

Lattice QCD Calculations of Generalized Form Factors with Dynamical Fermions

Sergey N. Syritsyn

Lawrence Berkeley National Laboratory
Nuclear Science Division

INT Workshop “*Orbital angular momentum in QCD*”
Seattle, Feb 7, 2012

- 1 QCD on a lattice
- 2 Generalized Form Factors
- 3 Quark energy-momentum tensor in the nucleon
- 4 Excited States Contamination
- 5 Summary

QCD on a Lattice: Numerical Feynman Integration

Monte Carlo sampling with $\text{Prob}[U, \psi, \bar{\psi}] \sim e^{-S[U, \psi, \bar{\psi}]}$

$$\begin{aligned} \langle \mathcal{O} \rangle &= \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{O}[U, \psi, \bar{\psi}] e^{-S[U, \psi, \bar{\psi}]} \\ &= \int \mathcal{D}U \tilde{\mathcal{O}} \Pi_f[\not{D} + m_f] e^{-S_g[U]} \rightarrow \frac{1}{N} \sum^N \tilde{\mathcal{O}}[U] \end{aligned}$$

QCD on a Lattice: Numerical Feynman Integration

Monte Carlo sampling with $\text{Prob}[U, \psi, \bar{\psi}] \sim e^{-S[U, \psi, \bar{\psi}]}$

$$\langle \mathcal{O} \rangle = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{O}[U, \psi, \bar{\psi}] e^{-S[U, \psi, \bar{\psi}]}$$

$$= \int \mathcal{D}U \tilde{\mathcal{O}} \Pi_f[\not{D} + m_f] e^{-S_g[U]} \rightarrow \frac{1}{N} \sum^N \tilde{\mathcal{O}}[U]$$

- Euclidean QFT:
$$\begin{cases} x^0 \equiv t & \rightarrow -ix_4 \equiv -i\tau \\ p^0 \equiv E & \rightarrow ip_4 \\ \langle N(t) \bar{N}(0) \rangle & \rightarrow e^{-E\tau} \end{cases}$$

QCD on a Lattice: Numerical Feynman Integration

Monte Carlo sampling with $\text{Prob}[U, \psi, \bar{\psi}] \sim e^{-S[U, \psi, \bar{\psi}]}$

$$\langle \mathcal{O} \rangle = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{O}[U, \psi, \bar{\psi}] e^{-S[U, \psi, \bar{\psi}]}$$

$$= \int \mathcal{D}U \tilde{\mathcal{O}} \Pi_f[\not{D} + m_f] e^{-S_g[U]} \rightarrow \frac{1}{N} \sum^N \tilde{\mathcal{O}}[U]$$

- Euclidean QFT:
$$\begin{cases} x^0 \equiv t & \rightarrow -ix_4 \equiv -i\tau \\ p^0 \equiv E & \rightarrow ip_4 \\ \langle N(t) \bar{N}(0) \rangle & \rightarrow e^{-E\tau} \end{cases}$$

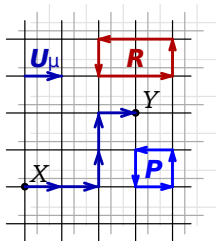
- Fields on a discrete space-time grid:

$$A_\mu^a(x) \rightarrow U_{x,\mu} = \mathcal{P} e^{-i \int_x^{x+\hat{\mu}} dx \cdot (A^a \frac{\lambda^a}{2})}$$

$$(D_\mu \varphi)_x \rightarrow \frac{1}{a} (U_{x,\mu} \varphi_{x+\hat{\mu}} - \varphi_x)$$

$$S_g[A_\mu] \sim (F_{\mu\nu}^a)^2 \rightarrow A \text{Tr}(\mathbf{P}) + B \text{Tr}(\mathbf{R})$$

- Fermions on a lattice: pick two from
no “doublers”; chiral symmetry; economy.



QCD on a Lattice: Numerical Feynman Integration

Monte Carlo sampling with $\text{Prob}[U, \psi, \bar{\psi}] \sim e^{-S[U, \psi, \bar{\psi}]}$

$$\langle \mathcal{O} \rangle = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{O}[U, \psi, \bar{\psi}] e^{-S[U, \psi, \bar{\psi}]}$$

$$= \int \mathcal{D}U \tilde{\mathcal{O}} \Pi_f[\not{D} + m_f] e^{-S_g[U]} \rightarrow \frac{1}{N} \sum^N \tilde{\mathcal{O}}[U]$$

- Euclidean QFT:
$$\begin{cases} x^0 \equiv t & \rightarrow -ix_4 \equiv -i\tau \\ p^0 \equiv E & \rightarrow ip_4 \\ \langle N(t)\bar{N}(0) \rangle & \rightarrow e^{-E\tau} \end{cases}$$

- Fields on a discrete space-time grid:

$$A_\mu^a(x) \rightarrow U_{x,\mu} = \mathcal{P} e^{-i \int_x^{x+\hat{\mu}} dx \cdot (A^a \frac{\lambda^a}{2})}$$

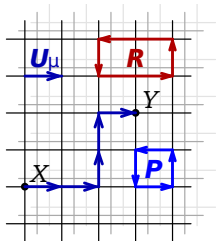
$$(D_\mu \varphi)_x \rightarrow \frac{1}{a} (U_{x,\mu} \varphi_{x+\hat{\mu}} - \varphi_x)$$

$$S_g[A_\mu] \sim (F_{\mu\nu}^a)^2 \rightarrow A \text{Tr}(\mathbf{P}) + B \text{Tr}(\mathbf{R})$$

- Fermions on a lattice: pick two from

no "doublers"; chiral symmetry; economy.

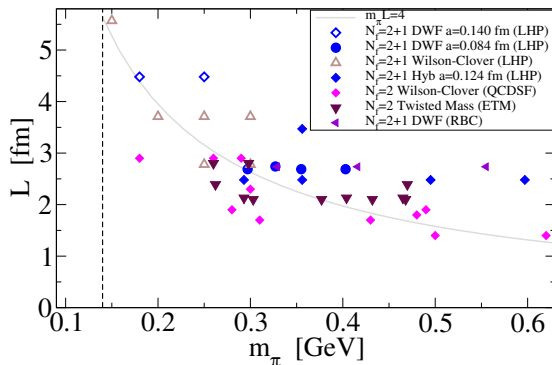
- Tune $(\alpha_S^{\text{lat}}, am_{ud}, am_s)$ to reproduce e.g. (m_π, m_K, m_Ω) .



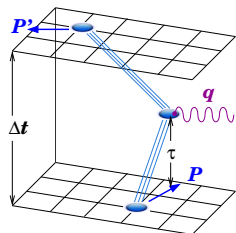
Lattice QCD is a Hard Problem

Solving QCD numerically is hard because

- **light quarks** are expensive: cost $\sim \frac{1}{m_\pi}$
- need **large physical size of the box** $L \gtrsim \frac{4}{m_\pi}$
- have to take **continuum limit** $a \rightarrow 0$, $L_{\text{lat}} = \frac{L}{a} \rightarrow \infty$
- **chiral symmetry** is expensive to preserve in lattice regularization



Hadron Matrix Elements



Extract $\langle P' | \mathcal{O} | P \rangle$ from 3-pt correlators

$$\sum_{\vec{x}, \vec{y}} e^{-i\vec{P}'\vec{x} + i\vec{q}\vec{y}} \langle N(\Delta t, \vec{x}) \mathcal{O}(\tau, \vec{y}) \bar{N}(0) \rangle$$

where for the proton

$$N_\alpha = \epsilon^{abc} u_\alpha^a [(u^b)^T C \gamma_5 d^c]$$

All QCD states are present:

$$\langle N(\Delta t) \mathcal{O}(\tau) \bar{N}(0) \rangle \sim \sum_{m,n} \sqrt{Z_m} \cdot e^{-E_m(\Delta t - \tau)} \cdot \mathcal{O}_{mn} \cdot e^{-E_n \tau} \cdot \sqrt{Z_n}^\dagger$$

Excited states can lead to systematic bias in m.e. :

$$\bar{N}_{\text{lat}} |\Omega\rangle = |N\rangle + C |X\rangle, \quad \Delta M = M_X - M_N,$$

$$\langle N | \mathcal{O} | N \rangle_{\text{lat}} \cong \langle N | \mathcal{O} | N \rangle + |C|^2 \langle X | \mathcal{O} | X \rangle e^{-\Delta M \cdot \Delta t} + \text{“tails”}$$

$$\text{Signal / noise} \sim e^{-(M_N - \frac{3}{2}m_\pi) \cdot \Delta t}$$

Hadron Matrix Elements are Challenging

- **2008:** The first calculation of hadron spectrum by the Budapest-Marseille-Wuppertal collaboration [Dürr et al, *Science*, 322:1224 (2008)]
- Hadron Structure \gg Hadron Spectrum

Quark-bilinear insertion

$$\langle P' | \bar{q} \Gamma q | P \rangle =$$

The diagram illustrates the quark-bilinear insertion $\langle P' | \bar{q} \Gamma q | P \rangle$. It shows two diagrams separated by a plus sign. The left diagram shows a quark bilinear insertion (wavy line) on a quark line between two vertices, with a gluon loop (green curly line) connecting the two vertices. The right diagram shows a quark bilinear insertion on a quark line, with a gluon loop (green curly line) connecting the two vertices and a ghost loop (black curly line) connecting the two vertices.

- Disconnected contractions are noisy
- Gluon operators are noisy (especially with dynamical fermions)

Only quenched calculations (no dynamical fermions) have been performed for gluon and disconnected quark EM tensors.

- 1 QCD on a lattice
- 2 Generalized Form Factors**
- 3 Quark energy-momentum tensor in the nucleon
- 4 Excited States Contamination
- 5 Summary

Quark GPDs

- Generalized Parton Distributions

$$\langle P' | \mathcal{O}^{[\gamma^5]}(x) | P \rangle \rightarrow \{ \mathcal{H}, \mathcal{E}, \tilde{\mathcal{H}}, \tilde{\mathcal{E}} \}(x, \xi, q^2),$$

$$\mathcal{O}^{[\gamma^5]}(x) = \int \frac{d\lambda}{2\pi} e^{2i\lambda x} \bar{q}_{(-\lambda n)} \left[\not{n} [\gamma^5] \mathcal{W}(-\lambda n, \lambda n) \right] q_{(\lambda n)}$$

- Moments $\mathcal{O}_n = \int dx x^n \mathcal{O}(x) \rightarrow \bar{q} \gamma^+ (i\overleftrightarrow{D}^+)^n q$

may be computed on a lattice using *local* operators

$$\mathcal{O}_n^{[\gamma^5]} = \bar{q} \left[\gamma_{\{\mu_1} [\gamma^5] i\overleftrightarrow{D}_{\mu_2} \cdots i\overleftrightarrow{D}_{\mu_n} \right] q$$

and reduced to **Generalized Form Factors**

$$\langle P' | \mathcal{O}_n | P \rangle \longrightarrow \{ A_{ni}, B_{ni}, C_n, \tilde{A}_{ni}, \tilde{B}_{ni} \}(Q^2)$$

Twist-2 Operators on a Hypercubic Lattice

Mellin moments of GPDs \iff symmetric, trace = 0 quark operators:

- In continuum: Lorentz symmetry preserves operators from mixing
- On a lattice: Hypercubic group has 20 irreducible representations

$$\begin{aligned}
 n = 1 & \quad \bar{q}\gamma_{\mu}q \rightarrow \mathbf{4}_1^- \\
 n = 2 & \quad \bar{q}[\gamma_{\{\mu}i\overleftrightarrow{D}_{\nu\}} - \langle\text{Tr}\rangle]q \rightarrow \mathbf{3}_1^+ \oplus \mathbf{6}_3^+ \\
 n = 3 & \quad \bar{q}[\gamma_{\{\mu}i\overleftrightarrow{D}_{\nu}i\overleftrightarrow{D}_{\rho\}} - \langle\text{Tr}\rangle]q \rightarrow \mathbf{8}_1^- \oplus \mathbf{4}_1^- \oplus \mathbf{4}_2^- \\
 n = 4 & \quad \bar{q}[\gamma_{\{\mu}i\overleftrightarrow{D}_{\nu}i\overleftrightarrow{D}_{\rho}i\overleftrightarrow{D}_{\sigma\}} - \langle\text{Tr}\rangle]q \rightarrow \mathbf{1}_1^+ \oplus \mathbf{3}_1^+ \oplus \mathbf{6}_3^+ \oplus \mathbf{2}_1^+ \oplus \mathbf{1}_2^+ \oplus \mathbf{6}_1^+ \oplus \mathbf{6}_2^+ \\
 \dots & \quad \hspace{10em} [\text{Göckeler et al, Phys.Rev.D54,5705(1996)}]
 \end{aligned}$$

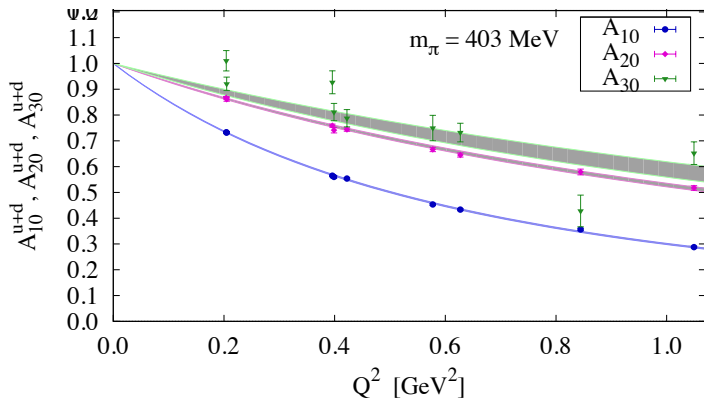
$$\text{Mixing coefficients} \sim \Lambda_{UV}^{d_1-d_2} = \left(\frac{1}{a}\right)^{d_1-d_2}$$

E.g. for $n = 2$ $\mathcal{O}^{\text{lat}} = \mathcal{O}^{\text{phys}} + O(a^2)$

For higher n :

- subtraction with non-perturbative mixing coefficients
- QCD on a more symmetric (Celmaster) 4D lattice

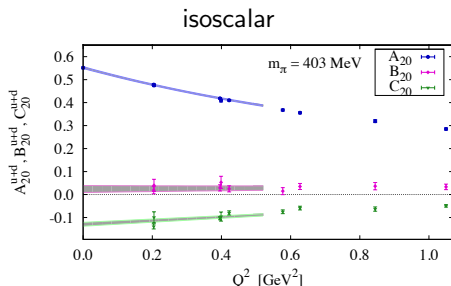
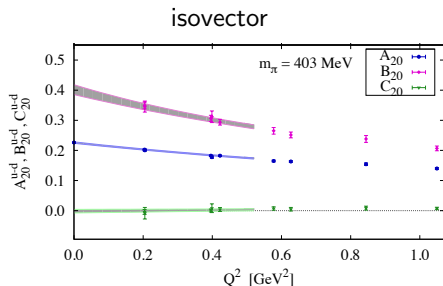
Generalized form factors $A_{n0}(Q^2)$



(normalized $A_{n,0}(Q^2)/A_{n,0}(0)$)

- Noise grows with n
- Generalized radii $\langle r_{n=1}^2 \rangle > \langle r_{n=2}^2 \rangle > \langle r_{n=3}^2 \rangle$

$n = 2$ Gen. Form Factors A_{20}, B_{20}, C_2



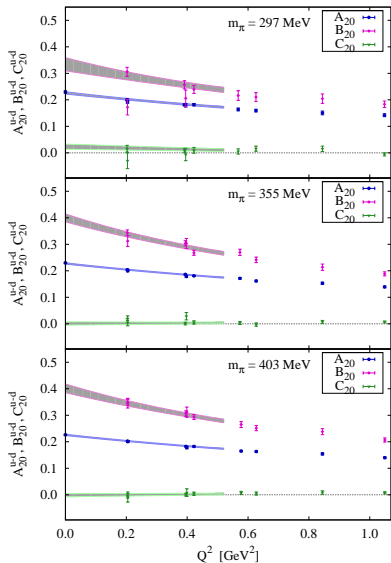
$$|A_{20}^{u+d}| \gg |A_{20}^{u-d}|, \quad |B_{20}^{u-d}| \gg |B_{20}^{u+d}| \approx 0, \quad |C_2^{u+d}| \gg |C_2^{u-d}| \approx 0.$$

agree with large- N_c scaling [Goeke et al, Prog. Part. Nucl. Phys. 47:401(2001)]

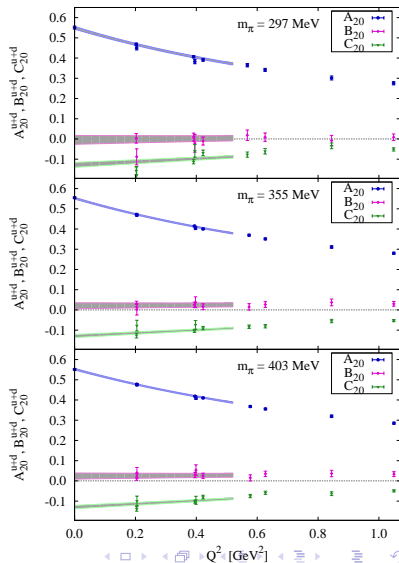
- fit with either *dipole* or *linear* form in $0 \leq Q^2 \leq 0.5$ GeV²
- extrapolate B_{20} and C_2 to $Q^2 \rightarrow 0$
- extract forward values ($Q^2 = 0$) and slopes $d\{A_{20}, B_{20}, C_2\} / dQ^2, Q^2 \rightarrow 0$

$n = 2$ Gen. Form Factors A_{20}, B_{20}, C_2 (cont.)

isovector

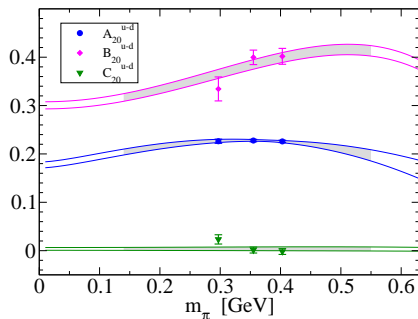


isoscalar

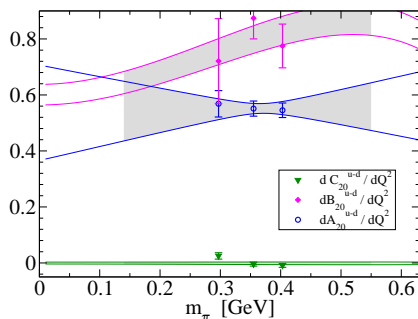


Chiral Extrapolations (isovector part)

forward values $Q^2 \rightarrow 0$



$d\{A_{20}, B_{20}, C_{20}\} / dQ^2, Q^2 \rightarrow 0$



- simultaneously fit *forward values* and *slopes* at $Q^2 \rightarrow 0$
- Cov. Baryon χ PT [Dorati et al Nucl. Phys. A798:96 (2008)]
- e.g., for $(u - d)$: 12 data points, 8 fit parameters, $\chi^2/dof \approx 1.5$

- 1 QCD on a lattice
- 2 Generalized Form Factors
- 3 Quark energy-momentum tensor in the nucleon**
- 4 Excited States Contamination
- 5 Summary

Quark Momentum and Angular momentum

Quark energy-momentum tensor $T_q^{\mu\nu}$

$$T_q^{\mu\nu} = \bar{q} \left[\gamma^{\{\mu} i \overleftrightarrow{D}^{\nu\}} - \langle \text{trace} \rangle \right] q$$

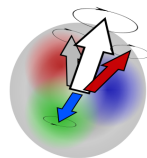
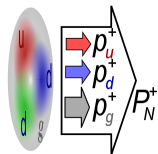
$$\langle N(P') | T_q^{\mu\nu} | N(P) \rangle \longrightarrow \{A_{20}, B_{20}, C_2\}(Q^2)$$

- quark momentum fraction

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

- quark angular momentum [X. Ji '97]:

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



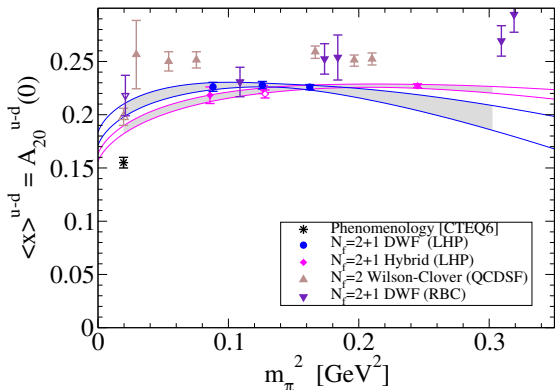
Separating contributions to nucleon spin:

- quark spin $S_q = \frac{1}{2} \Sigma_q = \frac{1}{2} \langle 1 \rangle_{\Delta q}$

- quark orbital angular momentum $L_q = J_q - \frac{1}{2} \Sigma_q$

- gluons : the rest $J_{\text{glue}} = \frac{1}{2} - \frac{1}{2} \Sigma_q - L_q$

Quark Momentum Fraction $\langle x \rangle_{u-d}$



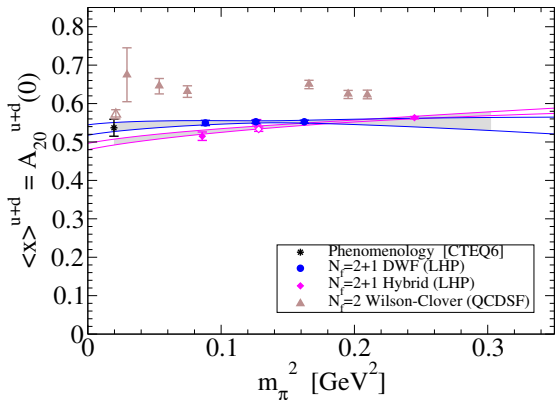
$$\begin{aligned}\langle x \rangle_q &= A_{20}^q(0) \\ &= \int dx x (q(x) + \bar{q}(x))\end{aligned}$$

Sources of discrepancy:

- renormalization?
- finite volume?
- sea quarks?
- fermion action?
- excited states?

- *perturbative vs. non-perturbative* renormalization
- agreement between $(2.5 \text{ fm})^3$ and $(3.5 \text{ fm})^3$ at $m_\pi = 350 \text{ MeV}$
- results are consistently above the phenomenological value by 15 – 25%.

Quark Momentum Fraction $\langle x \rangle_{u+d}$



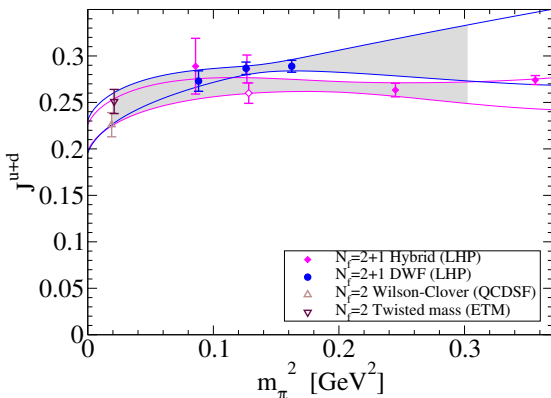
$$\begin{aligned}\langle x \rangle_q &= A_{20}^q(0) \\ &= \int dx x (q(x) + \bar{q}(x))\end{aligned}$$

Sources of discrepancy:

- renormalization?
- finite volume?
- sea quarks?
- fermion action?
- excited states?

- *perturbative vs. non-perturbative* renormalization
- agreement between $(2.5 \text{ fm})^3$ and $(3.5 \text{ fm})^3$ at $m_\pi = 350 \text{ MeV}$
- qualitative agreement with phenomenology (**no disc. contractions!**)

Quarks Angular Momentum (1): J^{u+d}



Following [X. Ji PRL '97],

$$J_q^3 = \langle N | \int d^3x M^{012} | N \rangle,$$

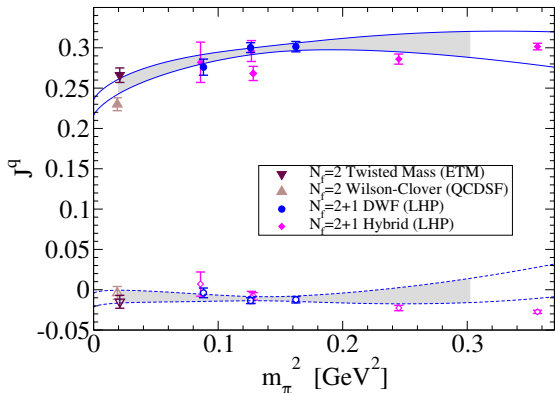
$$M^{\alpha\mu\nu} = x^\mu T_q^{\alpha\nu} - x^\nu T_q^{\alpha\mu}$$

and

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

- Gluon contribution $J^g = \frac{1}{2} - J^q \sim 52\%$ of the nucleon spin
- result agrees with QCD sum rule estimations [Balitsky, Ji (1997)]

Quarks Angular Momentum (2): J^u , J^d



Following [X. Ji PRL '97],

$$J_q^3 = \langle N | \int d^3x M^{012} | N \rangle,$$

$$M^{\alpha\mu\nu} = x^\mu T_q^{\alpha\nu} - x^\nu T_q^{\alpha\mu}$$

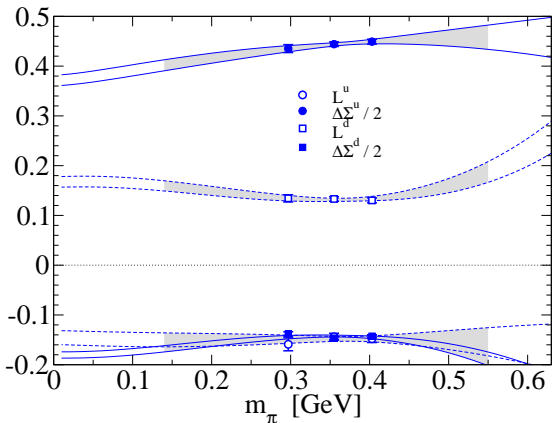
and

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

Most contribution to the nucleon spine comes from u -quarks:

$$|J^d| \ll |J^u|$$

Quark Spin and OAM



$$|J^d| \ll |S^d|, |L^d|$$

$$|L^{u+d}| \ll |L^u|, |L^d|$$

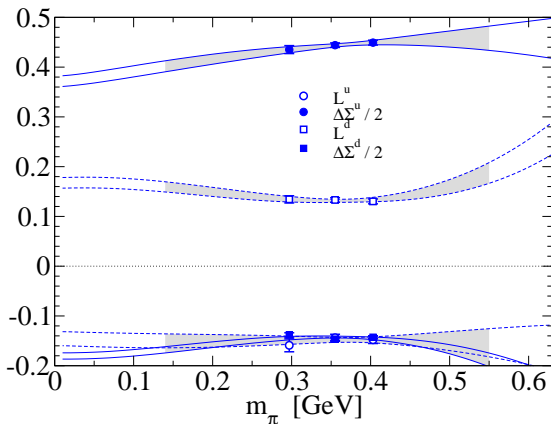
$$L^q = J^q - S^q,$$

$$S_q = \frac{1}{2} \Delta\Sigma_q$$

$$= \int dx (\Delta q(x) + \Delta \bar{q}(x))$$

In agreement with [\[Hägler et al \(2007\)\]](#)

Quark Spin and OAM



$$|J^d| \ll |S^d|, |L^d|$$

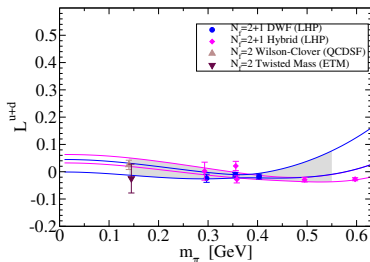
$$|L^{u+d}| \ll |L^u|, |L^d|$$

In agreement with [Hägler *et al* (2007)]

$$L^q = J^q - S^q,$$

$$S_q = \frac{1}{2} \Delta\Sigma_q$$

$$= \int dx (\Delta q(x) + \Delta \bar{q}(x))$$



$$|L^{u+d}| \ll \frac{1}{2}$$

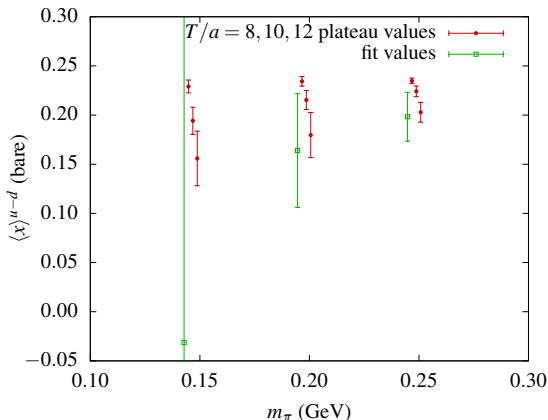
- 1 QCD on a lattice
- 2 Generalized Form Factors
- 3 Quark energy-momentum tensor in the nucleon
- 4 Excited States Contamination**
- 5 Summary

Mass Gap $\Delta M = M_{\text{exc}} - M_N$

Wilson-Clover $32^3 \times 48$, $m_\pi = 200$ MeV

	$M[\text{MeV}]$	aM	$a\Delta M$
π	200	0.118	
$2\pi/L$	334	0.196	
N	1021	0.600	
$N\pi\pi$	1421	0.835	0.235
$N\pi$	1463	0.860	0.260
" $N(1440)$ "	(?)1520	0.894	0.294
$N\pi$	1637	0.962	0.362
$N\pi$	1786	1.050	0.450
" $N(1710)$ "	(?)1790	1.052	0.452
	...		
$C_{2\text{pt}}$ best fit	≈ 2130	1.25(19)	0.65(19)

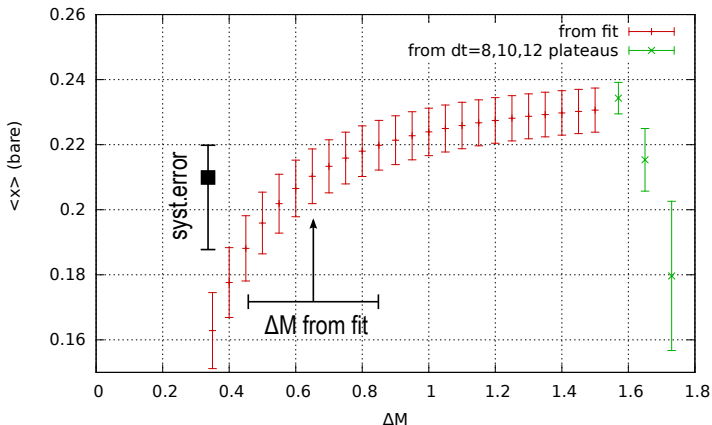
Momentum fraction $\langle x \rangle^{u-d}$: vary Δt



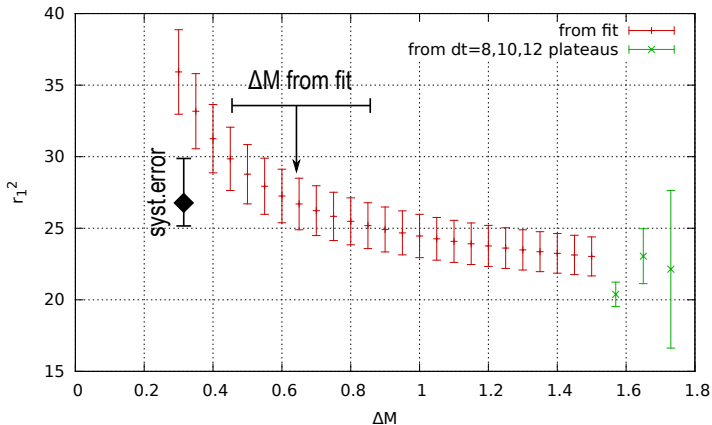
- Separate \bar{N} and N with $\Delta t = 0.93, 1.16, 1.39$ fm
- $m_\pi \approx 150, 200$ and 250 MeV, $m_N \approx 0.97 \dots 1.06$ GeV
- Fit to a 2-state model with *fixed* ΔM

Also reported in [\[Renner et al \(ETMC Collab\)\]](#)

Momentum fraction $\langle x \rangle^{u-d}$: fix ΔM



- Separate \bar{N} and N with $\Delta t = 0.93, 1.16, 1.39$ fm
- One point $m_\pi \approx 200$ MeV, $m_N \approx 1.00$ GeV
- Fit to a 2-state model with fixed ΔM

Dirac radius $\langle r_1^2 \rangle^{u-d}$: fix ΔM 

- $m_\pi \approx 200$ MeV, $m_N \approx 1.00$ GeV
- Separate \bar{N} and N with $\Delta t = 0.93, 1.16, 1.39$ fm
- Fit to a 2-state model with fixed ΔM

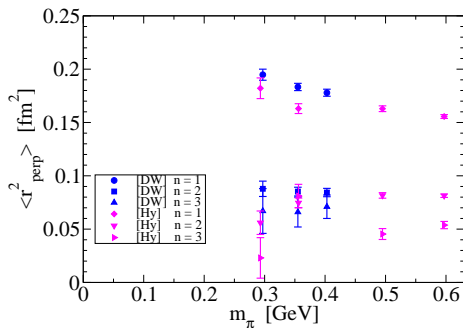
- 1 QCD on a lattice
- 2 Generalized Form Factors
- 3 Quark energy-momentum tensor in the nucleon
- 4 Excited States Contamination
- 5 Summary**

Summary

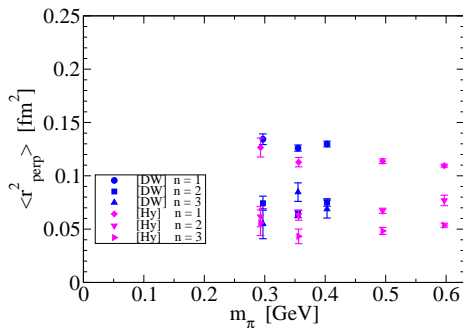
- Extrapolated results from different LQCD actions/volumes/discretizations agree near the physical point;
 - disagreement with phenomenology for $\langle x \rangle_{u-d}$
 - qualitative agreement with phenomenology for quark angular momentum
- Calculations at m_π^{phys} are necessary
- Systematic bias due to excited states is likely to increase towards m_π^{phys}
- Need a systematic “overhaul” of hadron structure calculations:
 - better control of excited states
 - additional statistics
 - disconnected contractions

BACKUP SLIDES

Generalized Radii



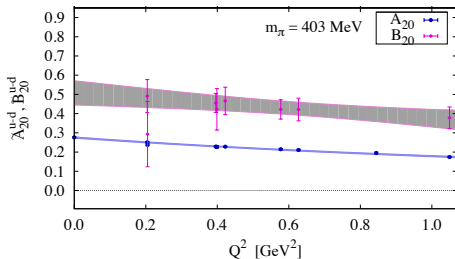
(spin-independent)



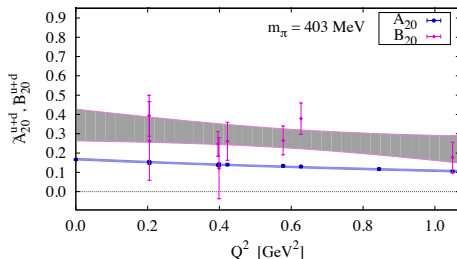
(spin-dependent)

$n = 2$ Spin-dependent GFFs $\tilde{A}_{20}, \tilde{B}_{20}$

isovector



isoscalar



- On a lattice, rotational symmetry is broken $O(4) \rightarrow H(4)$
- Tensors split into irred. reps. of $H(4)$

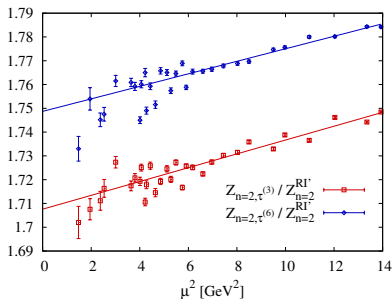
For energy-momentum tensor there are two irred. reps. of $H(4)$:

$$(\mathbf{4}_1)^{\otimes 2} = \mathbf{1}_1 \oplus \mathbf{6}_1 \oplus \underbrace{\mathbf{6}_3 \oplus \mathbf{3}_1}_{\text{trace}=0, \text{ symm.}}$$

[Göckeler et al, hep-lat/9602029]

(both $\mathbf{6}_3$ and $\mathbf{3}_1$ are needed to extract gen. form factors)

Use non-perturbative renormalization (RI/MOM) for quark-bilinear $T_q^{\mu\nu}$:



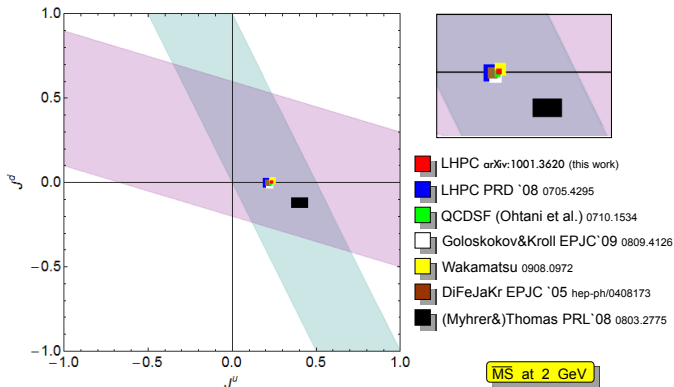
$$Z_O^{\text{scale-indep.}} = \frac{Z_O^{\text{lat}}(a\mu)}{Z_O^{\text{pert}}(\mu)}$$

$$Z_O^{\mathbf{3}_1} / Z_O^{\mathbf{6}_3} \approx 0.98$$

$$\text{Normalize to } \overline{\text{MS}} \text{ at } \mu^2 = (2 \text{ GeV})^2$$

Quark Angular Momentum: p,n-DVCS

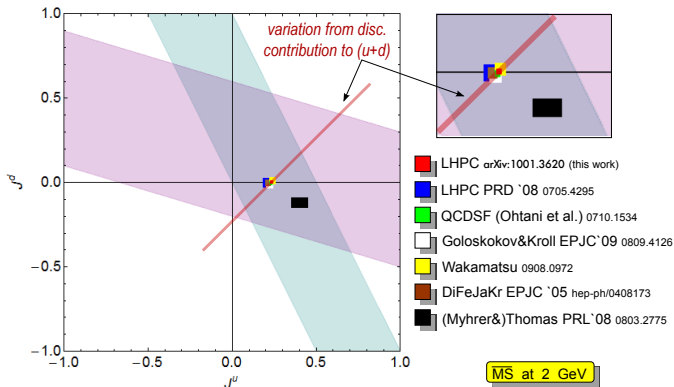
[Lab Hall A PRL '07; HERMES JHEP '08]



Picture: Ph. Hägler, MENU 2010, W&M, Virginia, USA; J.Phys.Conf.Ser.295:012009,2011

Quark Angular Momentum: p,n-DVCS

[Lab Hall A PRL '07; HERMES JHEP '08]



Picture: Ph. Hägler, MENU 2010, W&M, Virginia, USA; J.Phys.Conf.Ser.295:012009,2011