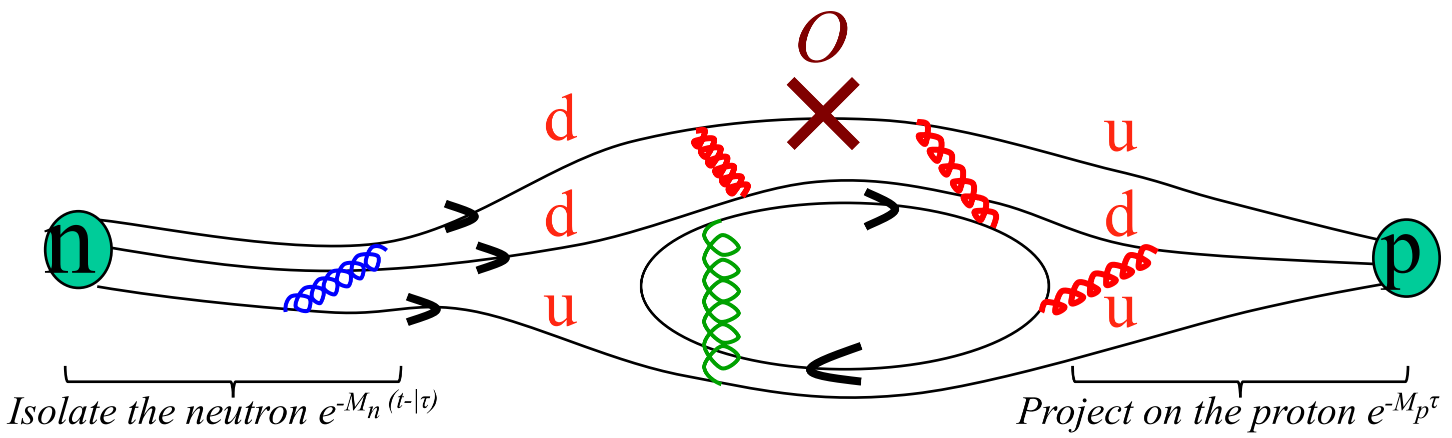
The spin of the proton from lattice QCD

Rajan Gupta
Laboratory Fellow
Theoretical Division
Los Alamos National Laboratory, USA



LA-UR 17-26064

SPIN2018, September 14, 2018

PNDME collaboration

(Clover-on-HISQ)

- Tanmoy Bhattacharya
- Vincenzo Cirigliano
- Yong-Chull Jang
- Huey-Wen Lin
- Boram Yoon

Bhattacharya et al, PRD85 (2012) 054512
Bhattacharya et al, PRD89 (2014) 094502
Bhattacharya et al, PRD92 (2015) 114026
Bhattacharya et al, PRL 115 (2015) 212002
Bhattacharya et al, PRD92 (2015) 094511
Bhattacharya et al, PRD94 (2016) 054508
Bhattacharya et al, PRD96 (2017) 114503
Gupta et al, Phys.Rev. D98 (2018) 034503
Huey-Wen Lin et al, arXiv:1806.10604
Gupta et al, arXiv:1808.07597

Spin of the Proton is known

Ji's gauge invariant decomposition of the proton spin is

$$\frac{1}{2} = \sum_{\{u,d,s,c\}} \underbrace{\left(\frac{1}{2}\Delta q + L_q\right)}_{J_q} + J_g$$

Ji, PRL (1999)

- Δq is the contribution of spin of quark flavor q
- L_q is the orbital angular momentum of quark q
- J_q is the total angular momentum of quarks
- J_g is the total angular momentum of gluons

- $\langle P | \bar{q} \; \gamma_\mu \gamma_5 \; q | P \rangle$

Goal: calculate each contribution using lattice QCD

$$\frac{1}{2} = \sum_{q=u,d,s,c} \underbrace{\left(\frac{1}{2}\Delta q + L_q\right)}_{J_q} + J_g$$

$\Delta q \equiv g_A^q$ **is best determined quantity**

$$\langle N | Z_A \overline{q} \gamma_\mu \gamma_5 q | N \rangle = g_A^q \, \overline{u}_{\mathrm{N}} \, \gamma_\mu \gamma_5 u_N$$

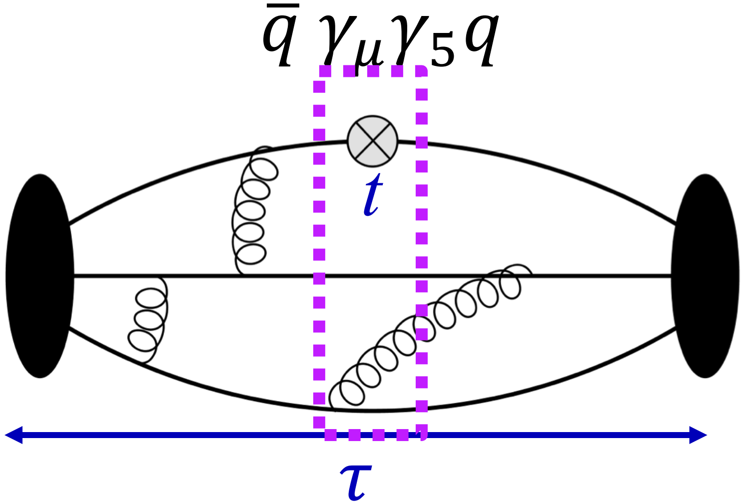
- $\overline{q}\gamma_\mu\gamma_5 q$ is the bare axial current for flavor q
- Z_A renormalization constant for axial current
- g_A^q axial charge for quark flavor q
- u_N nucleon spinor

COMPASS 2015 analysis @ 3GeV^2: $0.13 < \frac{1}{2}\Delta\Sigma < 0.18$

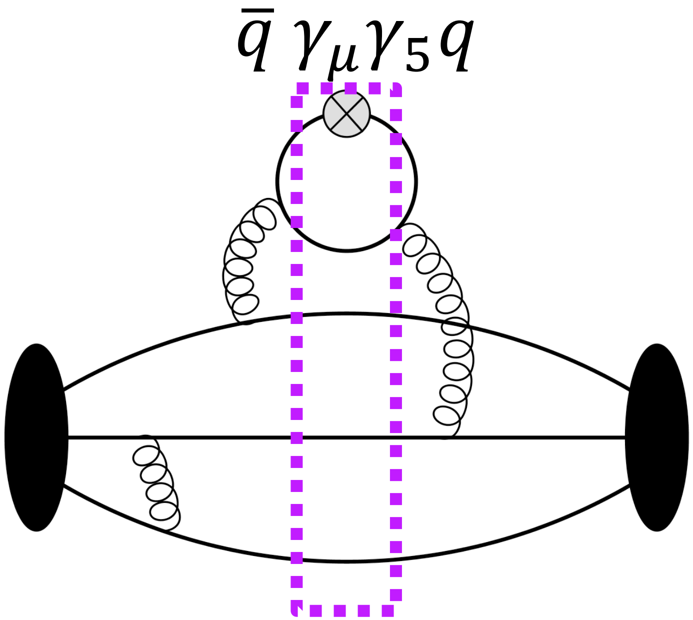
g_A is given by the matrix elements of quark bilinear axial current within the nucleon state: $\langle N|\bar{q}\,\gamma_\mu\gamma_5 q|\,N\rangle$

$$\langle N|Z_A\overline{q}\gamma_\mu\gamma_5 q|N\rangle = g_A^q\,\overline{u}_N\gamma_\mu\gamma_5 u_N$$

ME extracted from the 3-point correlation function $\langle N(\tau)A(t)N(0)\rangle$

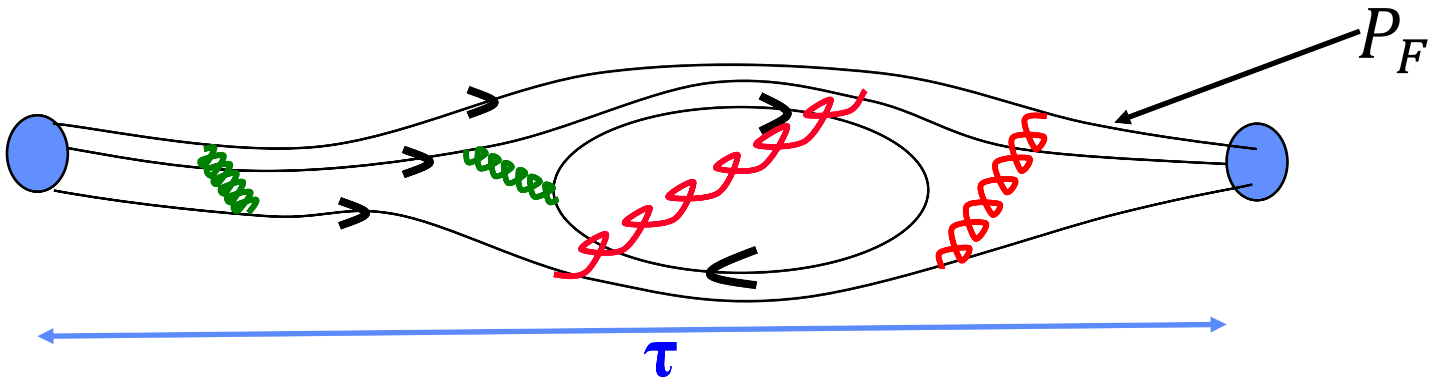


"Connected"



"Disconnected"

LQCD: Field theory in Euclidean time

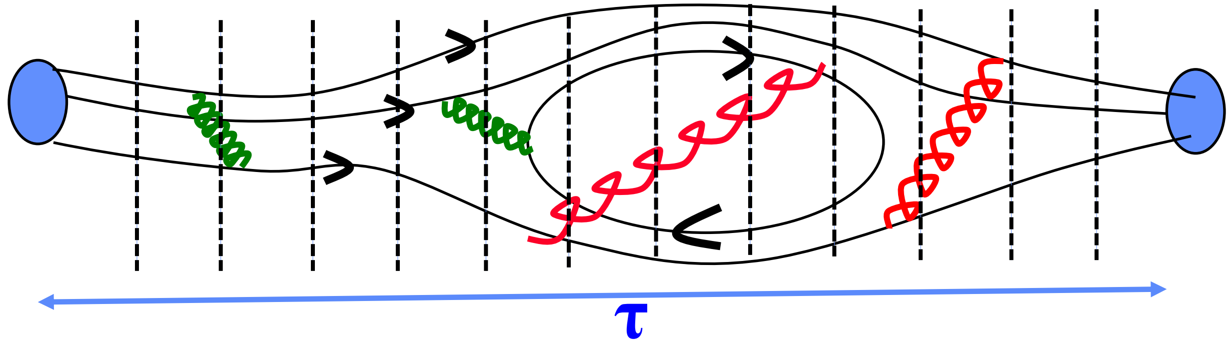


$$\langle 0 | N(\tau) \bar{N}(0) | 0 \rangle = \sum_n A_n^2 e^{-m_n \tau}$$

Choose any interpolating operator, $N = (\bar{u}^T C \gamma_5 \bar{d})\bar{u}$ with the right quantum numbers. It creates the nucleon state + all excited and multiparticle states

Key ingredients: **Ensemble of gauge configurations**
Feynman propagator $P_F = D^{-1}\eta$

LQCD: Field theory in Euclidean time



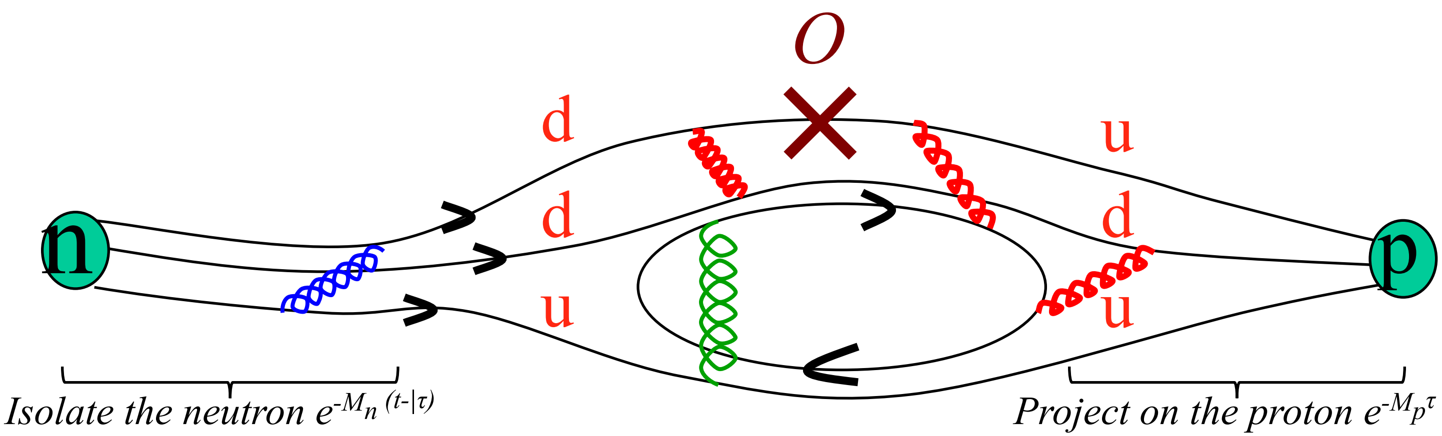
$$\Sigma_{i...f}\langle 0|N|n_f\rangle e^{-H\delta\tau}\,\langle n_f|n_{f-1}\rangle e^{-H\delta\tau}\;\ldots e^{-H\delta\tau}\langle n_{i+1}|n_i\rangle e^{-H\delta\tau}\,\langle n_i|N|0\rangle$$

$$\Sigma_{i...f}\langle 0|N|n_f\rangle e^{-E_f\delta\tau}\,\langle n_f|n_{f-1}\rangle e^{-E_{f-1}\delta\tau}\;\ldots e^{-E_{i+1}\delta\tau}\langle n_{i+1}|n_i\rangle e^{-H\delta\tau}\,\langle n_i|N|0\rangle$$

$$\Sigma_i\langle 0|N|n_i\rangle e^{-E_i\tau}\,\langle n_i|N|0\rangle = \Sigma_i A_i^2\, e^{-E_i\tau}$$

- Insert complete set of states $\Sigma_i|n_i\rangle\langle n_i| = 1$ of the transfer matrix at each intermediate time slice
- Propagate in Euclidean time: $e^{-H\delta\tau}$ with eigenvalues $e^{-E_n\delta\tau}$
- In a finite box these states are discrete with energy E_n
- At long time τ, only the ground state survives: $\lim_{\tau\to\infty} A_0^2 e^{-E_0\tau}$

matrix elements from 3-point functions



$$\langle \Omega | \hat{N}(t, p') \hat{O}(\tau, p'-p) \hat{N}(0, p) | \Omega \rangle =$$

$$\sum_{i,j} \langle \Omega | \hat{N}(p') | N_j \rangle e^{-\int dt\, H} \langle N_j | \hat{O}(\tau, p'-p) | N_i \rangle e^{-\int dt\, H} \langle N_i | \hat{N}(p) | \Omega \rangle =$$

$$\sum_{i,j} \langle \Omega | \hat{N}(p') | N_j \rangle e^{-E_j(t-\tau)} \underbrace{\langle N_j | \hat{O}(\tau, p'-p) | N_i \rangle}_{\text{Matrix element}} e^{-E_i \tau} \langle N_i | \hat{N}(p) | \Omega \rangle$$

Matrix element

Spectral decomposition of 2- and 3-point functions

$$\Gamma^2(t) = |A_0|^2 e^{-M_0 t} + |A_1|^2 e^{-M_1 t} + |A_2|^2 e^{-M_2 t} + |A_3|^2 e^{-M_3 t} + \ldots.$$

$$\Gamma^3(t,\Delta t) = |A_0|^2 \langle 0|O|0\rangle e^{-M_0 \Delta t} + |A_1|^2 \langle 1|O|1\rangle e^{-M_1 \Delta t} + A_0 A_1^* \langle 0|O|1\rangle e^{-M_0 \Delta t} e^{-\Delta M(\Delta t - t)} + A_0^* A_1 \langle 1|O|0\rangle e^{-\Delta M t} e^{-M_0 \Delta t} + \ldots$$

Gives amplitudes, energy levels, matrix elements

Flowchart: path integral method for calculating expectation values

- Generate ensemble of gauge configurations with weight e^{-S}
- On each configuration calculate Feynman quark propagator $P_F = D^{-1}\eta$
- 2-point function: Tie together 3 P_F with *Nucleon* interpolating operator N on either end
- Construct 2- and 3-point expectation values as ensemble averages
- Extract matrix elements using the spectral decomposition

Lattice QCD is QCD on a finite 4-d Euclidean lattice with spacing a

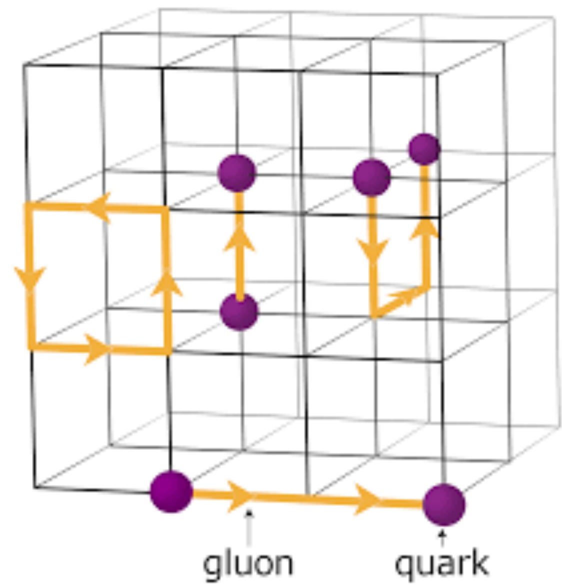
Theory defined by 6 free parameters

- Bare coupling $g \leftrightarrow a$
- u, d, s, c, b quark masses

Fix a, m_q using 6 physical quantities

8 gluon degrees of freedom

- SU(3) matrices $U = e^{iagA\cdot\lambda}$



Dirac action $S_F = \bar{\psi}\,\partial_\mu A^\mu\,\psi(x) + m_q\overline{\psi}\,\psi(x)$

- $\bar{\psi}\,\partial_\mu A^\mu\,\psi(x) \rightarrow \dfrac{\bar{\psi} U_\mu(x)\psi(x + a\hat{\mu})}{a} = \dfrac{\overline{\psi_i} D_{ij}\psi_j}{a}$

Simulate using Markov Chain Monte Carlo method

- Action $A = e^{-\frac{1}{4}F^{\mu\nu}\ F_{\mu\nu}+S_F}$
- Integrate out the fermions
- $A = e^{-\frac{1}{4}(F^{\mu\nu}\ F_{\mu\nu})+\ln detD_F} = e^{-S}$
- Use e^{-S} as Boltzmann weight to generate importance sampled gauge configurations
- Feynman quark propagator $P_F = 1/D$
- Stitching *P* and *U* construct gauge invariant correlation functions on ensembles of gauge configurations
- Calculate expectation values as ensemble averages
- These give $O(a, m_u, m_d, m_s, m_c, m_b)$
- Take the continuum limit $a \rightarrow 0$ keeping physics constant
- Tune m_u, m_d, m_s, m_c, m_b to their physical value to get O_{physical}

Simulations of lattice QCD provide the non-perturbative wavefunction of hadrons→ME.

➤ precise lattice data for $g_A(a, M_\pi, M_\pi L)$ at multiple values of $a, M_\pi^2, M_\pi L$

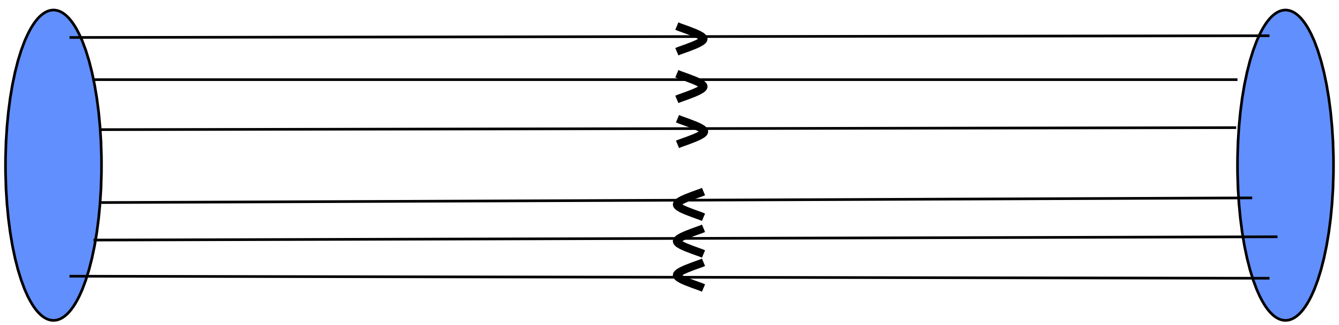
Calculations done in the isospin symmetric limit $m_u = m_d$

m_s , m_c tuned to physical value using M_Ω or $M_{s\bar{s}}$ and $M\eta_c$

Ignore bottom quarks as m_b is heavy for this physics

The challenge: signal to noise

The lowest state in the squared correlation function is the 3 pion state ($3M_\pi$) which is much lighter than the 2 nucleon ($2M_N$) state



$$\frac{signal}{noise} \sim e^{-(M_N - 1.5M_\pi)\tau}$$

Need very high statistics to reach large τ at which excited state contribution becomes negligible

Systematic uncertainties in matrix elements within nucleon states

- **High Statistics: O(100,000) measurements**
- **Demonstrating control over all Systematic Errors:**
  - Contamination from excited states
  - Non-perturbative renormalization of bilinear operators (RI_{smom} scheme)
  - Finite volume effects
  - Chiral extrapolation to physical m_u and m_d (simulate at physical point)
  - Extrapolation to the continuum limit (lattice spacing $a \rightarrow 0$)

Perform simulations on ensembles with multiple values of

- Lattice sizes and take $M_\pi L \rightarrow \infty$
- Light quark masses $\rightarrow$ physical m_u and m_d $\rightarrow M_\pi = 135$ MeV
- Lattice spacings and take $a \rightarrow 0$

Toolkit

- Multigrid Dirac invertor → propagator $P_F = D^{-1}\eta$
- Truncated solver method with bias correction (TSM)
- Coherent source sequential propagator
- Deflation + hierarchical probing (for disconnected)
- 3-5 values of τ with smeared sources
- 2-state and 3-state fits to multiple values of τ
- Non-perturbative renormalization constant Z_A
- Combined extrapolation in a, M_π, $M_\pi L$
- Variation of results with extrapolation ansatz

HISQ Ensembles $N_f = 2+1+1$

PNDME collaboration

m_s tuned to the physical mass using $M_{s\bar{s}}$

Ensemble ID	a (fm)	$M_\pi^{\rm sea}$ (MeV)	$M_\pi^{\rm val}$ (MeV)	$L^3 \times T$	$M_\pi^{\rm val} L$	τ/a	$N_{\rm conf}$	$N_{\rm meas}^{\rm HP}$	$N_{\rm meas}^{\rm LP}$
a15m310	0.1510(20)	306.9(5)	320(5)	$16^3 \times 48$	3.93	$\{5,6,7,8,9\}$	1917	7668	122,688
$a12m310$	0.1207(11)	305.3(4)	310.2(2.8)	$24^3 \times 64$	4.55	$\{8,10,12\}$	1013	8104	64,832
a12m220S	0.1202(12)	218.1(4)	225.0(2.3)	$24^3 \times 64$	3.29	$\{8,10,12\}$	946	3784	60,544
a12m220	0.1184(10)	216.9(2)	227.9(1.9)	$32^3 \times 64$	4.38	$\{8,10,12\}$	744	2976	47,616
a12m220L	0.1189(09)	217.0(2)	227.6(1.7)	$40^3 \times 64$	5.49	$\{8,10,12,14\}$	1000	4000	128,000
a09m310	0.0888(08)	312.7(6)	313.0(2.8)	$32^3 \times 96$	4.51	$\{10,12,14,16\}$	2263	9052	144,832
a09m220	0.0872(07)	220.3(2)	225.9(1.8)	$48^3 \times 96$	4.79	$\{10,12,14,16\}$	964	7712	123,392
$a09m130$	0.0871(06)	128.2(1)	138.1(1.0)	$64^3 \times 96$	3.90	$\{10,12,14\}$	883	7064	84,768
a09m130W						$\{8,10,12,14,16\}$	1290	5160	165,120
$a06m310$	0.0582(04)	319.3(5)	319.6(2.2)	$48^3 \times 144$	4.52	$\{16,20,22,24\}$	1000	8000	64,000
a06m310W						$\{18,20,22,24\}$	500	2000	64,000
$a06m220$	0.0578(04)	229.2(4)	235.2(1.7)	$64^3 \times 144$	4.41	$\{16,20,22,24\}$	650	2600	41,600
a06m220W						$\{18,20,22,24\}$	649	2596	41,536
a06m135	0.0570(01)	135.5(2)	135.6(1.4)	$96^3 \times 192$	3.7	$\{16,18,20,22\}$	675	2700	43,200

$$a: \quad 0.15, 0.12, 0.09, 0.06\ fm$$

$$M_\pi: \quad 310, 220, 135\ MeV$$

$$3.3 < M_\pi L < 5.5$$

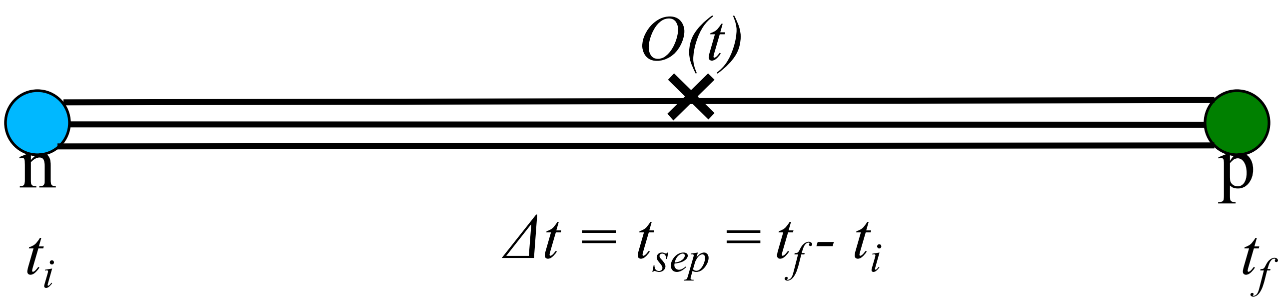
Gupta et al, Phys. Rev. D98 (2018) 034503

Controlling excited-state contamination: n-state fit

$$\Gamma^2(t) = |A_0|^2 e^{-M_0 t} + |A_1|^2 e^{-M_1 t} + |A_2|^2 e^{-M_2 t} + |A_3|^2 e^{-M_3 t} + \ldots.$$

$$\Gamma^3(t, \Delta t) = |A_0|^2 \langle 0|O|0\rangle e^{-M_0 \Delta t} + |A_1|^2 \langle 1|O|1\rangle e^{-M_1 \Delta t} + A_0 A_1^* \langle 0|O|1\rangle e^{-M_0 \Delta t} e^{-\Delta M(\Delta t - t)} + A_0^* A_1 \langle 1|O|0\rangle e^{-\Delta M t} e^{-M_0 \Delta t} + \ldots$$

M_0, M_1, … masses of the ground & excited states
A_0, A_1, … corresponding amplitudes

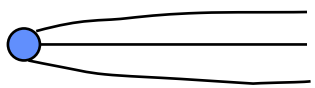


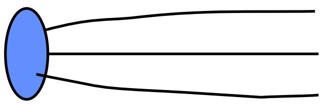
Make a simultaneous fit to data at multiple t and $\tau \equiv \Delta t$

Controlling excited-state contamination

- Reduce A_n/A_0 in an n-state fit by tuning N
  - Tune source smearing size σ in

$$P_F = D^{-1}\eta_\sigma = D^{-1}\, S_\sigma \delta(x)$$



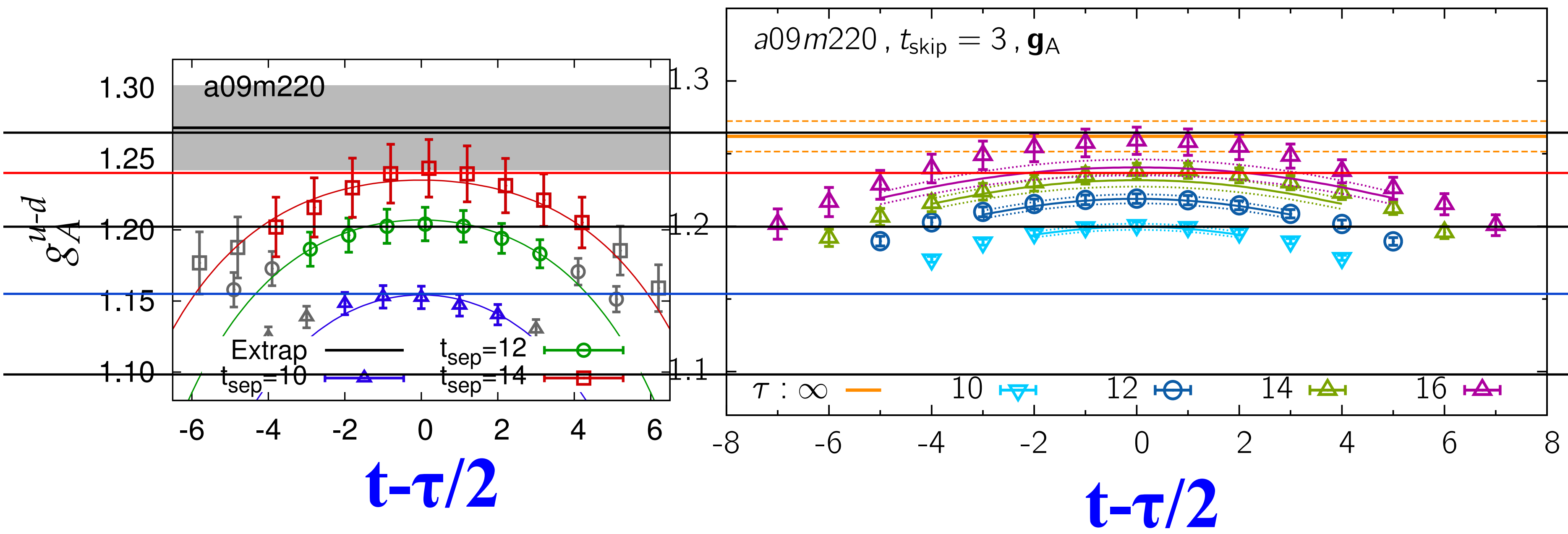


- Generate data at multiple values of τ
- 2 → 3 → n-state fits to data at many t and τ

Yoon et al, PRD D93 (2016) 114506
Yoon el al, PRD D95 (2017) 074508

Toolkit: Controlling Excited State Contamination

- Better smearing
- Higher statistics (10K 100K) with TSM
- 4-5 values of source-sink separation τ
- 4-state fits to 2-point functions
- 3-state fits to 3-point functions
- Full covariance error matrix



Gupta et al, Phys. Rev. D98 (2018) 034503

Analyzing lattice data $g_A(a, M_\pi, M_\pi L)$:
Simultaneous CCFV fits versus a, M_π^2, $M_\pi L$

Take into account corrections to lattice data due to

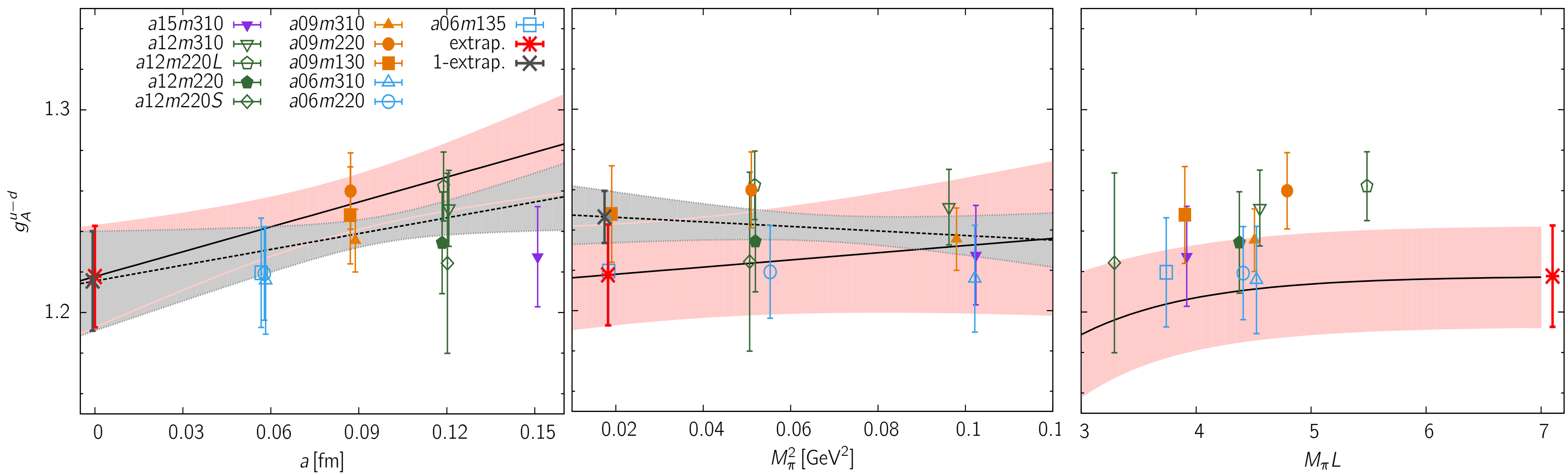
- Lattice spacing: a
- Dependence on light quark mass: $m_q \sim M_\pi^2$
- Finite volume: $M_\pi L$

Get physical result using the fit with lowest order term in each

$$g_A^{u,d,s}(a, M_\pi, M_\pi L) = c_0 + c_1 \mathrm{a} + c_2\, M_\pi^2 + c_3 M_\pi^2\, e^{-M_\pi L} + \ldots$$

Simultaneous extrapolation in $a,\ M_\pi^2,\ M_\pi L$

Fits using 11 clover-on-HISQ ensembles:



$$g_A^{u-d} = \quad 1.218(25)(30) \qquad g_A^{u+d}\Big|_{conn} = 0.575(24)$$

g_A^{u-d} smaller than experimental value 1.277(2) by 5%

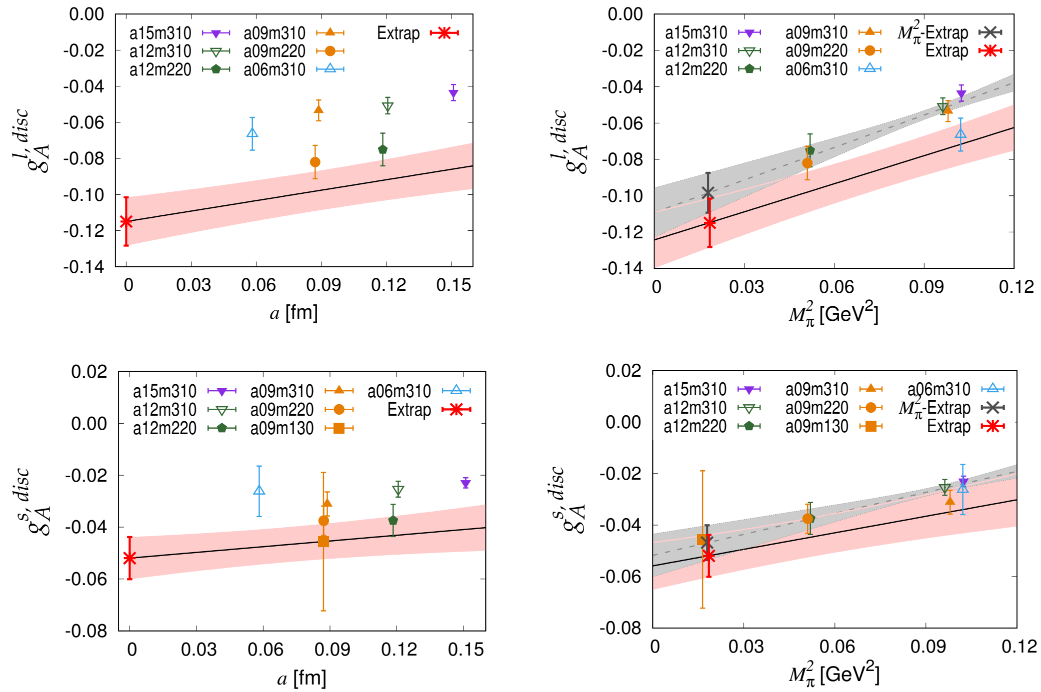
PNDME collaboration Phys. Rev. D98 (2018) 034503

Disconnected Contribution

PNDME collaboration arXiv:1806:10604

$$g_A^q = \langle p(0)|\bar{q}\gamma_\mu\gamma_5 q|p(0)\rangle$$

- $g_A^l = -0.118(14)$
- $g_A^s = -0.053(8)$



- $g_A^u = \quad 0.777(25)$
- $g_A^d = -0.438(18)$
- $g_A^s = -0.053(8)$

$$\frac{1}{2}\Delta\Sigma = (g_A^u + g_A^d + g_A^s + \cdots)/2 = 0.143(31)(36)$$

COMPASS Analysis (2016): 0.13 < ΔΣ/2 < 0.18

Only lattice QCD result with continuum and chiral extrapolation

Detailed Summary of Results

	$g_A^u\big\vert_{conn}$	$g_A^d\big\vert_{conn}$	$g_A^l\big\vert_{disc}$	$g_A^s\big\vert_{disc}$	$g_A^u\big\vert_{sum}$	$g_A^d\big\vert_{sum}$	$g_A^s\big\vert_{sum}$
PNDME	0.895(21)	-0.320(12)	-0.118(14)	-0.053(8)	0.777(25)	-0.438(18)	-0.053(8)
ETMC	0.904(30)	-0.305(28)	-0.075(14)	-0.042(10)	0.830(26)	-0.386(18)	-0.042(10)
χQCD	0.917 (13)(28)	-0.337 (10)(10)	-0.070 (12)(15)	-0.035 (6)(7)	0.847 (18)(32)	-0.407 (16)(18)	-0.035 (6)(7)

PNDME
1806.10604

$$\frac{1}{2}\Delta\Sigma = (g_A^u + g_A^d + g_A^s)/2 = 0.143(31)(36)$$

ETMC
1706.02973

$$\frac{1}{2}\Delta\Sigma = (g_A^u + g_A^d + g_A^s)/2 = 0.201(17)(5)$$

χQCD
1806.08366

$$\frac{1}{2}\Delta\Sigma = (g_A^u + g_A^d + g_A^s)/2 = 0.202(13)(19)$$

Not “equal”: systematics are different?

- PNDME: 0.143(31)(36) (2+1+1 flavor clover-on-HISQ)
- ETMC: 0.201(17)(5) (2 flavor twisted mass)
- χQCD: 0.202(13)(19) (2+1 flavor overlap-on-Domain Wall)

	g_A^{u-d}	$a \to 0$	M_π MeV	$M_\pi L$	Z_A
PNDME N_f =2+1+1	1.218(25)(30)	Yes 11 ensembles 0.15 – 0.06 fm	135 220 310	3.3 – 5.5	Assume $Z_A^s = Z_A^{ns}$
ETMC N_f =2	1.212(40)	0.094 fm	130	2.93	Checked $Z_A^s = Z_A^{ns}$
χQCD N_f =2+1	1.254(16)(30)	“No” a variation 0.143 fm 0.11 fm 0.083 fm	171 337 302	3.97 4.53 4.06	Checked $Z_A^s = Z_A^{ns}$

In perturbation theory $Z_A^s \neq Z_A^{ns}$ at 2 loops . ETMC & χQCD show a ~1% difference

Ji: Total angular momentum

$$J^i_{q,g} = \frac{1}{2}\epsilon^{ijk}\int d^3x\,(T^{0k}_{q,g}\,x^j - T^{0j}_{q,g}x^k)$$

$$\vec{J}_q = \int d^3x\,\psi^\dagger[\vec{\gamma}\gamma_5 + \vec{x}\times(-i\vec{D})]\psi$$

$$\vec{J}_g = \int d^3x\,[\vec{x}\times\left(\vec{E}\times\vec{B}\right)]$$

Total angular momentum $J_{q(g)}$ of quark (gluon)

EXPT: 2nd Mellin moment of unpolarized nucleon PDF

Lattice: $\left\langle N(p',s') \left| O_V^{\{\mu\nu\}} \right| N(p,s) \right\rangle = \overline{u}_N(p',s')\Lambda^{\{\mu\nu\}} u_N(p,s)$

$$O_V^{\{\mu\nu\}} = \overline{q}\gamma\{^{\mu}\, i\overleftrightarrow{D}^{\nu} q\} \qquad O_g^{\{\mu\nu\}} = \frac{g^{\mu\nu}G^2}{4} - G^{\mu\sigma}G_{\sigma}^{\nu}$$

Decompose $\Lambda^{\{\mu\nu\}}$ in terms of three form factors

$$\Lambda_q^{\{\mu\nu\}}(Q^2) = A_{20}^q(Q^2)\{\gamma^{\mu} P^{\nu}\} + \frac{B_{20}^q(Q^2)\{\sigma^{\mu\alpha}q_{\alpha}P^{\nu}\}}{2M_N} + \frac{C_{20}^q(Q^2)\{Q^{\mu}Q^{\nu}\}}{M_N}$$

Where $Q = (p' - p)$; $P = (p' + p)/2$

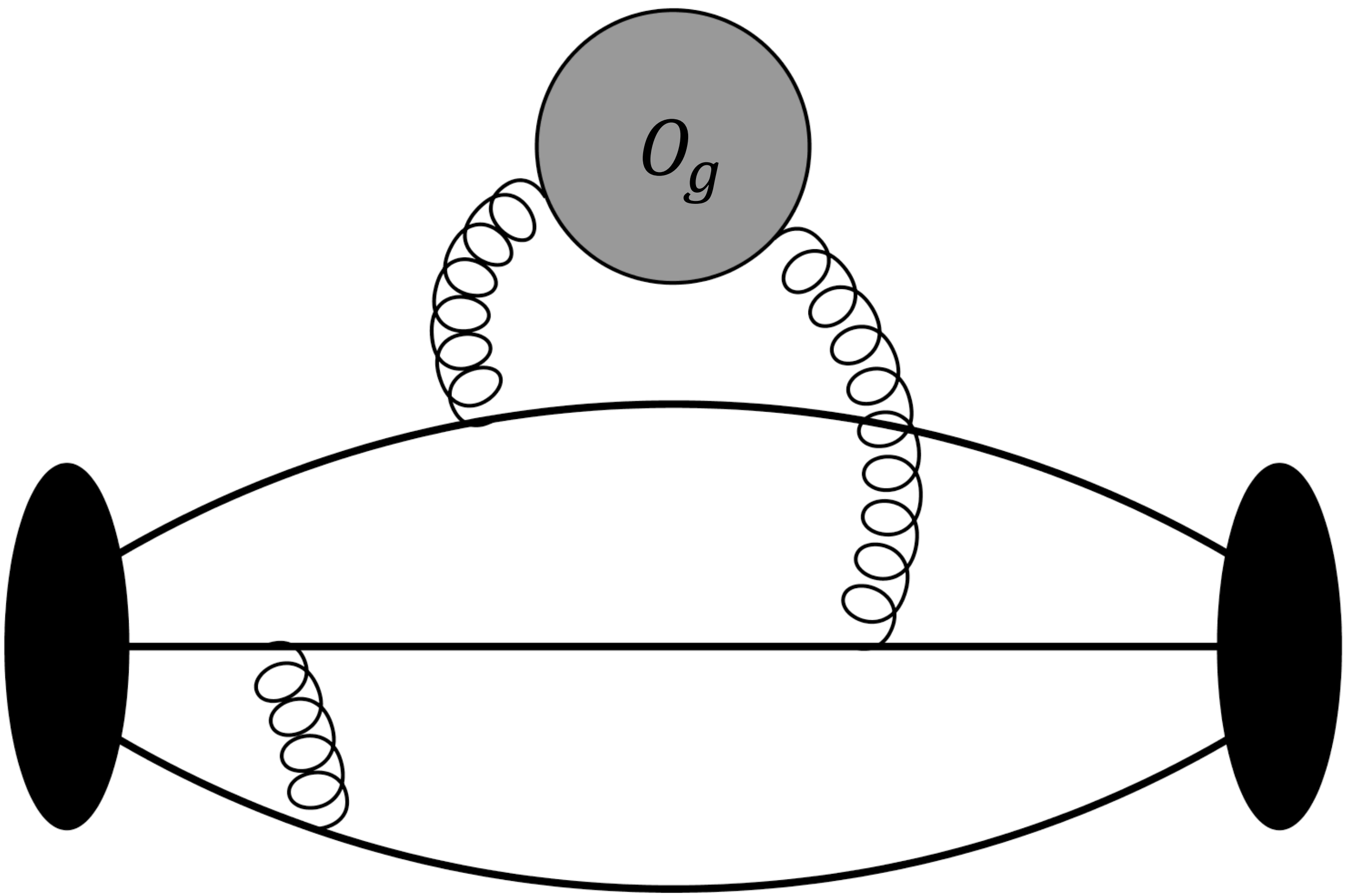
The total angular momentum $J_{q(g)}$ of quark (gluon)

$$J_{q(g)} = \frac{1}{2}[A_{20}^{q(g)}(0) + B_{20}^{q(g)}(0)]$$

$$\langle x \rangle_{q(g)} = A_{20}^{q(g)}(0)$$

Form factors calculated using LQCD

Signal in the gluon diagram (disconnected only) is noisy



$J_q + J_g$

$$J_g \approx \frac{1}{2}\langle x\rangle_g = 0.133(11)(14)$$

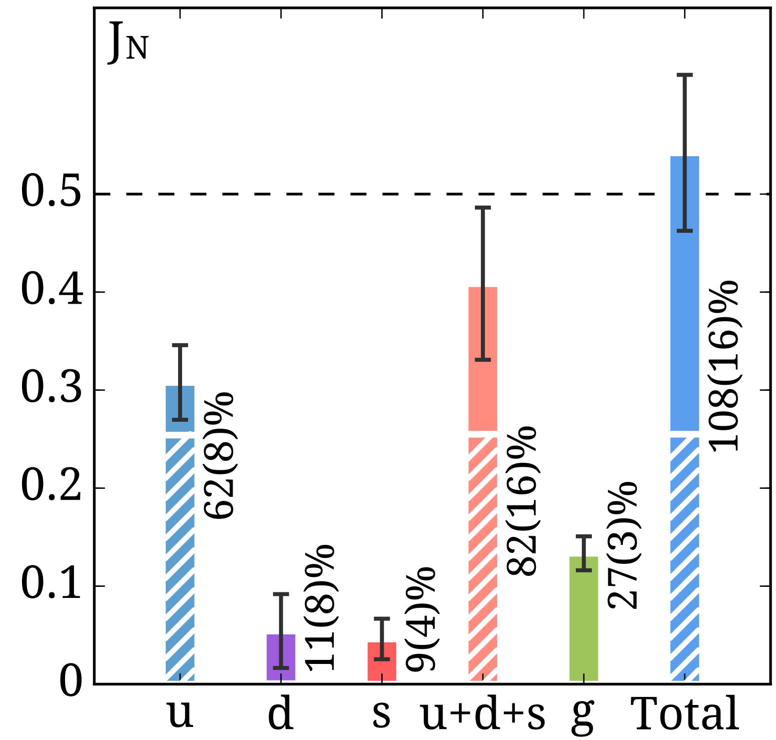
ETMC: PRL 119 (2017) 142002
Fernanda Steffens @ SPIN 2018

$$J_{u+d+s} = 0.255(12)(3)\Big|_{conn} + 0.153(60)(47)\Big|_{disc}$$

$$= 0.408(61)(48)$$

$$\frac{1}{2}\Delta\Sigma = \frac{g_A^u + g_A^d + g_A^s}{2} = 0.201(17)(5)$$

$$J_N = \sum_q J_q + J_g = 0.541(62)(49)$$



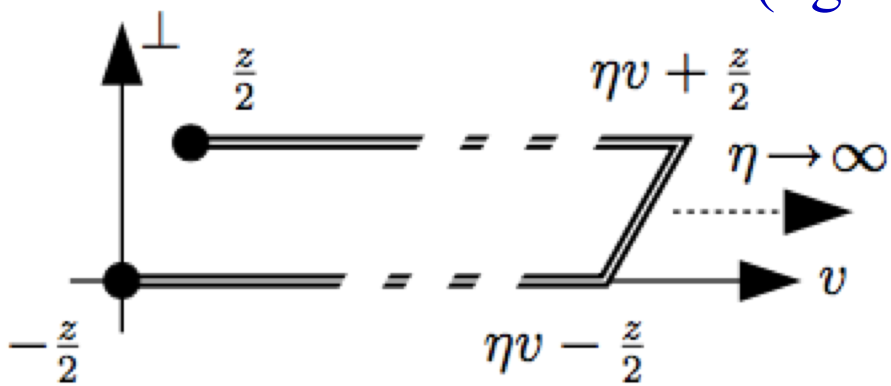
Also χQCD: Work in progress
Yi-Bo Yang @ Lattice 2018

Orbital Angular momentum

$\int d^3x\, \psi^\dagger [\vec{x} \times i\vec{D}]\psi$ versus $\int d^3x\, \psi^\dagger [\vec{x} \times i\vec{\nabla}]\psi$

Ji

Jaffe-Manohar
(light cone gauge)



$p' = P + \Delta_T \quad p = P - \Delta_T$

Engelhardt PRD (2017)

P and s in the z-direction

Straight path $\eta = 0$ gives Ji′s OAM

Staple $\eta \to \infty$ gives Jaffe − Manohar OAM

The difference is the accumulated torque due to FSI

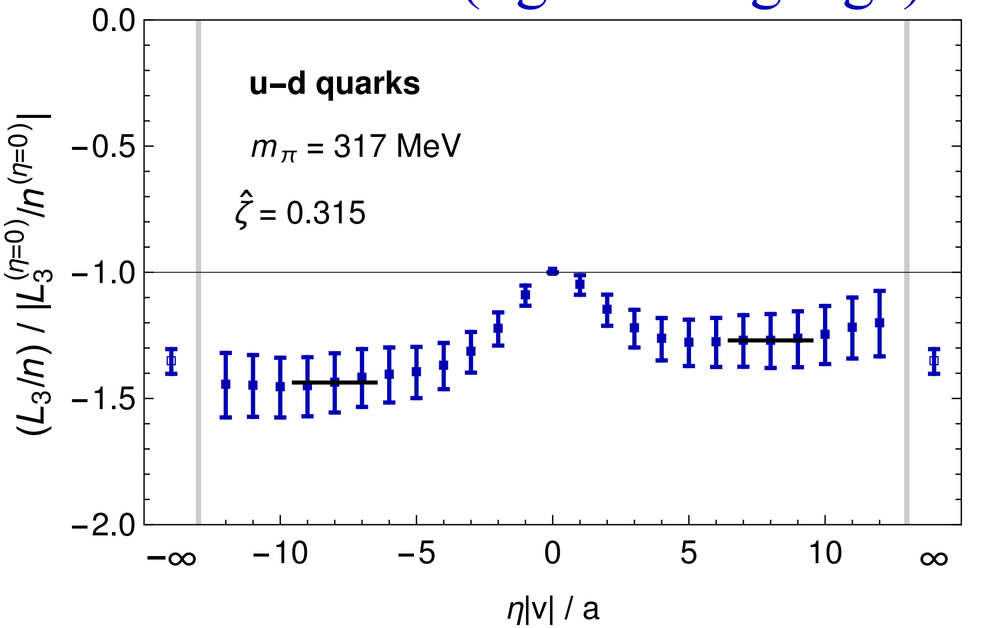
Orbital Angular momentum

$$\int d^3x\, \psi^\dagger [\vec{x} \times i\vec{D}]\psi \quad \text{versus} \quad \int d^3x\, \psi^\dagger [\vec{x} \times i\vec{\nabla}]\psi$$

Ji

Jaffe-Manohar
(light cone gauge)

$$\frac{\text{Jaffe} - \text{Manohar}}{|\text{Ji}|}$$



The difference is the extra torque accumulated as the struck quark flies out of the proton

Engelhardt Lattice 2018, Spin 2018

Summary

- With O(10^5) measurements, the statistical precision reached allows us to understood and control all systematics in the contribution of the quark spin
- Results on $\frac{1}{2}\Delta\Sigma$ will improve steadily
- Glue and OAM are more challenging.
- Significant progress in the last 2 years (computer time and algorithms) has led to first results

Acknowledgement: Computing Resources

- Clover-on-Clover:
- Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.
- Institutional Computing at Los Alamos National Laboratory.
- The USQCD Collaboration, funded by the Office of Science, U.S. DOE

- Clover-on-HISQ
- The National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. DOE under Contract No. DE-AC02-05CH11231
- Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.
- The USQCD Collaboration, funded by the Office of Science, U.S. DOE
- Institutional Computing at Los Alamos National Laboratory.
- The Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1053575