Improving Hadron Matrix Element Determination using the Variational Method

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CSSM/QCDSF/UKQCD

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Lattice QCD Motivation

- Calculation of g_A, g_S and $\langle x \rangle$ have been difficult.

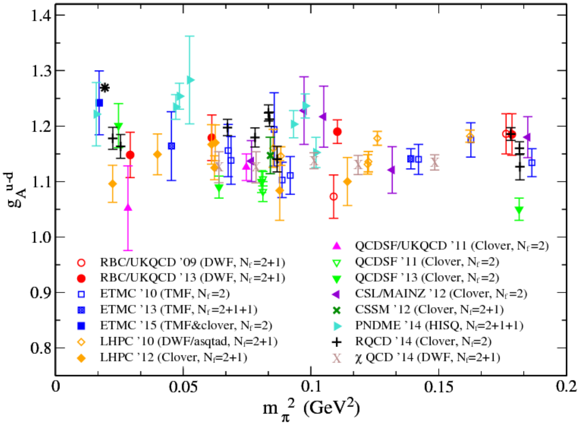


Figure: Constantinou 2015

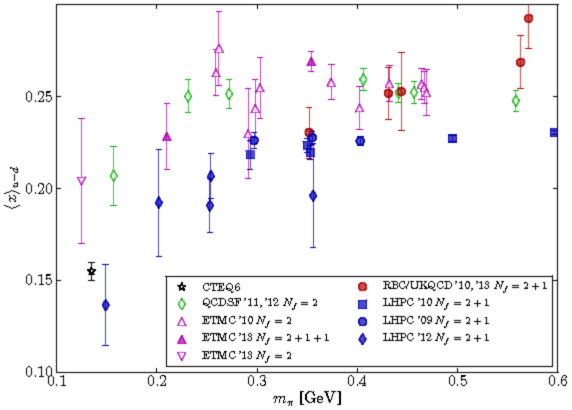


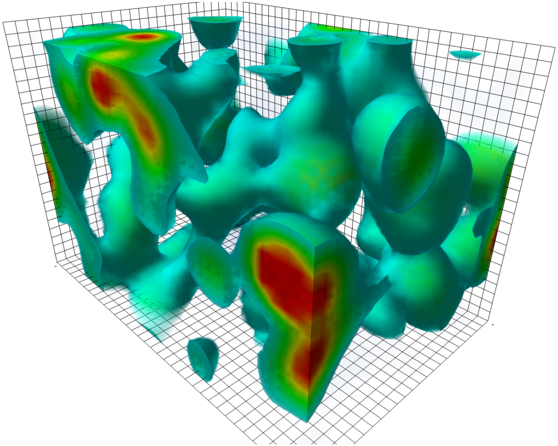
Figure: Syritsyn 2014

Aim

- Some problems associated with calculating these include:
  - Finite size effects
  - Renormalisation
  - Continuum extrapolation
  - Excited-state contamination
- This talk:
  - g_A, g_S, $\langle x \rangle$
  - form factors, G_E, G_M, G_A, G_P
- Emphasis on excited-state contamination effects
- Some proposed methods to improve this include:
  - Summation method
  - Two-state fit method
  - Variational method
- The aim of this work is to systematically compare 3 three methods for all quantities extracted.

Calculation Parameters

- QCDSF/UKQCD/CSSM gauge fields.
- SU(3)-symmetric point
- $m_\pi \approx 470$ MeV.
- Lattice Spacing of 0.074 fm
- $32^3 \times 64$ volume.
- Gauge-invariant Gaussian smearing.



Calculation Parameters

- Summation / two-state fit methods:
  - $t_{sink} - t_{source} = 10, 13, 16, 19, 22$ (0.74 fm $\leq$ t $\leq$ 1.63 fm)
  - Smearing = 32 sweeps (rms radius = 0.248 fm)
- Variational method:
  - $t_{sink} - t_{source} = 13, 16$ (0.96 fm , 1.184 fm)
  - Smearings = 32, 64, 128 sweeps (rms radius = 0.248 fm, 0.351 fm, 0.496 fm)

N_{smear} \ t	10	13	16	19	22
32	⋆	⋆	⋆	⋆	⋆
64		⋆			
128		⋆			
variational		⋆	⋆		

Two-Point Correlators

Defined as:

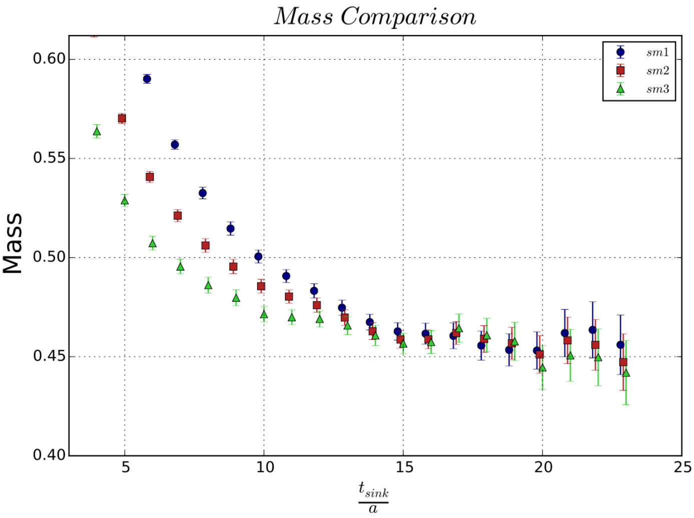
$$G_2(\Gamma;\vec{p},t) =$$
$$\sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}} \mathrm{Tr}\left\{\Gamma \langle\Omega|\, \chi(\vec{x},t)\overline{\chi}(0)\, |\Omega\rangle\right\}$$

Which reduces to:

$$G_2(\Gamma_4;\vec{p},t) = \sum_{\alpha} e^{-E^{\alpha}_{\vec{p}}t}\overline{\mathcal{Z}}^{\alpha}_{\vec{p}}\mathcal{Z}^{\alpha}_{\vec{p}}$$

Can find the mass m, via:

$$\log\left(\frac{G_2(\Gamma_4;\vec{0},t)}{G_2(\Gamma_4;\vec{0},t+\Delta t)}\right) \xrightarrow{t\gg 0} m\Delta t$$



Variational Method

Create a linear combination that strongly couples to state α

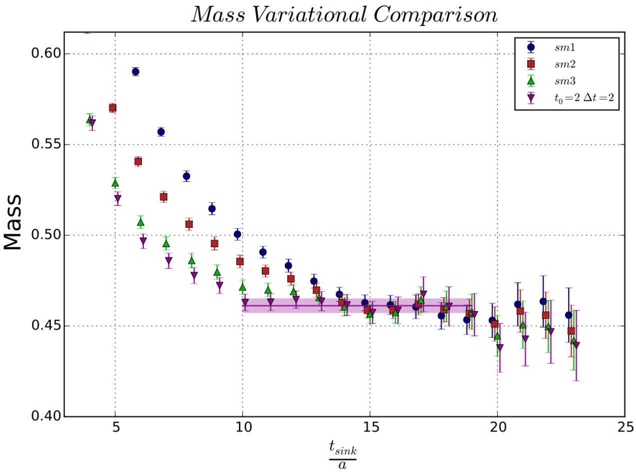
$$\phi^{\alpha}(x,\vec{p}) \equiv \sum_i v_i^{\alpha}(\vec{p})\chi_i(x),$$

$$\overline{\phi}^{\alpha}(0,\vec{p}) \equiv \sum_i u_i^{\alpha}(\vec{p})\overline{\chi}_i(0)$$

u and v obtained by solutions to a Generalised Eigenvalue Problem.

Optimal 2 point correlator is produced by projecting with u and v:

$$G_2^{\alpha}(\vec{p},t;\Gamma) = v_i^{\alpha}(\vec{p})\left(G_2\right)_{ij}(\Gamma;\vec{p},t)u_j^{\alpha}(\vec{p}),$$



Three-point correlators

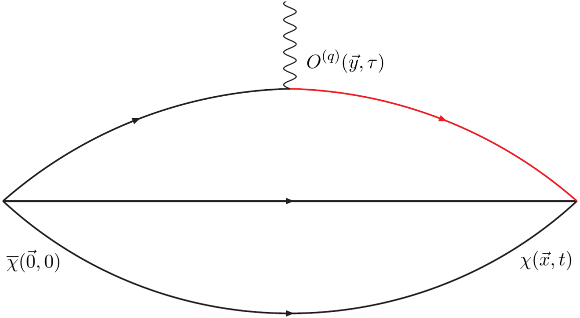
Three-point correlator defined as:

$$G_3(\Gamma;\vec{p}',t;\vec{q},\tau;O^{(q)}) = \sum_{\vec{x},\vec{y}} e^{-i\vec{p}'\cdot\vec{x}} e^{i\vec{q}\cdot\vec{y}} \mathrm{Tr}\left\{\Gamma \langle\Omega|\,\chi(\vec{x},t) O^{(q)}(\vec{y},\tau)\overline{\chi}(\vec{0},0)\,|\Omega\rangle\right\}$$

For zero momentum, a simple ratio gives us an extracted value

$$R(\Gamma;t;\tau;O^{(q)}) \equiv \frac{G_3(\Gamma;t;\tau;O^{(q)})}{G_2(\Gamma_4;t)} \xrightarrow{t\gg\tau\gg0} FF$$

Selecting appropriate $O^{(q)}$ and Γ gives access to $FF = g_A$, g_S etc..



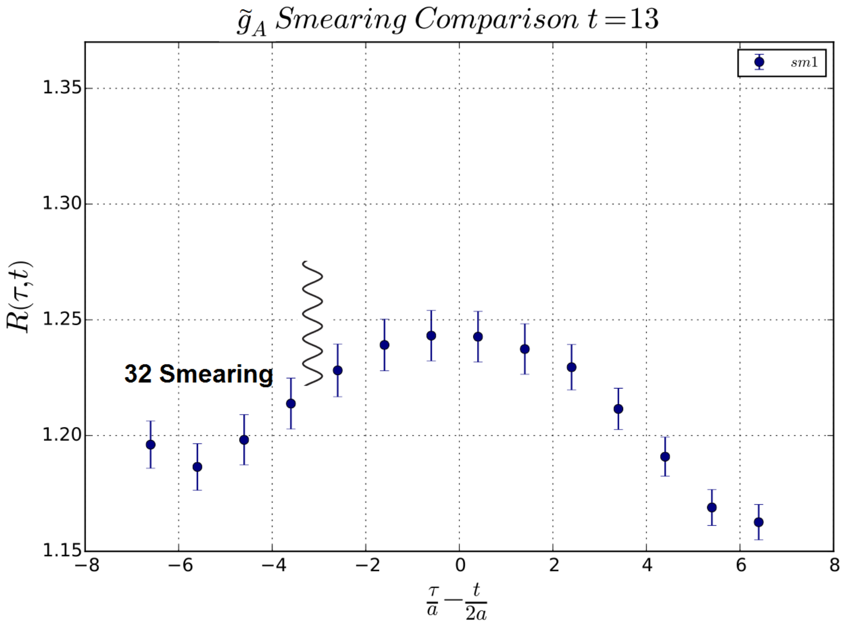
Variational Method for Three-Point Correlators

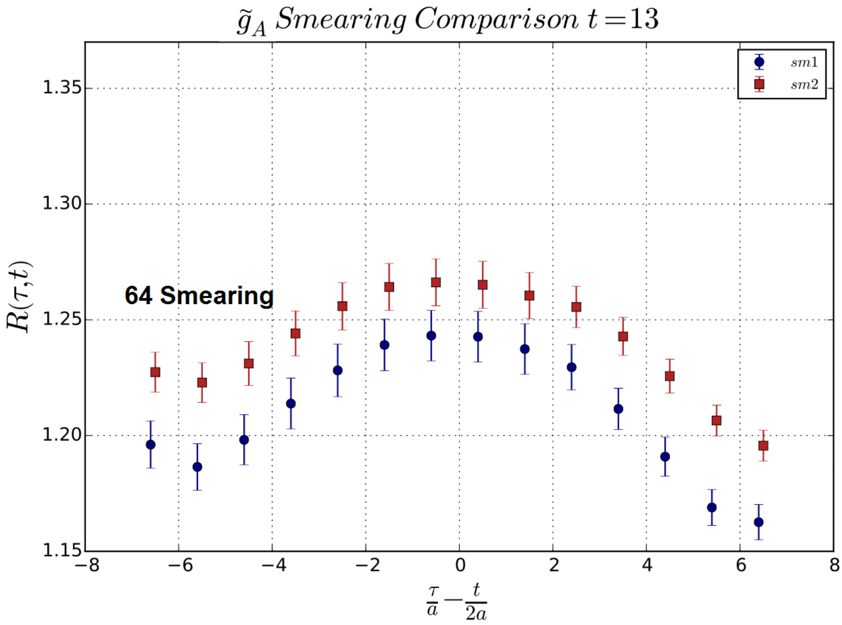
Extending the variational method to three-point correlators, we have:

$$G_3^{\alpha}(\Gamma;\vec{p}',t;\vec{q},\tau;O^{(q)}) = \sum_{\vec{x},\vec{y}} e^{-i\vec{p}'\cdot\vec{x}} e^{i\vec{q}\cdot\vec{y}} \mathrm{Tr}\left\{\Gamma \langle\Omega|\, \phi^{\alpha}(x,\vec{p}) O^{(q)}(y) \overline{\phi}^{\,\alpha}(0,\vec{p})\, |\Omega\rangle\right\}$$

So in terms of calculation, we can use the same u and v vectors in the three-point correlator construction via the projection:

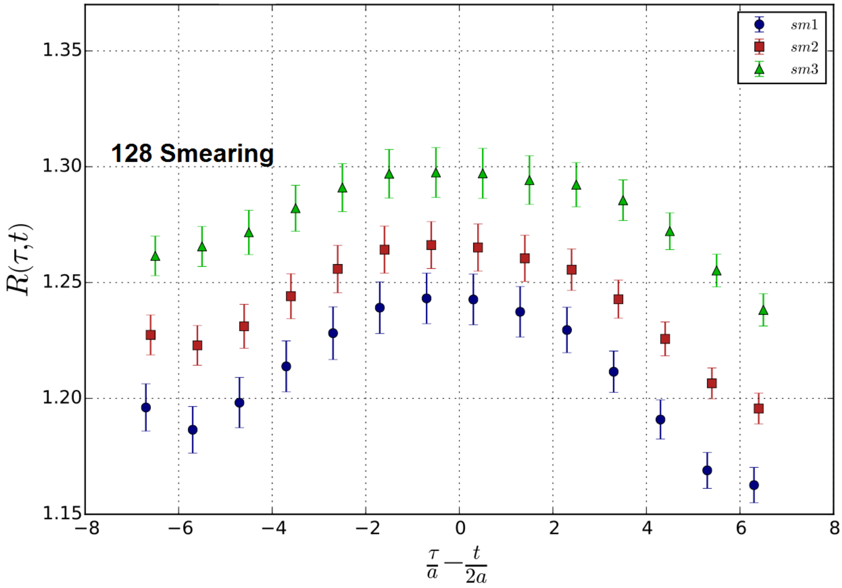
$$G_3^{\alpha}(\Gamma;\vec{p}',t;\vec{q},\tau;O^{(q)}) = v_i^{\alpha}(\vec{p}')\,(G_3)_{ij}\,(\Gamma;\vec{p}',t;\vec{q},\tau;O^{(q)}) u_j^{\alpha}(\vec{p})$$

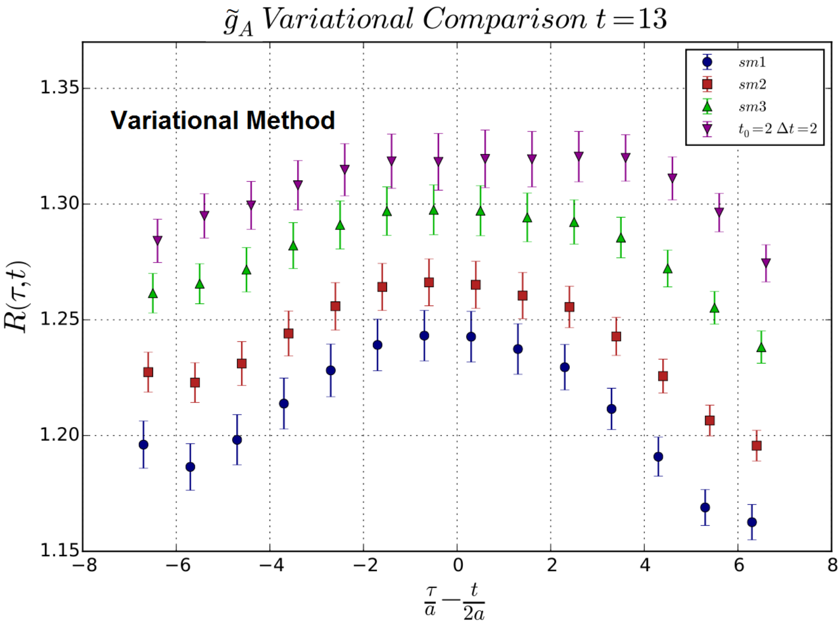

$\tilde{g}_A$ Smearing Comparison $t=13$
sm1
32 Smearing
1.35
1.30
1.25
1.20
1.15
$R(\tau,t)$
−8
−6
−4
−2
0
2
4
6
8
$\frac{\tau}{a} - \frac{t}{2a}$



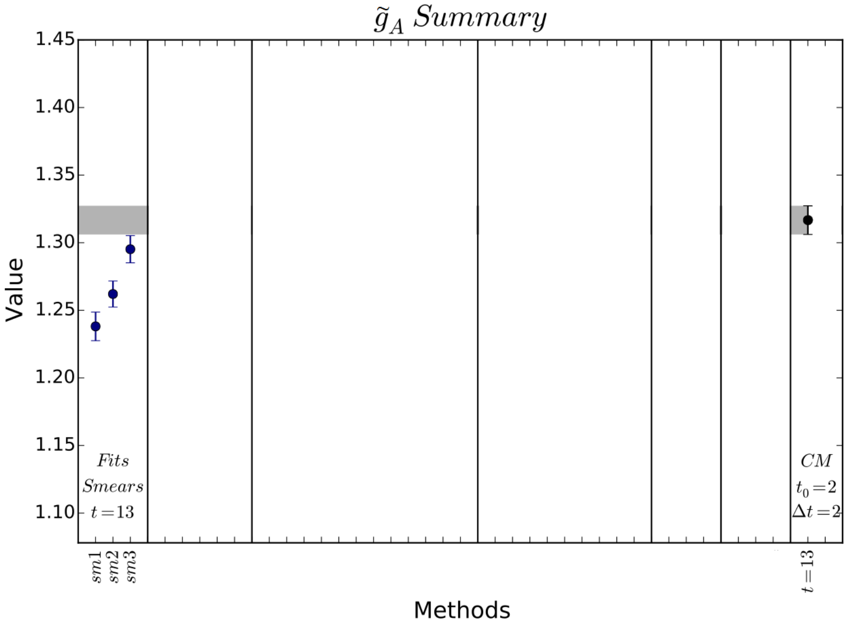
$\tilde{g}_A$ Smearing Comparison $t = 13$
sm1
sm2
64 Smearing
$R(\tau, t)$
1.35
1.30
1.25
1.20
1.15
−8
−6
−4
−2
0
2
4
6
8
$\frac{\tau}{a} - \frac{t}{2a}$

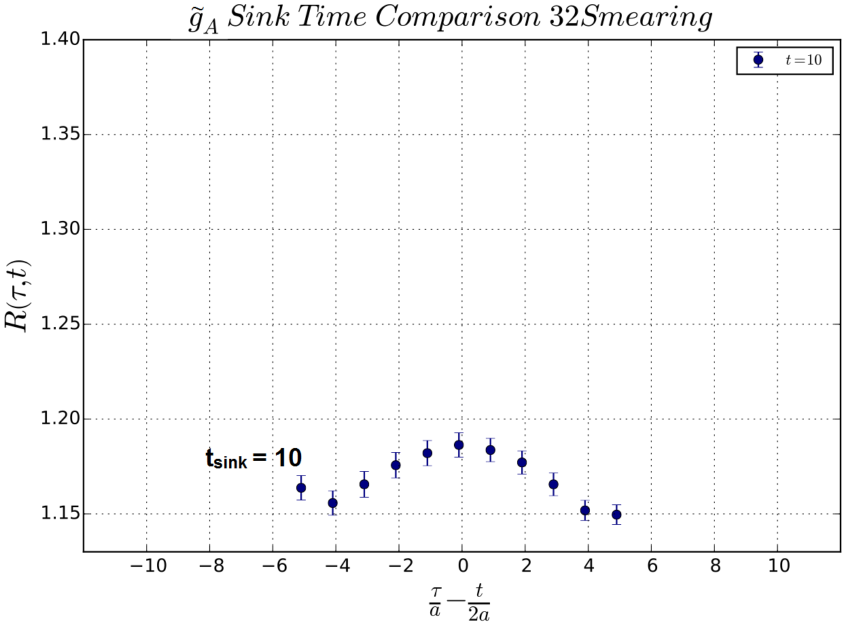
$\tilde{g}_A$ Smearing Comparison $t = 13$

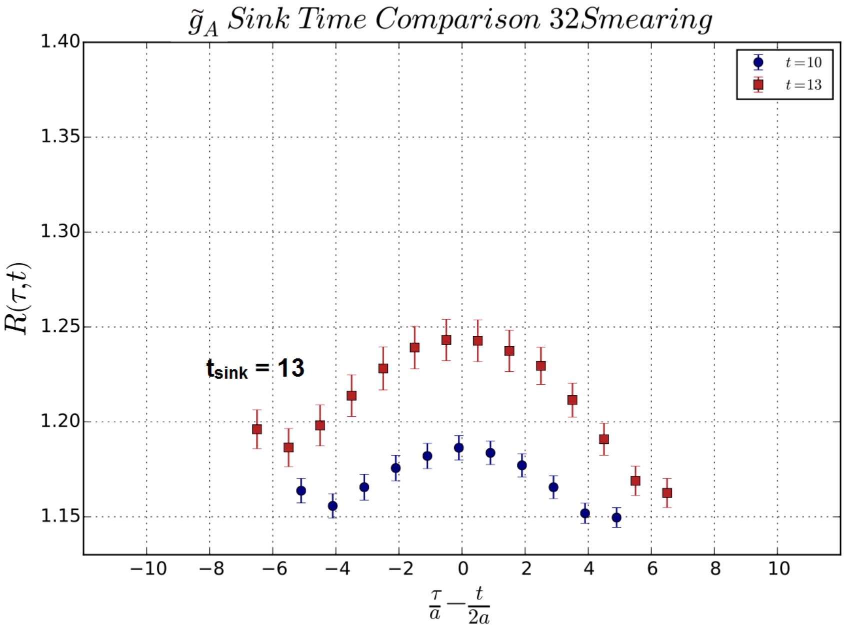




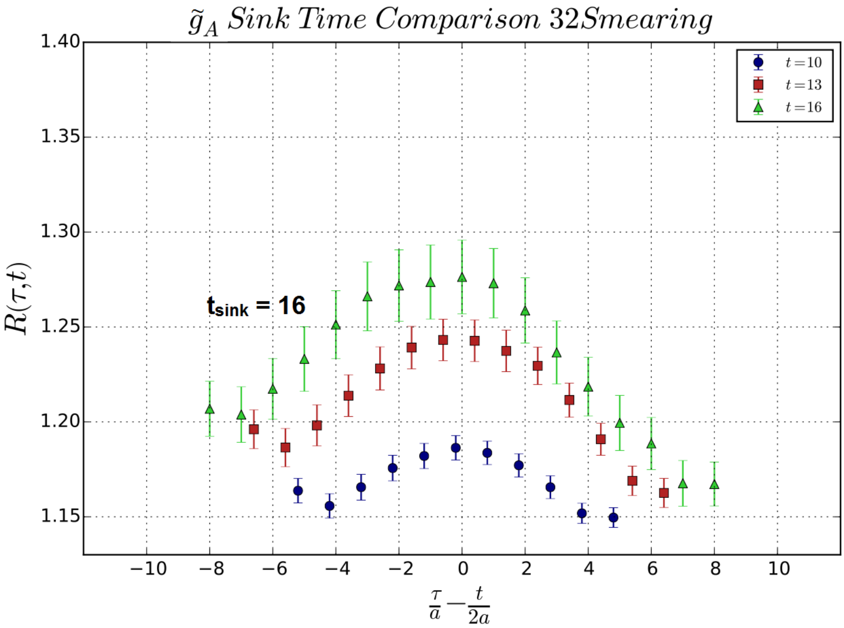
$\tilde{g}_A$ Variational Comparison $t=13$
Variational Method
sm1
sm2
sm3
$t_0=2\ \Delta t=2$
$R(\tau,t)$
$\frac{\tau}{a}-\frac{t}{2a}$
1.35
1.30
1.25
1.20
1.15
−8
−6
−4
−2
0
2
4
6
8

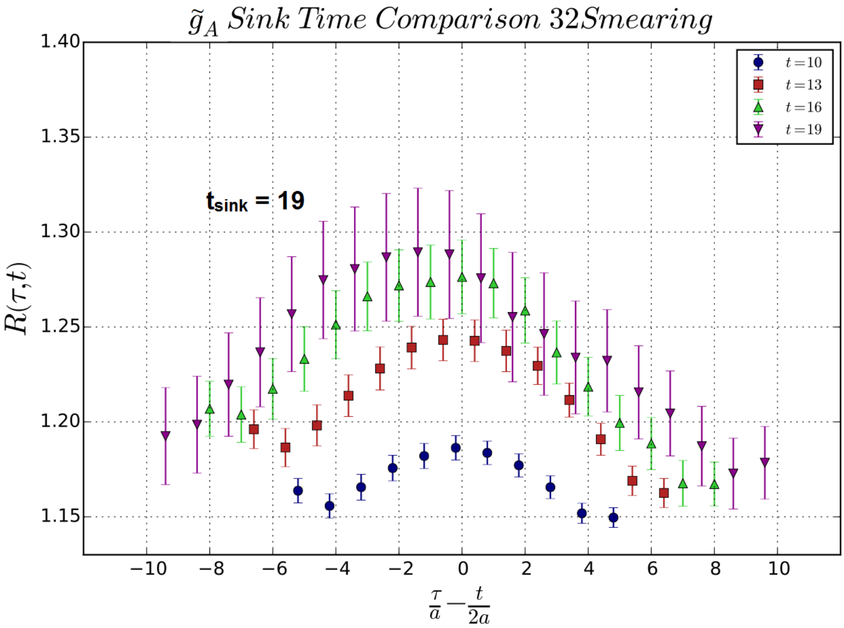

$\tilde{g}_A$ Summary
1.45
1.40
1.35
1.30
1.25
1.20
1.15
1.10
Value
Fits
Smears
$t = 13$
CM
$t_0 = 2$
$\Delta t = 2$
sm1
sm2
sm3
$t = 13$
Methods

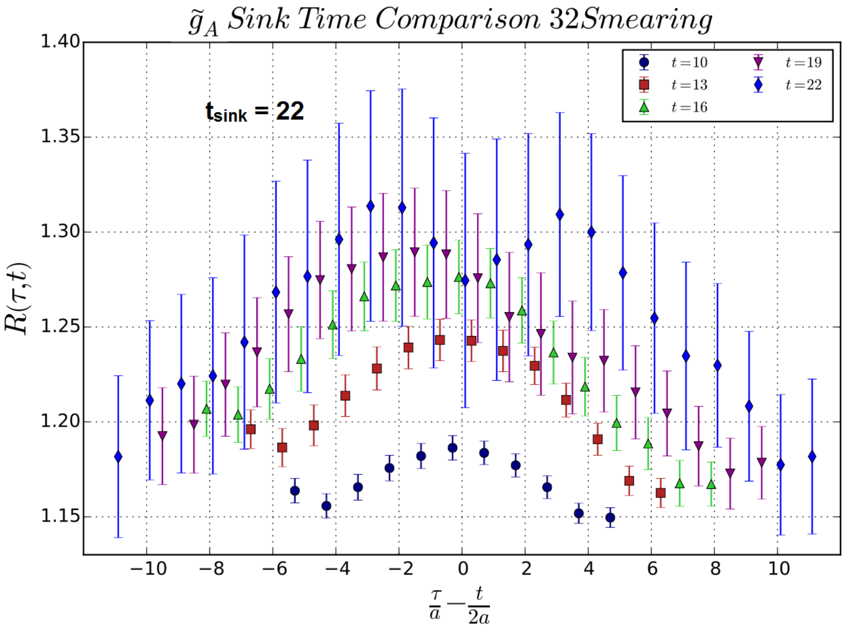

$\tilde{g}_A$ Sink Time Comparison 32Smearing
$t = 10$
$t_{sink} = 10$
$R(\tau,t)$
$\frac{\tau}{a} - \frac{t}{2a}$
1.40
1.35
1.30
1.25
1.20
1.15
−10 −8 −6 −4 −2 0 2 4 6 8 10

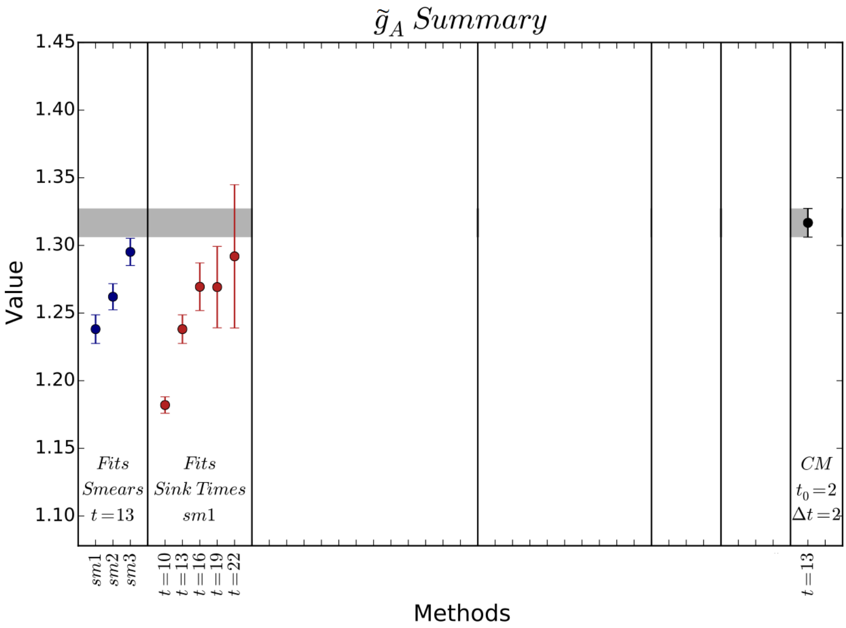


$\tilde{g}_A$ Sink Time Comparison 32Smearing
1.40
1.35
1.30
1.25
1.20
1.15
$R(\tau,t)$
$t=10$
$t=13$
$t_{sink} = 13$
−10
−8
−6
−4
−2
0
2
4
6
8
10
$\frac{\tau}{a} - \frac{t}{2a}$


$\tilde{g}_A$ Sink Time Comparison 32Smearing
1.40
1.35
1.30
1.25
1.20
1.15
$R(\tau,t)$
t_{sink} = 16
−10
−8
−6
−4
−2
0
2
4
6
8
10
$\frac{\tau}{a} - \frac{t}{2a}$
$t = 10$
$t = 13$
$t = 16$


$\tilde{g}_A$ Sink Time Comparison 32Smearing
t=10
t=13
t=16
t=19
t_{sink} = 19
$R(\tau,t)$
$\frac{\tau}{a} - \frac{t}{2a}$
1.40
1.35
1.30
1.25
1.20
1.15
−10
−8
−6
−4
−2
0
2
4
6
8
10


$\tilde{g}_A$ Sink Time Comparison 32Smearing
t_{sink} = 22
$t=10$
$t=13$
$t=16$
$t=19$
$t=22$
$R(\tau,t)$
$\frac{\tau}{a}-\frac{t}{2a}$
1.40
1.35
1.30
1.25
1.20
1.15
−10 −8 −6 −4 −2 0 2 4 6 8 10

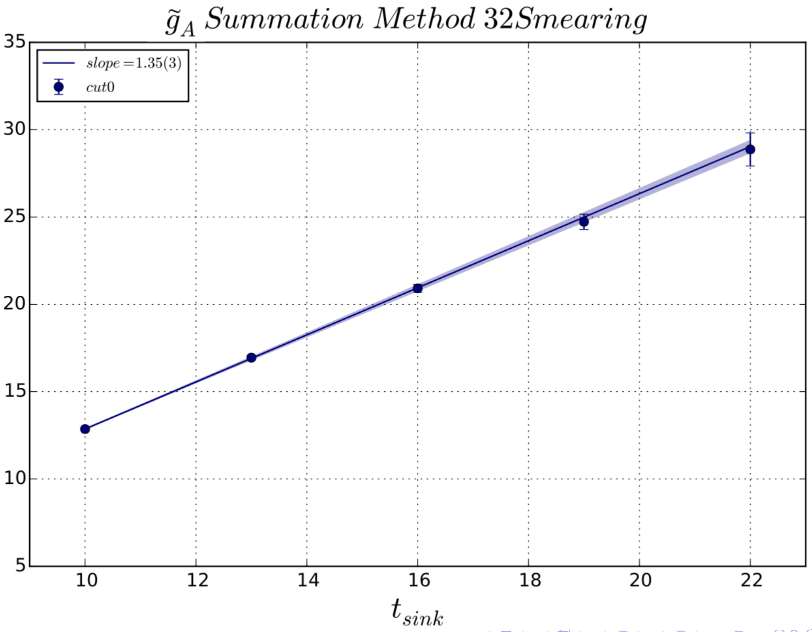


$\tilde{g}_A$ Summary
Value
Methods
1.45
1.40
1.35
1.30
1.25
1.20
1.15
1.10
Fits
Smears
$t=13$
Fits
Sink Times
$sm1$
CM
$t_0=2$
$\Delta t=2$
$sm1$
$sm2$
$sm3$
$t=10$
$t=13$
$t=16$
$t=19$
$t=22$
$t=13$

$$S(t) = \sum_{\tau=\delta t}^{t-\delta t} R(t,\tau) \rightarrow$$

$$c + t\left\{FF + \mathcal{O}\left(e^{-\Delta m t}\right)\right\}$$

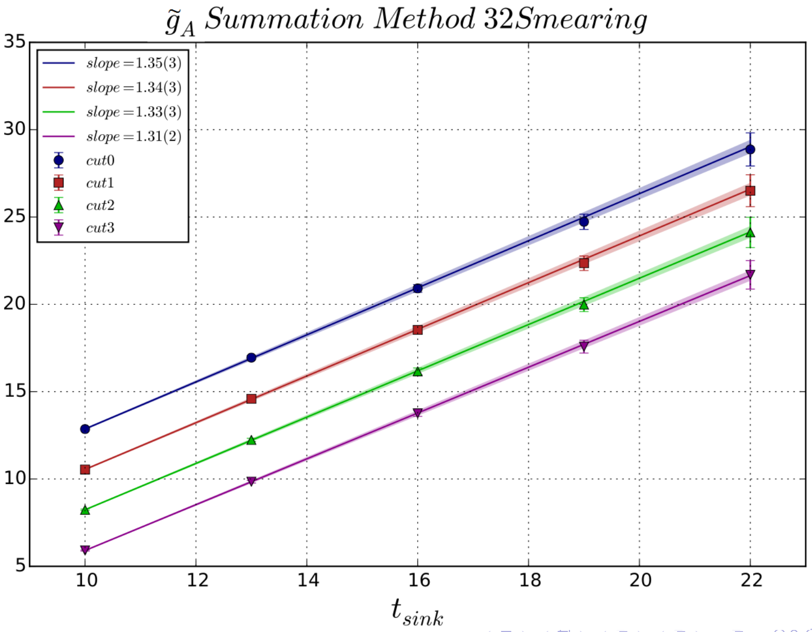
- Where $\Delta m = m^1 - m^0$.
- Free to choose δt (or cut value).

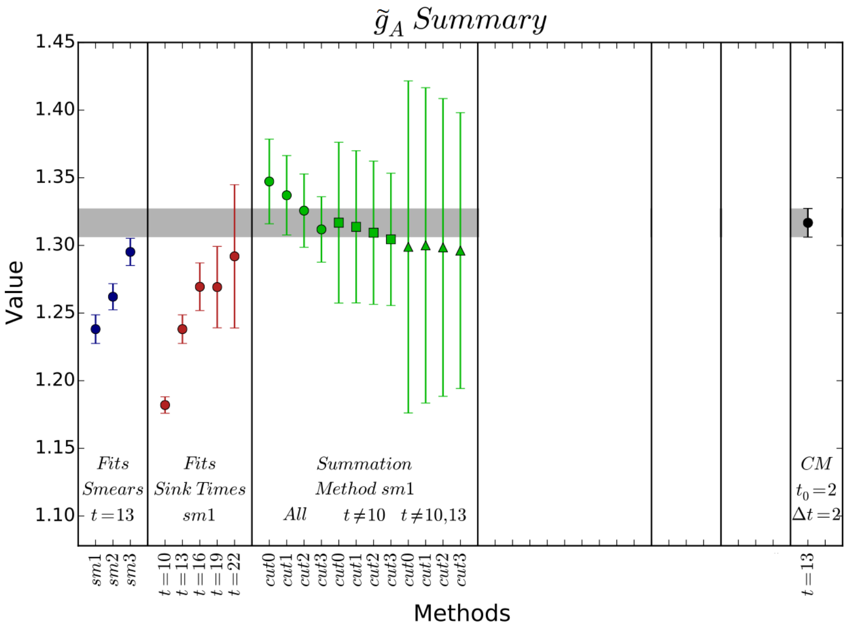


$$S(t) = \sum_{\tau=\delta t}^{t-\delta t} R(t,\tau) \rightarrow$$

$$c + t\left\{FF + \mathcal{O}\left(e^{-\Delta m t}\right)\right\}$$

- Where $\Delta m = m^1 - m^0$.
- Free to choose δt (or cut value).





$\tilde{g}_A$ Summary
1.45
1.40
1.35
1.30
1.25
1.20
1.15
1.10
Value
Fits Smears $t=13$
Fits Sink Times sm1
Summation Method sm1
All
$t \neq 10$
$t \neq 10,13$
CM $t_0=2$ $\Delta t=2$
sm1 sm2 sm3
$t=10$ $t=13$ $t=16$ $t=19$ $t=22$
cut0 cut1 cut2 cut3 cut0 cut1 cut2 cut3 cut0 cut1 cut2 cut3
$t=13$
Methods

Two-Exponential Fit

Fitting an expected function for the two states produces mass and coefficient parameters

$$G_2(\vec{0}, t) = A_m e^{-mt} + A'_m e^{-(m+\Delta m)t}$$

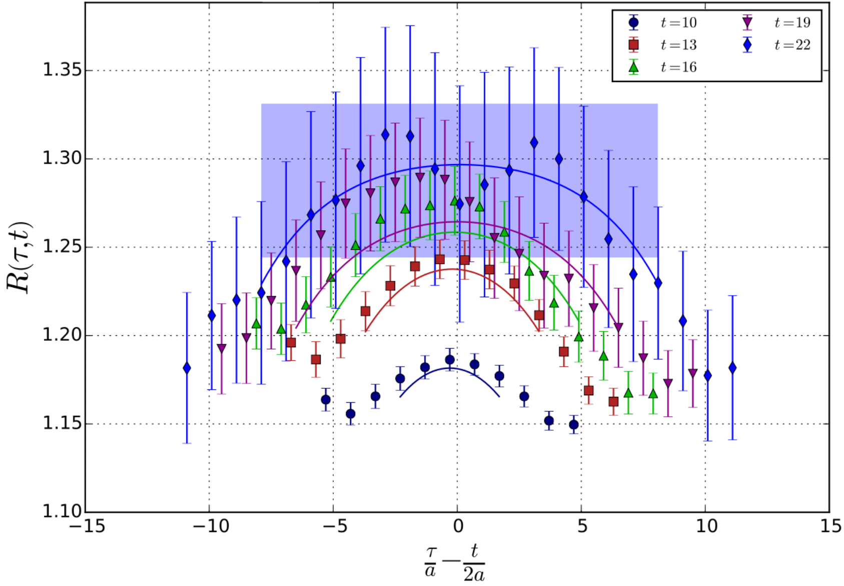
Then use the fit parameters above to fit another expected function for the three-point case

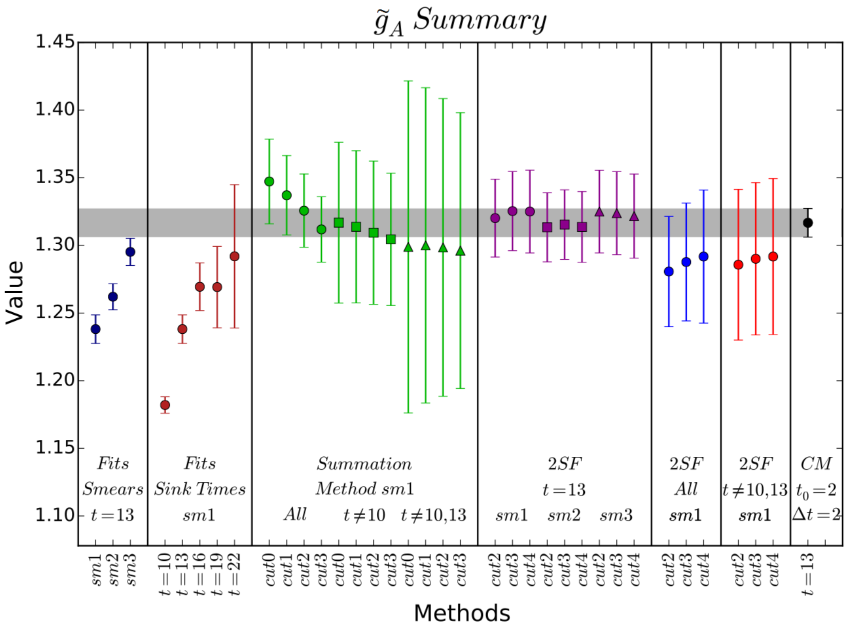
$$G_3(\Gamma; \vec{0}, t; \vec{0}, \tau; O^{(q)}) = A_m e^{-mt} \left\{ B_0 + B_1 \left(e^{-\Delta m \tau} + e^{-\Delta m (t-\tau)} \right) + B_2 e^{-\Delta m t} \right\}.$$

Where B_0 is proportional to the matrix element in question,

B_2 can only be calculated if fitting over multiple sink times.

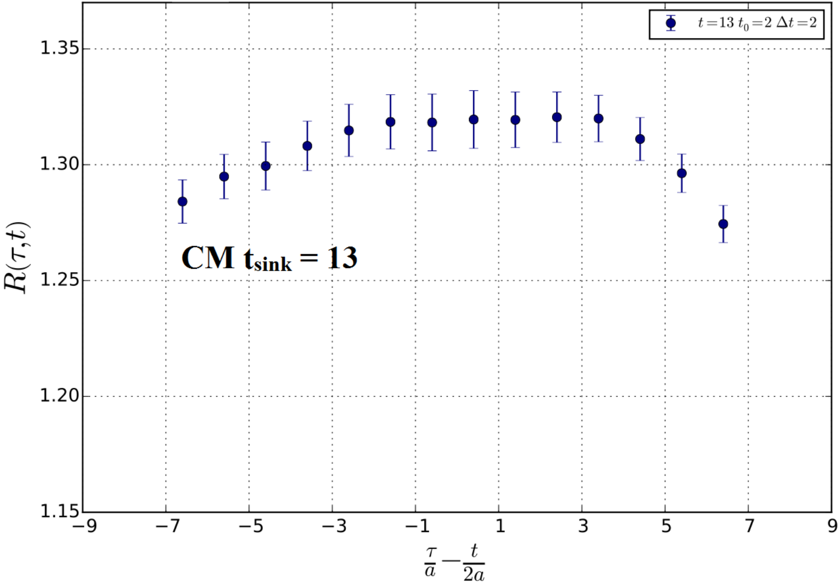
$\tilde{g}_A$ 2SF TSink Comparison

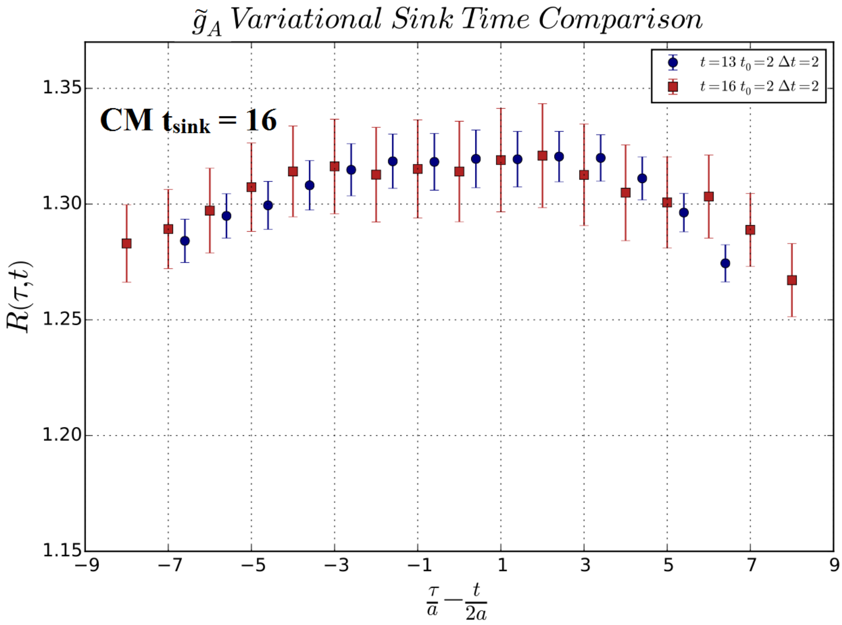


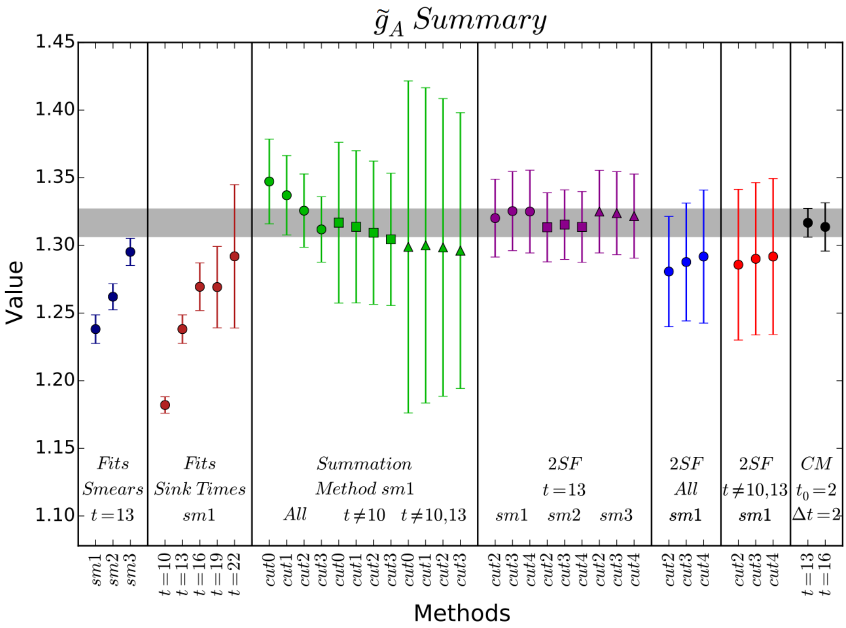


$\tilde{g}_A$ Summary
Value
1.45
1.40
1.35
1.30
1.25
1.20
1.15
1.10
Fits Smears $t=13$
Fits Sink Times $sm1$
Summation Method $sm1$
All
$t \neq 10$
$t \neq 10,13$
2SF $t=13$
$sm1$ $sm2$ $sm3$
2SF All $sm1$
2SF $t \neq 10,13$ $sm1$
CM $t_0=2$ $\Delta t=2$
$sm1$ $sm2$ $sm3$
$t=10$ $t=13$ $t=16$ $t=19$ $t=22$
$cut0$ $cut1$ $cut2$ $cut3$ $cut0$ $cut1$ $cut2$ $cut3$ $cut0$ $cut1$ $cut2$ $cut3$
$cut2$ $cut3$ $cut4$ $cut2$ $cut3$ $cut4$ $cut2$ $cut3$ $cut4$
$cut2$ $cut3$ $cut4$
$cut2$ $cut3$ $cut4$
$t=13$
Methods

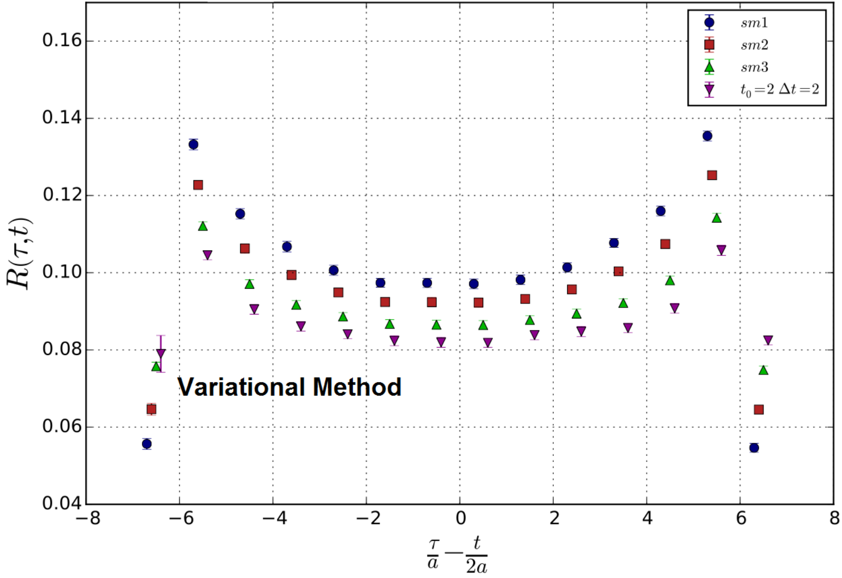
$\tilde{g}_A$ Variational Sink Time Comparison



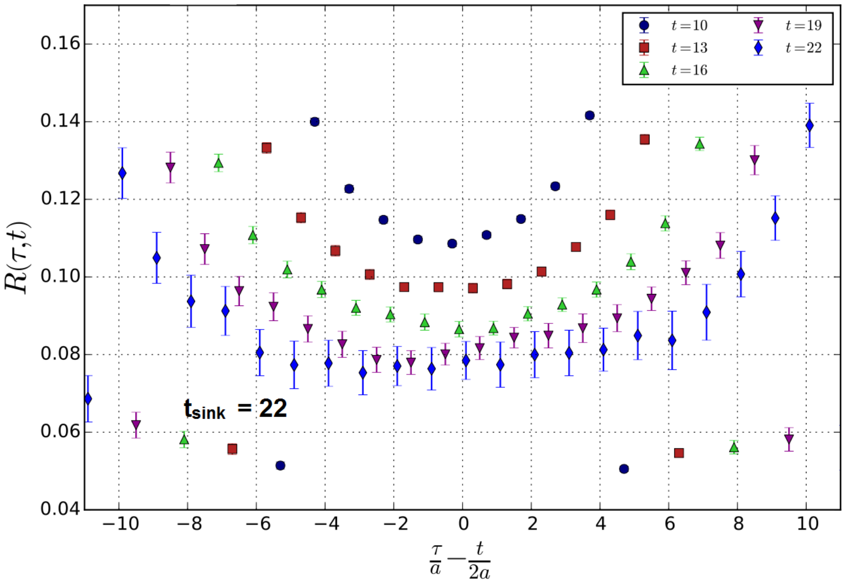

$\tilde{g}_A$ Variational Sink Time Comparison
CM t_{sink} = 16
$t=13$ $t_0=2$ $\Delta t=2$
$t=16$ $t_0=2$ $\Delta t=2$
$R(\tau,t)$
1.35
1.30
1.25
1.20
1.15
−9
−7
−5
−3
−1
1
3
5
7
9
$\frac{\tau}{a}-\frac{t}{2a}$


$\tilde{g}_A$ Summary
Value
1.45
1.40
1.35
1.30
1.25
1.20
1.15
1.10
Fits Smears $t=13$
Fits Sink Times $sm1$
Summation Method $sm1$
All
$t\neq10$
$t\neq10,13$
2SF $t=13$
$sm1$ $sm2$ $sm3$
2SF All $sm1$
2SF $t\neq10,13$ $sm1$
CM $t_0=2$ $\Delta t=2$
$sm1$ $sm2$ $sm3$
$t=10$ $t=13$ $t=16$ $t=19$ $t=22$
$cut0$ $cut1$ $cut2$ $cut3$ $cut0$ $cut1$ $cut2$ $cut3$ $cut0$ $cut1$ $cut2$ $cut3$
$cut2$ $cut3$ $cut4$ $cut2$ $cut3$ $cut4$ $cut2$ $cut3$ $cut4$
$cut2$ $cut3$ $cut4$
$cut2$ $cut3$ $cut4$
$t=13$ $t=16$
Methods

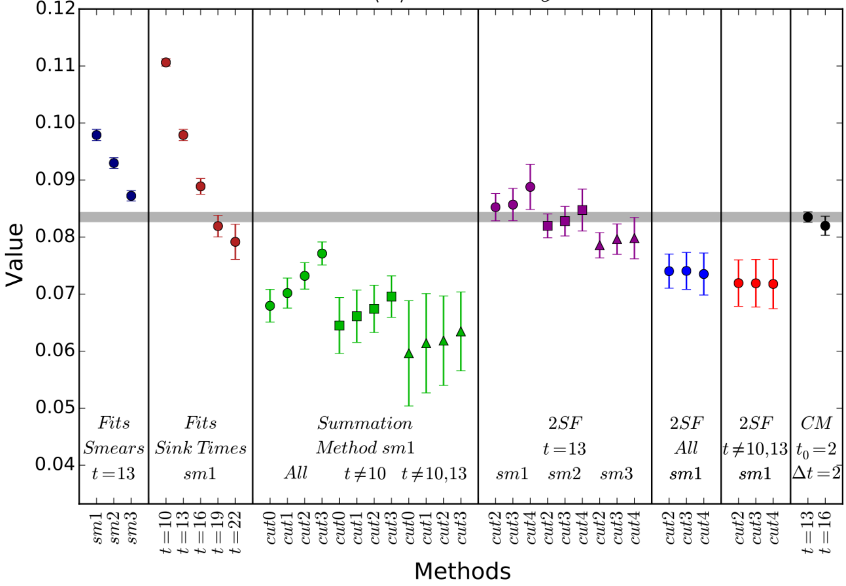
$\langle \tilde{x} \rangle$ Variational Comparison $t=13$

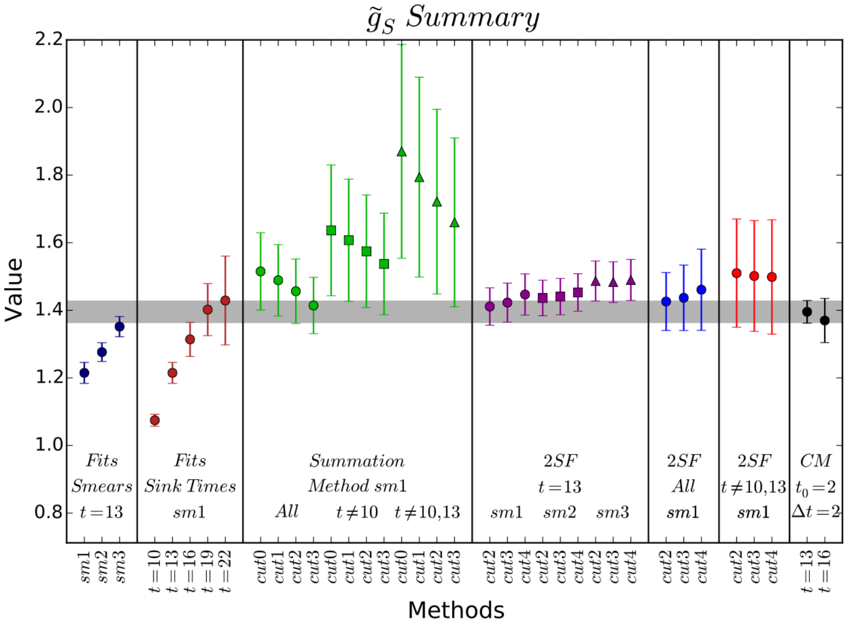


$\langle \tilde{x} \rangle$ Sink Time Comparison 32Smearing



$\langle \tilde{x} \rangle$ Summary





$\tilde{g}_S$ Summary
Value
Methods
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
Fits Smears $t=13$
Fits Sink Times $sm1$
Summation Method $sm1$
All
$t\neq10$
$t\neq10,13$
2SF $t=13$
$sm1$
$sm2$
$sm3$
2SF All $sm1$
2SF $t\neq10,13$ $sm1$
CM $t_0=2$ $\Delta t=2$
sm1 sm2 sm3
$t=10$ $t=13$ $t=16$ $t=19$ $t=22$
cut0 cut1 cut2 cut3 cut0 cut1 cut2 cut3 cut0 cut1 cut2 cut3
cut2 cut3 cut4 cut2 cut3 cut4 cut2 cut3 cut4
cut2 cut3 cut4
cut2 cut3 cut4
$t=13$ $t=16$

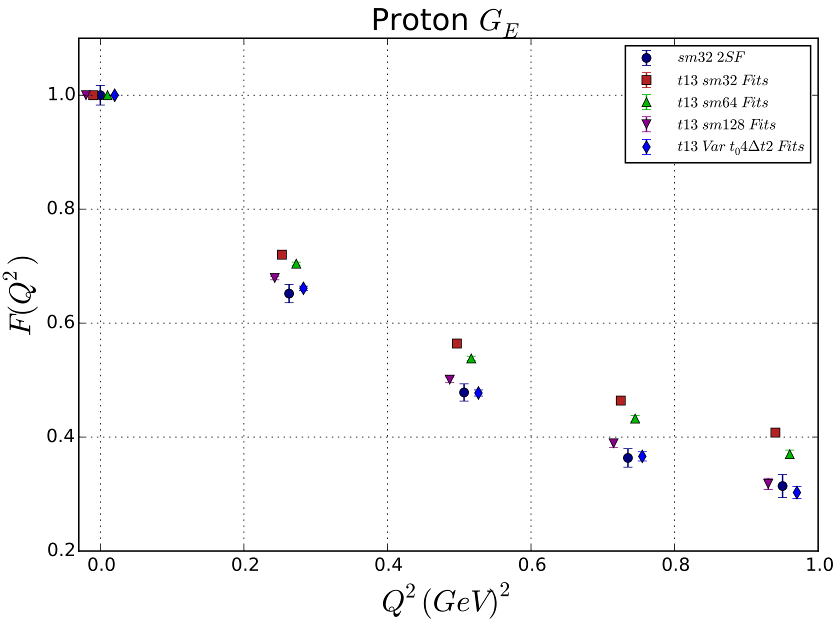
Form Factors

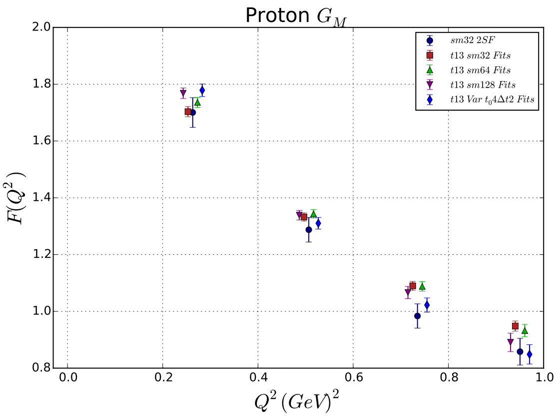
- No disconnected quark loop contributions for proton and neutron combinations.
- Solve system of equations for γ_μ / $\gamma_5\gamma_\mu$, Γ and $\vec{q}$ in q^2

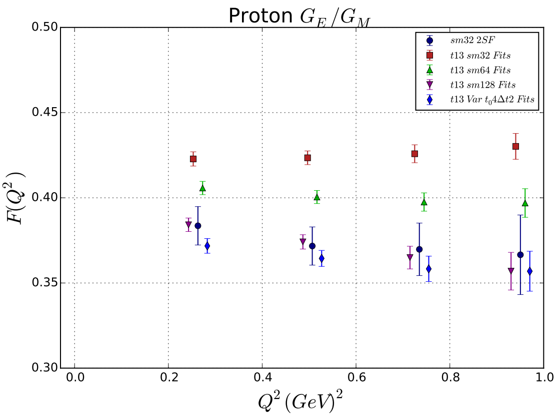
$$\mathcal{A}_E G_E(q^2) + \mathcal{A}_M G_M(q^2) = R(\Gamma; \vec{0}, t; \vec{q}, \tau; \overline{u}\gamma_\mu u),$$

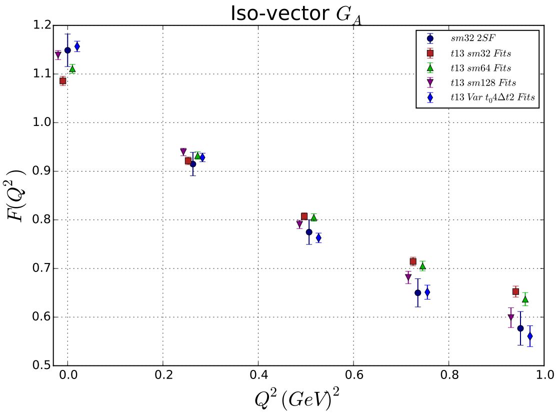
$$\mathcal{A}_A G_A(q^2) + \mathcal{A}_P G_P(q^2) = R(\Gamma; \vec{0}, t; \vec{q}, \tau; \overline{u}\gamma_5\gamma_\mu u),$$

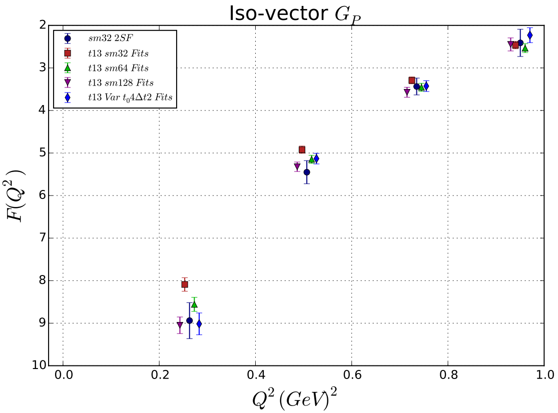
- Comparing the excited-state contamination effects by comparing:
  - 32, 64, 128 sweeps of smearing at $t = 13$
  - Variational method at $t = 13$
  - Two-exponential fit method over 32 sweeps of smearing using $t = 10, 13, 16, 19, 22$


Proton G_E
$sm32\ 2SF$
$t13\ sm32\ Fits$
$t13\ sm64\ Fits$
$t13\ sm128\ Fits$
$t13\ Var\ t_0 4\Delta t2\ Fits$
$F(Q^2)$
$Q^2\ (GeV)^2$
1.0
0.8
0.6
0.4
0.2
0.0
0.2
0.4
0.6
0.8
1.0


Proton G_M
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.0
0.2
0.4
0.6
0.8
1.0
$F(Q^2)$
$Q^2\ (GeV)^2$
sm32 2SF
t13 sm32 Fits
t13 sm64 Fits
t13 sm128 Fits
t13 Var $t_0 4\Delta t2$ Fits


Proton G_E/G_M
0.50
0.45
0.40
0.35
0.30
0.0
0.2
0.4
0.6
0.8
1.0
$F(Q^2)$
$Q^2\ (GeV)^2$
sm32 2SF
t13 sm32 Fits
t13 sm64 Fits
t13 sm128 Fits
t13 Var $t_0 4\Delta t2$ Fits


Iso-vector G_A
$F(Q^2)$
$Q^2\ (GeV)^2$
sm32 2SF
t13 sm32 Fits
t13 sm64 Fits
t13 sm128 Fits
t13 Var $t_0 4\Delta t2$ Fits


Iso-vector G_P
$F(Q^2)$
$Q^2\ (GeV)^2$
sm32 2SF
t13 sm32 Fits
t13 sm64 Fits
t13 sm128 Fits
t13 Var $t_0 4\Delta t2$ Fits

Summary

- We have systematically undertaken all 3 methods in this analysis.
- Variational method can reach the ground state solution by optimising our interpolating fields.
- The two-state fit and summation methods are sufficient for removing "*minimal*" excited-state contamination.
- Careful consideration is needed when analysing correlators with insufficient source-sink separations.
- Excited-state systematics is crucial if we hope to undertake precise calculations of:
  - Form factors at larger Q^2
  - Complicated operators $O^{(q)} = \overline{q}\gamma_{\mu_1} D_{\mu_2} \ldots D_{\mu_n} q$

Cost/Benefit Discussion

- The biggest contributor to calculation time is associated with matrix inversions.
- Assume we use the same number of gauge fields per calculation.
- Creating a G_2 requires 1 set of inversion for a point to all propagator.
- Creating a G_3 requires $4\vec{p}'$ sets of inversions to account for up/down quark contributions and spin projections.

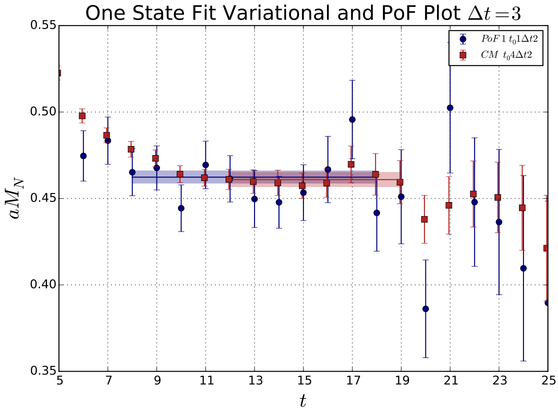
Create	Standard	2exp & SM (over n_t)	CM (over n_{basis})
C_2	1	1	n_{basis}
C_3	4	$4n_t$	$4n_{basis}$
Total	5	$1 + 4n_t$	$5n_{basis}$
This Work	5	21	15

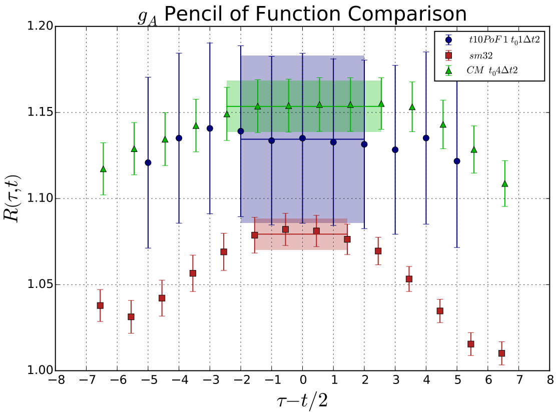
Pencil of Function

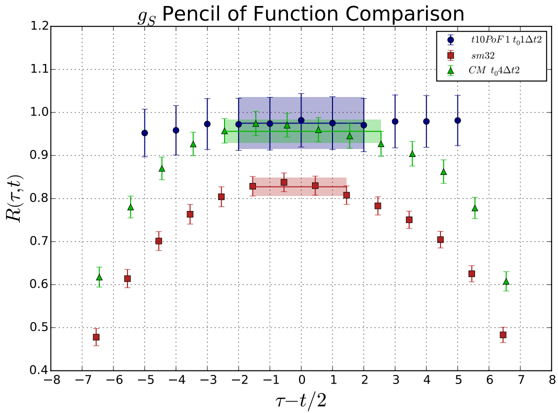
- A Pencil of Function can be utilised as shown in Phys. Rev. D 90, 074507 (2014) J. R. Green et al.
- As done in the variational method, we create a matrix of 2 point correlators of the form:

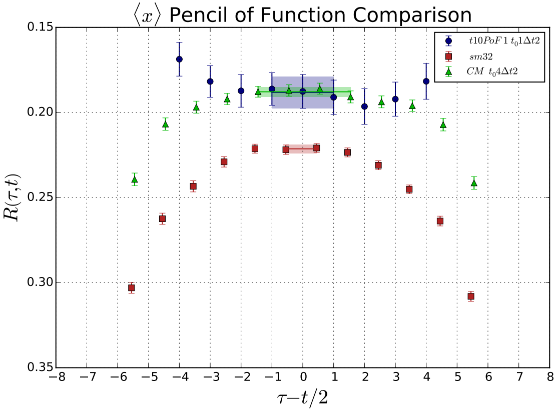
$$G_2(\vec{p},t) = \begin{bmatrix} (G_2)_{ij}(\vec{p},t) & (G_2)_{ij}(\vec{p},t+\delta) \\ (G_2)_{ij}(\vec{p},t+\delta) & (G_2)_{ij}(\vec{p},t+2\delta) \end{bmatrix}_{kl}.$$

- We can visualise the above equation as a block matrix equation, with indices running over both the sink shifts kl and the smearings ij.


One State Fit Variational and PoF Plot $\Delta t = 3$
aM_N
t
$PoF\,1\ t_0 1 \Delta t 2$
$CM\ t_0 4 \Delta t 2$
0.55
0.50
0.45
0.40
0.35
5
7
9
11
13
15
17
19
21
23
25


g_A Pencil of Function Comparison
$R(\tau, t)$
$\tau - t/2$
$t10PoF\,1\ t_0 1 \Delta t 2$
$sm32$
$CM\ t_0 4 \Delta t 2$
1.20
1.15
1.10
1.05
1.00
−8
−7
−6
−5
−4
−3
−2
−1
0
1
2
3
4
5
6
7
8


g_S Pencil of Function Comparison
$t10PoF1\ t_0 1\Delta t2$
$sm32$
$CM\ t_0 4\Delta t2$
$R(\tau,t)$
$\tau - t/2$


$\langle x \rangle$ Pencil of Function Comparison
$t10PoF1\ t_0 1\Delta t2$
$sm32$
$CM\ t_0 4\Delta t2$
$R(\tau,t)$
$\tau - t/2$