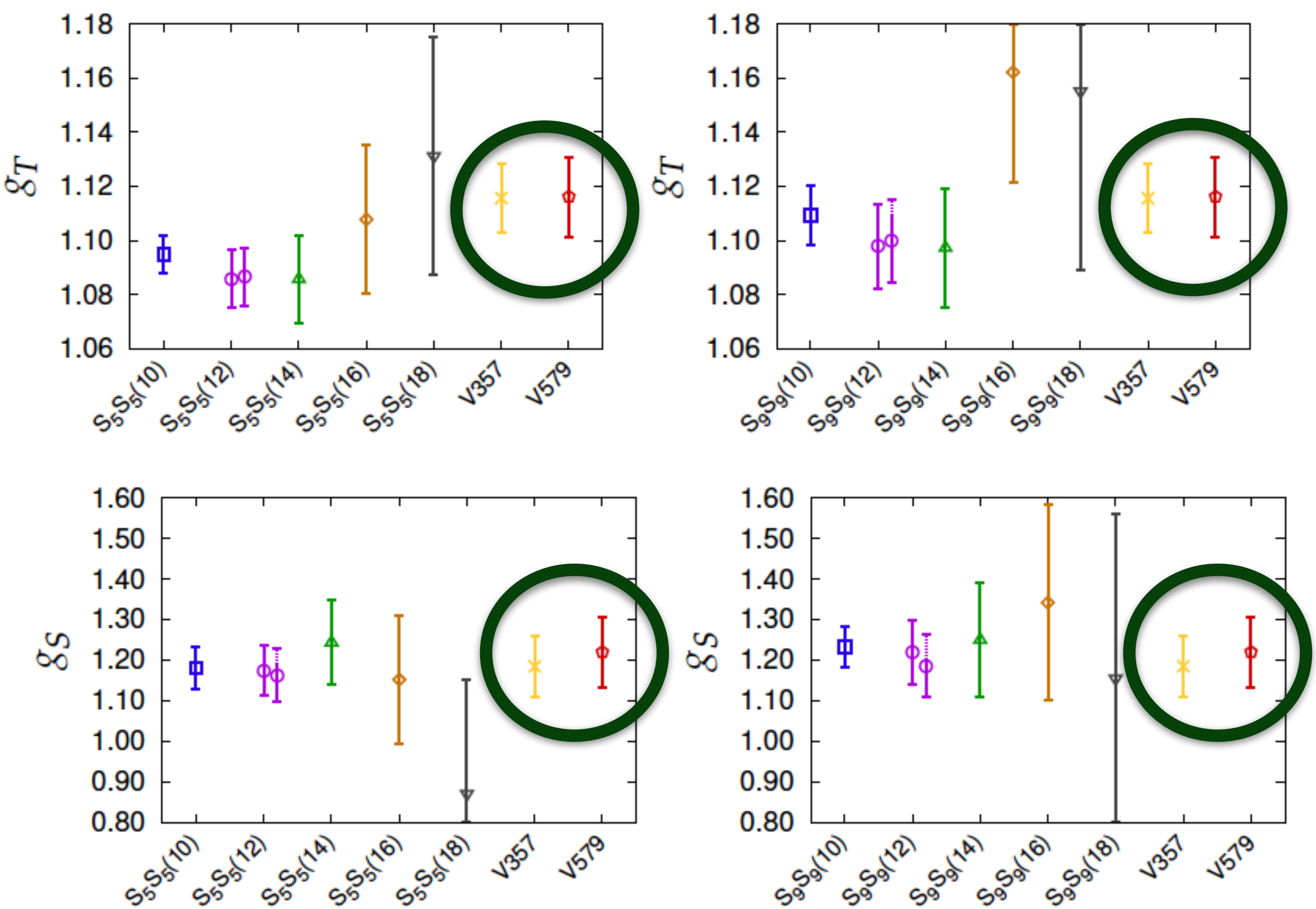
Variational Method



Variational Comparison - II



Variational - III



Controlling excited states essential for precision calculations!

Renormalized Charges

Yoon et al., Phys. Rev. D 95, 074508 (2017)

ID	Lattice Theory	a fm	M_π(MeV)	g_A^{u-d}	g_S^{u-d}	g_T^{u-d}	g_V^{u-d}
$a127m285$	2+1 clover-on-clover	0.127(2)	285(6)	1.249(28)	0.89(5)	1.023(21)	1.014(2
$a12m310$	2+1+1 clover-on-HISQ	0.121(1)	310(3)	1.229(14)	0.84(4)	1.055(36)	0.969(2
$a094m280$	2+1 clover-on-clover	0.094(1)	278(3)	1.208(33)	0.99(9)	0.973(36)	0.998(2
$a09m310$	2+1+1 clover-on-HISQ	0.089(1)	313(3)	1.231(33)	0.84(10)	1.024(42)	0.975(3
$a091m170$	2+1 clover-on-clover	0.091(1)	166(2)	1.210(19)	0.86(9)	0.996(23)	1.012(2
$a09m220$	2+1+1 clover-on-HISQ	0.087(1)	226(2)	1.249(35)	0.80(12)	1.039(36)	0.969(3
$a09m130$	2+1+1 clover-on-HISQ	0.087(1)	138(1)	1.230(29)	0.90(11)	0.975(38)	0.971(3

Consistency between different actions

Matrix Elements of 1st excited state?

ID	Type	$\langle 0\vert\mathcal{O}_A\vert 1\rangle$	$\langle 0\vert\mathcal{O}_S\vert 1\rangle$	$\langle 0\vert\mathcal{O}_T\vert 1\rangle$	$\langle 0\vert\mathcal{O}_V\vert 1\rangle$	$\langle 1\vert\mathcal{O}_A\vert 1\rangle$	$\langle 1\vert\mathcal{O}_S\vert 1\rangle$	$\langle 1\vert\mathcal{O}_T\vert 1\rangle$	$\langle 1\vert\mathcal{O}_V\vert 1\rangle$
		−0.179(21)		0.182(16)		−0.9(2.4)		−0.2(1.2)	
			−0.35(4)		−0.014(2)		0.6(1.1)		0.80(34)
a127m285	S_5S_5	−0.172(18)	−0.37(4)	0.210(15)	−0.015(2)	0.75(48)	0.8(9)	0.42(27)	0.87(28)
		−0.295(58)	−0.45(15)	0.167(40)	−0.014(6)	1.5(3.0)	1.8(1.4)	0.54(86)	0.86(55)
		−0.295(57)	−0.45(15)	0.166(47)	−0.014(6)	1.46(54)	1.8(1.4)	0.54(41)	0.86(28)

arXiv:1704.01114, Berkowitz et al

Feynman-Hellman Method proceeds through looking at variation of a spectral function w.r.t external current.

$$\frac{\partial E_n}{\partial \lambda} = \langle n \mid H_\lambda \mid n \rangle \text{ where } H = H_0 + \lambda H_\lambda$$

See talk by K. Orginos

Nucleon Charge Radius

Bouchard, Chang, Orginos, Richards, PoS LATTICE2016 (2016) 170

Proton EM form factors

- Nucleon Pauli and Dirac Form Factors described in terms of matrix element of vector current

$$\langle N \mid V_\mu \mid N\rangle(\vec{q}) = \bar{u}(\vec{p}_f)\left[F_q(q^2)\gamma_\mu + \sigma_{\mu\nu}q_\nu \frac{F_2(q^2)}{2m_N}\right]u(\vec{p}_i)$$

- Alternatively, Sach's form factors determined in experiment

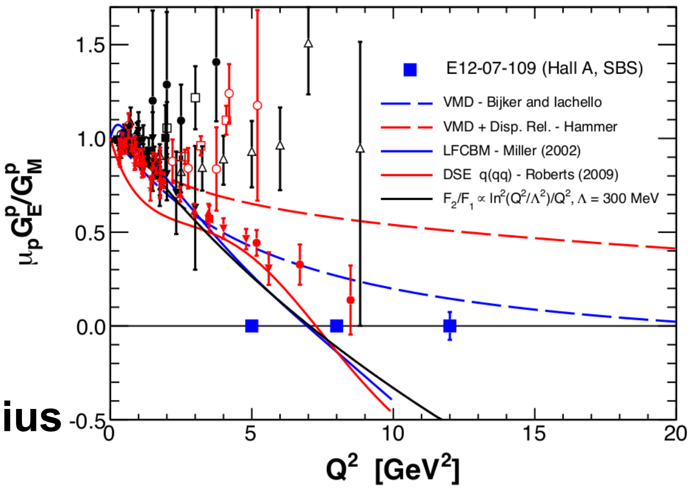
$$\begin{aligned} G_E(Q^2) &= F_1(Q^2) - \frac{Q^2}{4M^2}F_2(Q^2) \\ G_M(Q^2) &= F_1(Q^2) + F_2(Q^2) \end{aligned}$$

Charge radius is slope at $Q^2 = 0$

$$\left.\frac{\partial G_E(Q^2)}{\partial Q^2}\right|_{Q^2=0} = -\frac{1}{6}\langle r^2\rangle = \left.\frac{\partial F_1(Q^2)}{\partial Q^2}\right|_{Q^2=0} - \frac{F_2(0)}{4M^2}$$

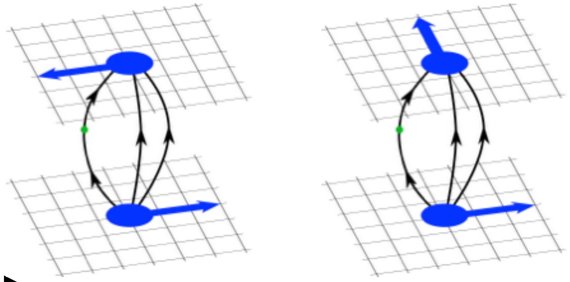
EM Form factors

PRAD: E12-11-106



Approved expt E12-07-109

$Q^2 \lesssim 8.2$ GeV^2 $\quad Q^2 \lesssim 4.1$ GeV^2



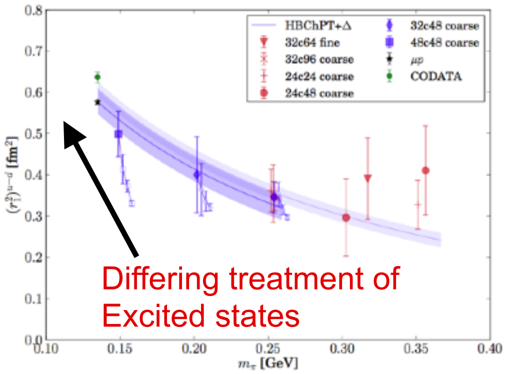
Nucleon Charge Radius

Boosted interpolating operators

Bali *et al*., Phys. Rev. D 93, 094515 (2016)

LHPC, Syritsyn, Gambhir, Orginos et al, Lattice 2016

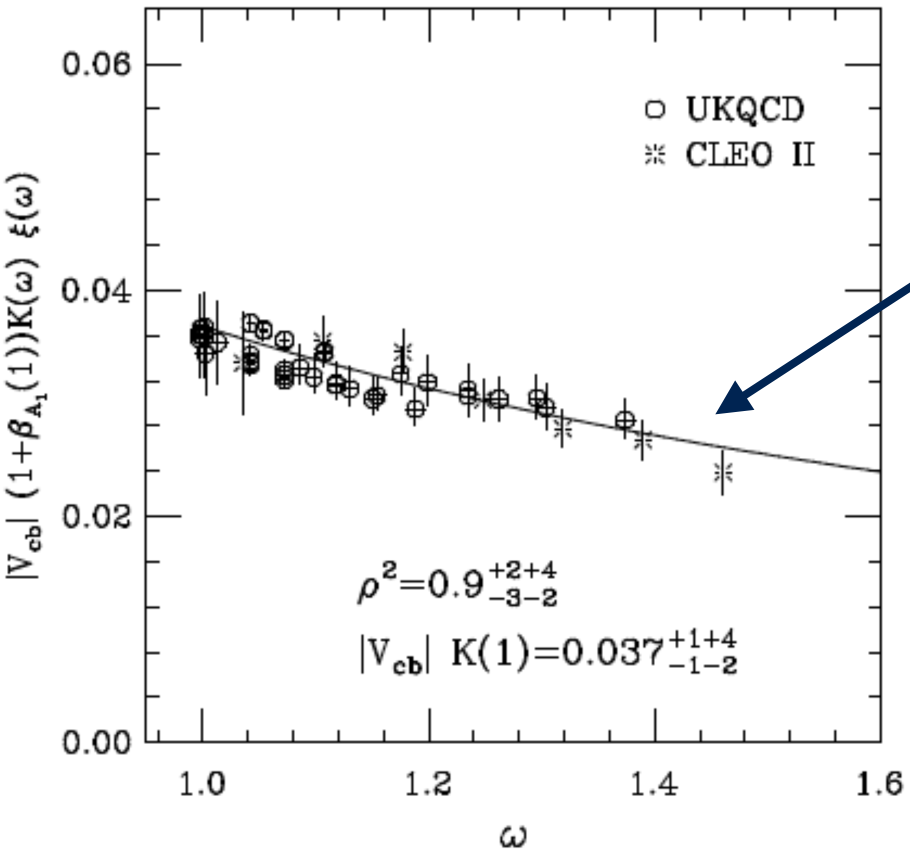
Green et al, arXiv:1404.40



Direct calculation of charge radius through coordinate-space moments

UKQCD, Lellouch, Richards *et al.*, NPB444 (1995) 401

Isgur-Wise Function and CKM matrix



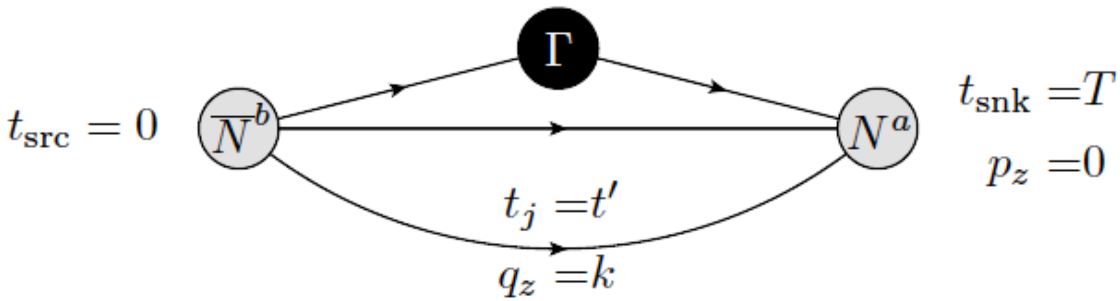
Extract V_{cb} if know intercept at zero recoil

Lattice

Calculate slope at zero recoil..

UKQCD, L. Lellouch et al., Nucl. Phys. B444, 401 (1995), hep-lat/9410013

Moment Methods



- Introduce three-momentum projected three-point function

$$C^{3\text{pt}}(t,t') = \sum_{\vec{x},\vec{x}'} \left\langle N^a_{t,\vec{x}} \Gamma_{t',\vec{x}'} \overline{N}^b_{0,\vec{0}} \right\rangle e^{-ikx'_z}$$

- Now take derivative w.r.t. *k*²

$$C'_{3\text{pt}}(t,t') = \sum_{\vec{x},\vec{x}'} \frac{-x'_z}{2k} \sin(kx'_z) \left\langle N^a_{t,\vec{x}} \Gamma_{t',\vec{x}'} \overline{N}^b_{0,\vec{0}} \right\rangle$$

whence

$$\lim_{k^2 \to 0} C'_{3\text{pt}}(t,t') = \sum_{\vec{x},\vec{x}'} \frac{-x'^2_z}{2} \left\langle N^a_{t,\vec{x}} \Gamma_{t',\vec{x}'} \overline{N}^b_{0,\vec{0}} \right\rangle .$$

Odd moments vanish by symmetry

Moment Methods - II

- Analogous expressions for two-point functions:

$$C_{2\mathrm{pt}}(t) = \sum_{\vec{x}} \left\langle N^b_{t,\vec{x}} \overline{N}^b_{0,\vec{0}} \right\rangle e^{-ikx_z}$$

$$\Longrightarrow$$

$$C'_{2\mathrm{pt}}(t) = \sum_{\vec{x}} \frac{-x_z}{2k} \sin\left(kx_z\right) \left\langle N^b_{t,\vec{x}} \overline{N}^b_{0,\vec{0}} \right\rangle$$

$$\Longrightarrow$$

$$\lim_{k^2 \to 0} C'_{2\mathrm{pt}}(t) = \sum_{\vec{x}} \frac{-x_z^2}{2} \left\langle N^b_{t,\vec{x}} \overline{N}^b_{0,\vec{0}} \right\rangle .$$

Lowest coordinate-space moment ⇔ slope at zero momentum

Moment Methods - II

- Analogous expressions for two-point functions:

$$C_{2\mathrm{pt}}(t) = \sum_{\vec{x}} \left\langle N^b_{t,\vec{x}} \overline{N}^b_{0,\vec{0}} \right\rangle e^{-ikx_z}$$

$$\Longrightarrow$$

$$C'_{2\mathrm{pt}}(t) = \sum_{\vec{x}} \frac{-x_z}{2k} \sin(kx_z) \left\langle N^b_{t,\vec{x}} \overline{N}^b_{0,\vec{0}} \right\rangle$$

$$\Longrightarrow$$

$$\lim_{k^2 \to 0} C'_{2\mathrm{pt}}(t) = \sum_{\vec{x}} \frac{-x_z^2}{2} \left\langle N^b_{t,\vec{x}} \overline{N}^b_{0,\vec{0}} \right\rangle .$$

Lowest coordinate-space moment ⇔ slope at zero momentum

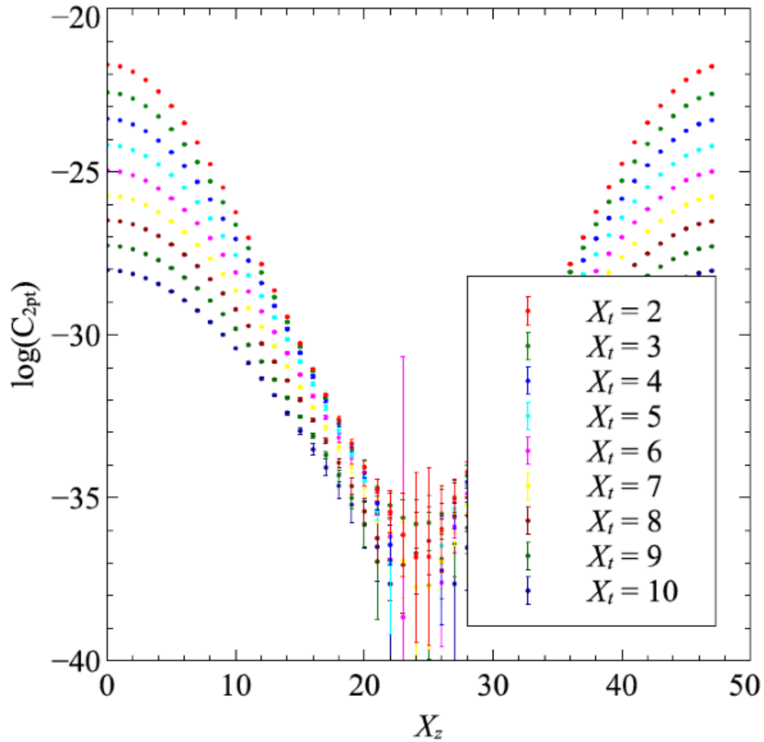
Lattice Details

- Two degenerate light-quark flavors, and strange quark set to its physical value

$$\begin{aligned} a &\simeq 0.12\ \mathrm{fm} \\ m_\pi &\simeq 400\ \mathrm{MeV} \\ \text{Lattice Size} &: 24^3 \times 64 \end{aligned}$$

- To gain control over finite-volume effects, replicate in z direction: $24 \times 24 \times 48 \times 64$

Two-point correlator

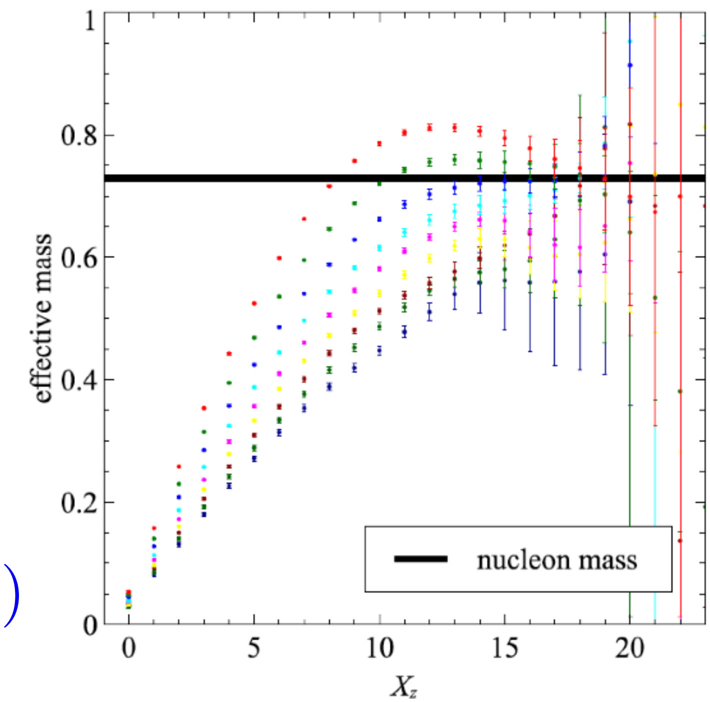


$\ln\left[C_{\mathrm{2pt}}(t, x_z)\right]$

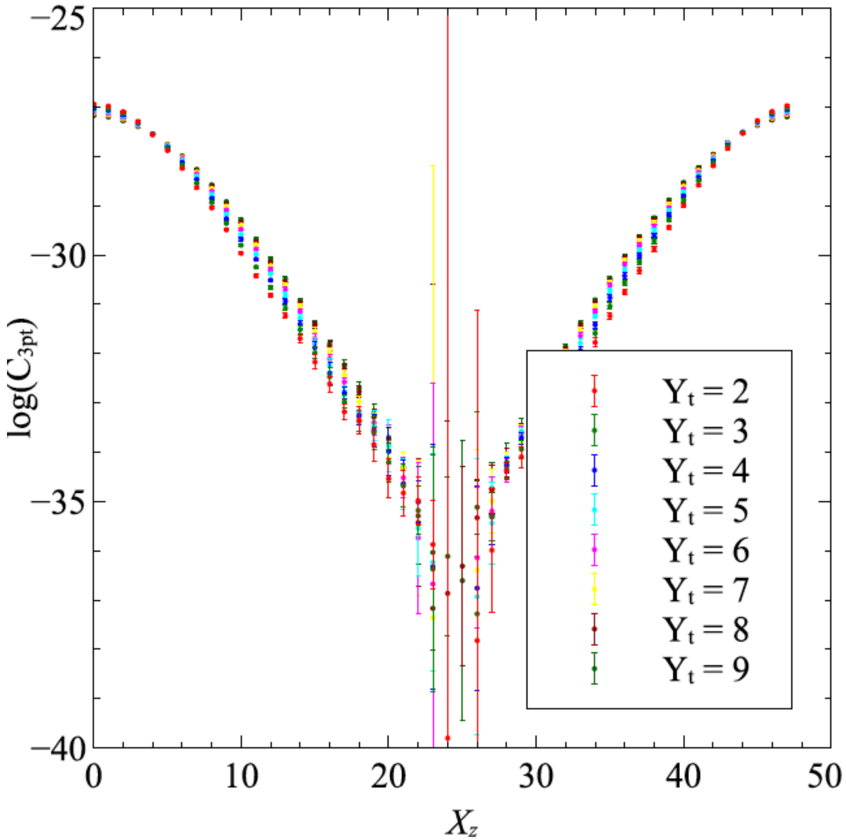
Any polynomial moment in x_z converges

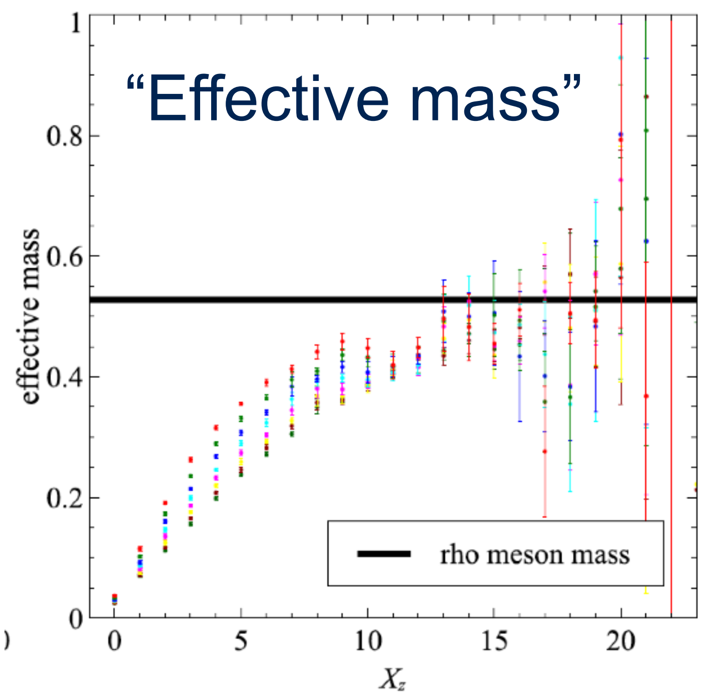
"Effective mass"

$\ln C_{\mathrm{2pt}}(t, x_z)/C_{\mathrm{2pt}}(t, x_z+1)$



Three-point correlator





- Spatial moments push the peak of the correlator away from origin
- Larger finite volume corrections compared to regular correlators

Fitting the data...

$$C^{3\mathrm{pt}}(t,t') = \sum_{n,m} \frac{Z_n^{\dagger a}(0)\Gamma_{nm}(k^2)Z_m^b(k^2)}{4M_n(0)E_m(k^2)} e^{-M_n(0)(t-t')} e^{-E_m(k^2)t'}$$

$$C_{2\mathrm{pt}}(t) = \sum_m \frac{Z_m^{b\dagger}(k^2)Z_m^b(k^2)}{2E_m(k^2)} e^{-E_m(k^2)t}$$

where

$$Z_n^{\dagger a}(0) \equiv \langle \Omega | N^a | n, p_i = (0,0,0) \rangle$$

$$Z_m^b(k^2) \equiv \langle m, p_i = (0,0,k) | \overline{N}^b | \Omega \rangle$$

$$\boxed{\Gamma_{nm}(k^2) \equiv \langle n, p_i = (0,0,0) | \Gamma | m, p_i = (0,0,k) \rangle}$$

Allow for multi-state contributions in the fit

Fitting - II

- Now look at the functional form of derivatives:

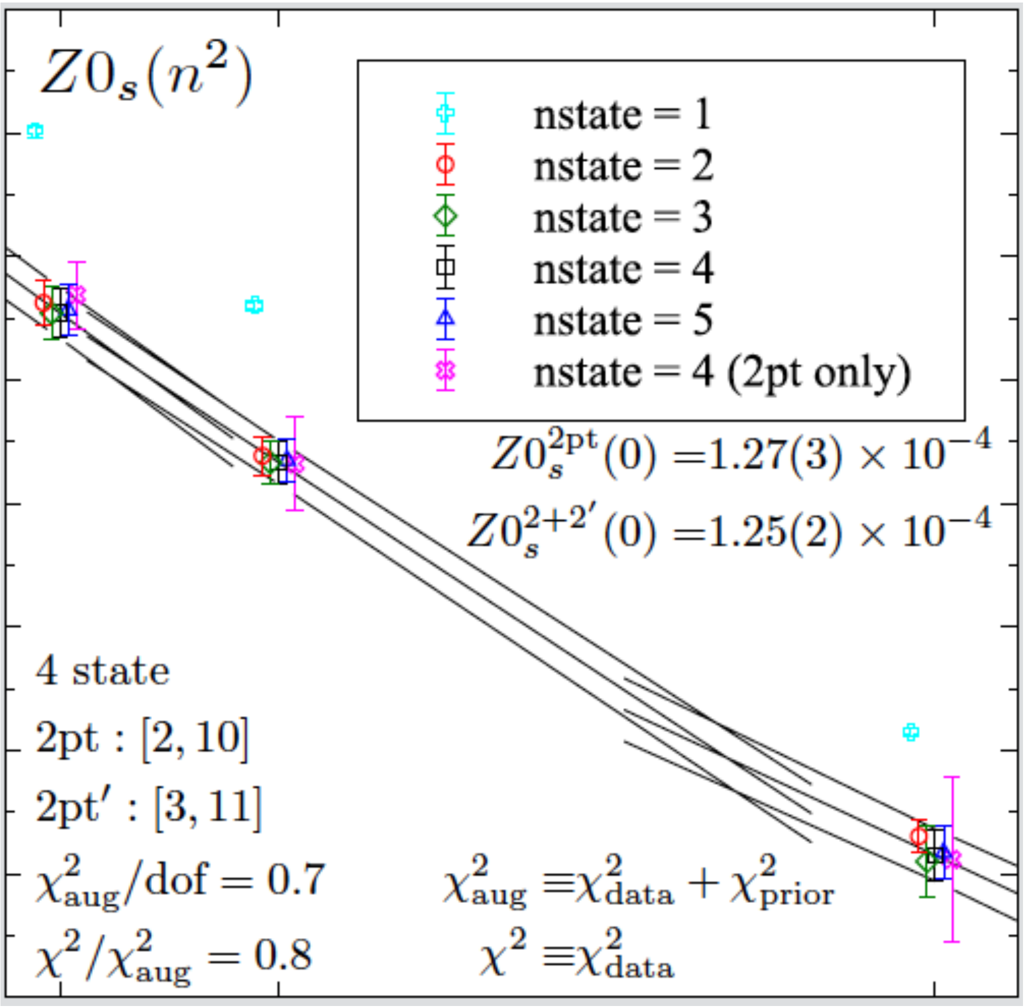
$$C'_{2\mathrm{pt}}(t) = \sum_m C_m^{2\mathrm{pt}}(t) \left(\frac{2Z_m^{b\prime}(k^2)}{Z_m^b(k^2)} - \frac{1}{2[E_m(k^2)]^2} - \frac{t}{2E_m(k^2)} \right)$$

$$C'_{3\mathrm{pt}}(t,t') = \sum_{n,m} C_{nm}^{3\mathrm{pt}}(t,t') \left\{ \frac{\Gamma'_{nm}(k^2)}{\Gamma_{nm}(k^2)} + \frac{Z_m^{b\prime}(k^2)}{Z_m^b(k^2)} - \frac{1}{2[E_m(k^2)]^2} - \frac{t'}{2E_m(k^2)} \right\}$$

spatially extended sources

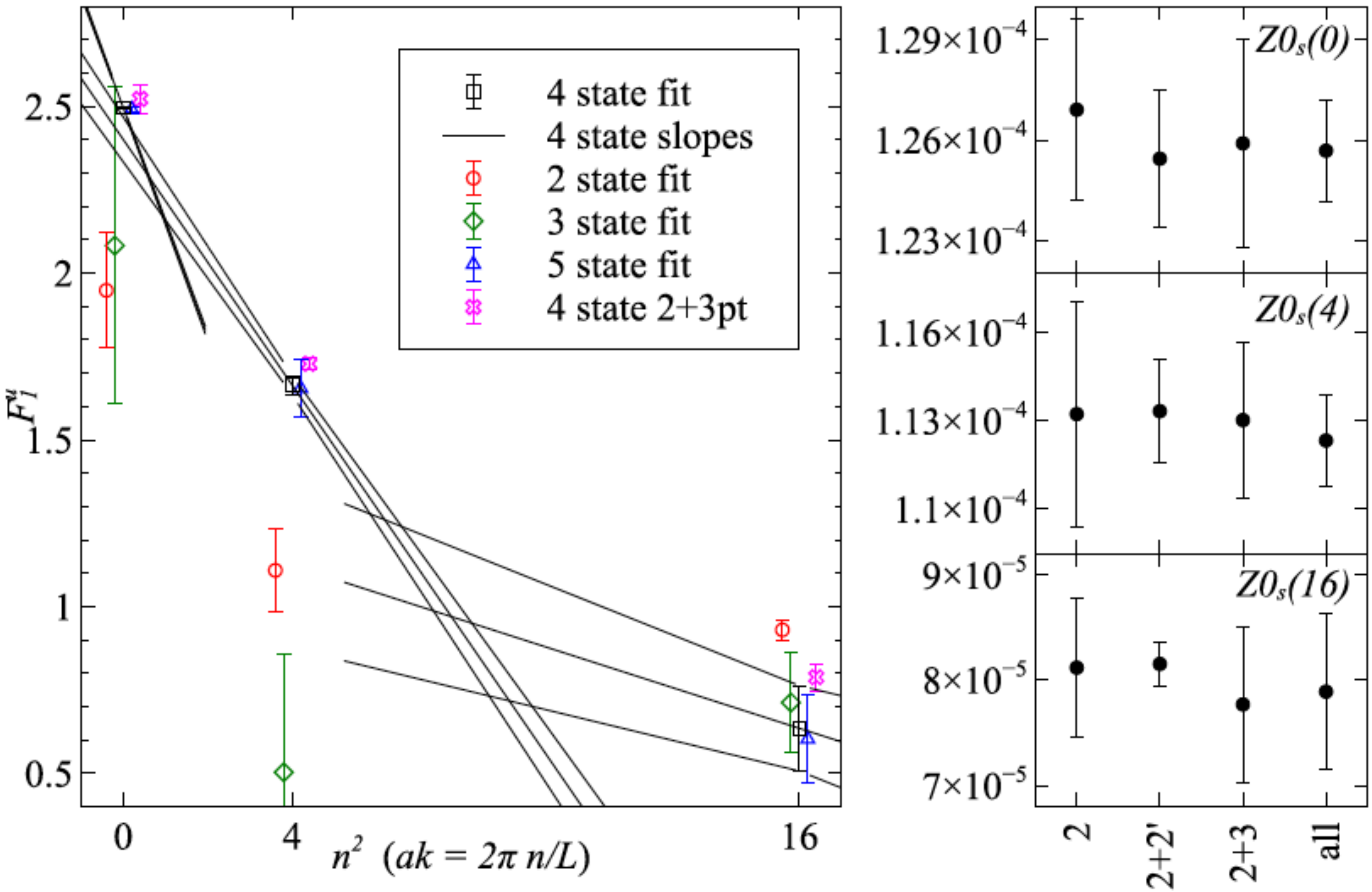
Second distance scale

Fitting - III



In practice we use multi-exponential, Bayesian fits

F_1 Form Factor



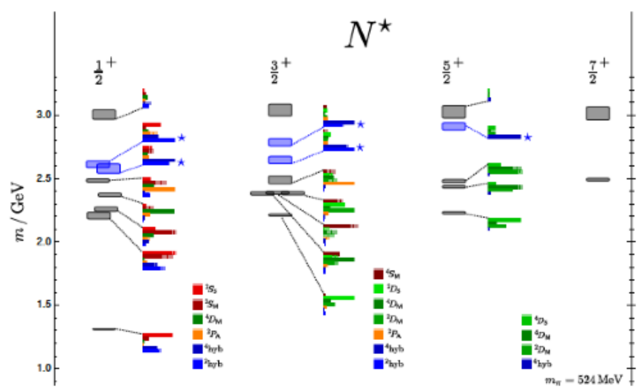
Outlook

- Controlling the contribution from excited states in study of hadron structure is a crucial for precise and accurate calculations
- The approach of the variational method is a powerful way of addressing systematic uncertainties due to excited state
- Current basis of operators based on quasi-local sources. Exploring basis that admits non-zero orbital structure

Starting point $$B = \left(\mathcal{F}_{\Sigma_F} \otimes \mathcal{S}_{\Sigma_S} \otimes \mathcal{D}_{\Sigma_D}\right)\{\psi_1\psi_2\psi_3\}$$

Introduce circular basis:

$$\overleftrightarrow{D}_{m=-1} = \frac{i}{\sqrt{2}}\left(\overleftrightarrow{D}_x - i\overleftrightarrow{D}_y\right)$$
$$\overleftrightarrow{D}_{m=0} = i\overleftrightarrow{D}_z$$
$$\overleftrightarrow{D}_{m=+1} = -\frac{i}{\sqrt{2}}\left(\overleftrightarrow{D}_x + i\overleftrightarrow{D}_y\right).$$



R.G.Edwards et al., arXiv:1104.5152
Dudek, Edwards, arXiv:1201.2349

- Structure of Excited States - *Raul Briceno*