

# Lattice QCD

Kostas Orginos

The College of William and Mary/Jlab



# Summary

- Introduction
- Hadron spectrum
  - What are the low energy degrees of freedom of QCD
- Hadronic structure
  - Moments of structure functions
  - Form factors
  - Generalized Parton Distributions
- Nucleon-Nucleon interactions
  - Scattering lengths and phase shifts
  - Existence of 2 body bound states
- Resources needed
- Outlook

# Lattice QCD

- Lattice QCD: QCD on a discrete space time
- QCD: The continuum limit of Lattice QCD
- High energy regime:
  - Asymptotic freedom: Weak coupling
  - Perturbative calculations
- Low energy: Lattice QCD powerful tool for calculations
  - Lots of very important physics can be explored theoretically
  - Requires significant resources
- Recent theoretical and computer technology advances together with investment in computer resources and personnel make lattice QCD a tool available to us today.

# Physics we can do

- Hadronic spectrum and quark masses
- Low energy constants for EFTs
- Hadronic structure
  - Form factors and moments of GPDs
- Hadronic interactions
  - Scattering lengths and phase shifts
- Thermodynamics and finite density QCD
  - RHIC physics
- Weak matrix elements and new physics
  - Aid experimental effort to discover new physics

$f_\pi, f_K, g_A \dots$

# Computation break up

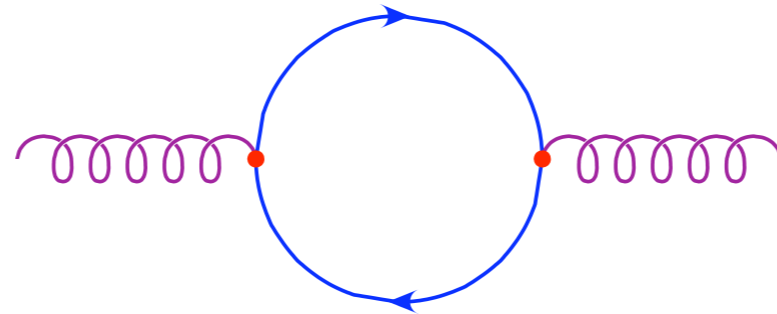
$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \prod_{\mu, x} dU_{\mu}(x) \mathcal{O}[U, D(U)^{-1}] \det (D(U)^{\dagger} D(U))^{n_f/2} e^{-S_g(U)}$$

- Gauge field configuration generation: **The accelerator**
  - Can be used by several collaborations
- Correlation function calculation: **The detector**
  - Used for specific calculations

# Realistic Calculations

- Include the vacuum polarization effects
  - 2 light (up down) 1 heavy (strange)
- Finite Volume
  - Compute in multiple and large volume
- Continuum Limit
  - Compute with several lattice spacings
- Chiral Limit
  - Compute with several values for the quark masses
  - Study quark mass dependence of QCD
- Need effective field theory for all the above
  - Light quark masses:  $m_\pi < 400\text{MeV}$  (?)

Past: Ignore vacuum polarization -- **Quenched approximation**

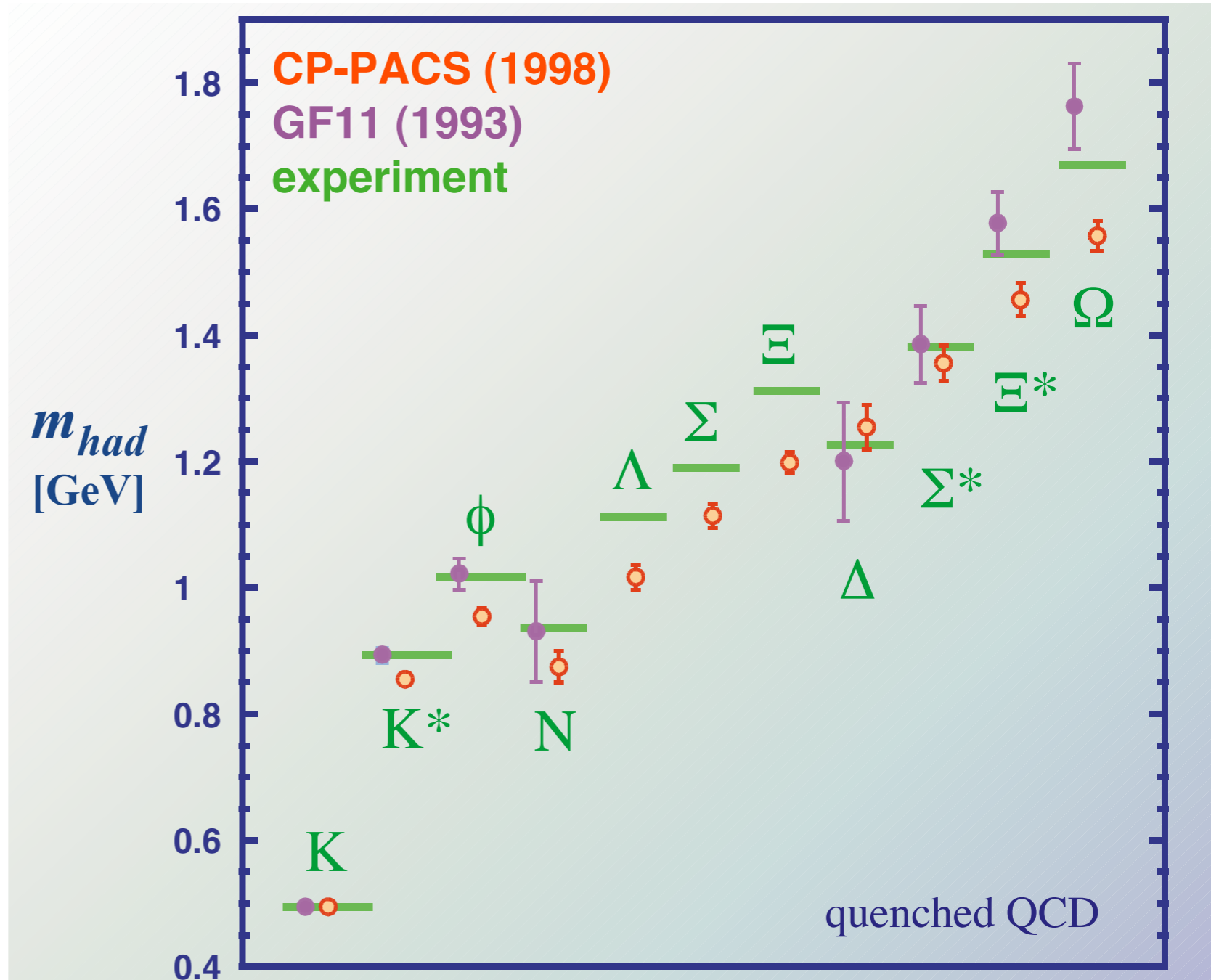


Last 5 years: Include vacuum polarization -- **Dynamical calculations**

Future: Light quark masses -- Systematics -- New calculations

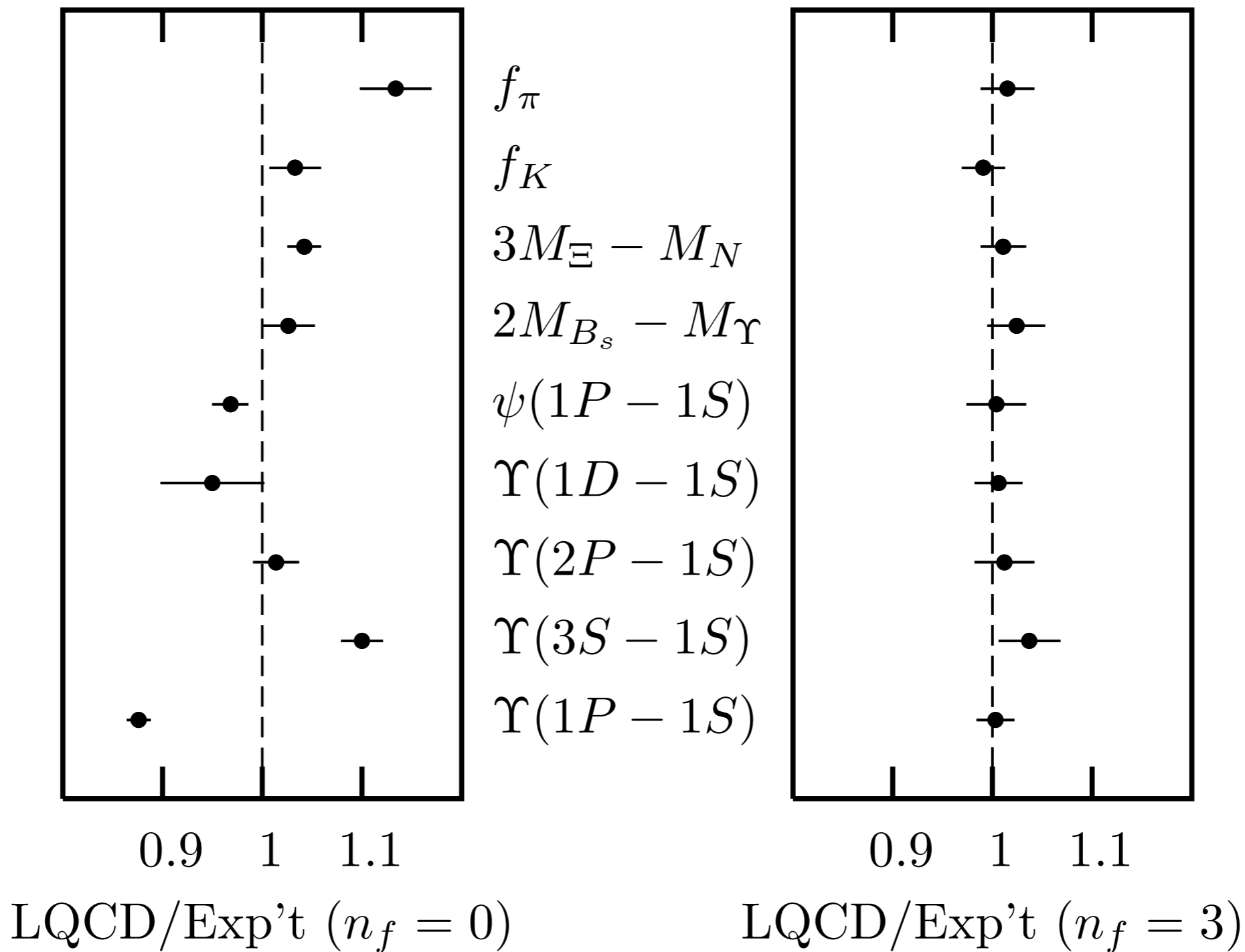
# Spectrum (past)

- Computation of similar results with dynamical quarks is under way.
- Meson spectrum
  - See [J. Dudek](#)
- Heavy quarkonia spectrum (MILC, UKQCD HPQCD .... )

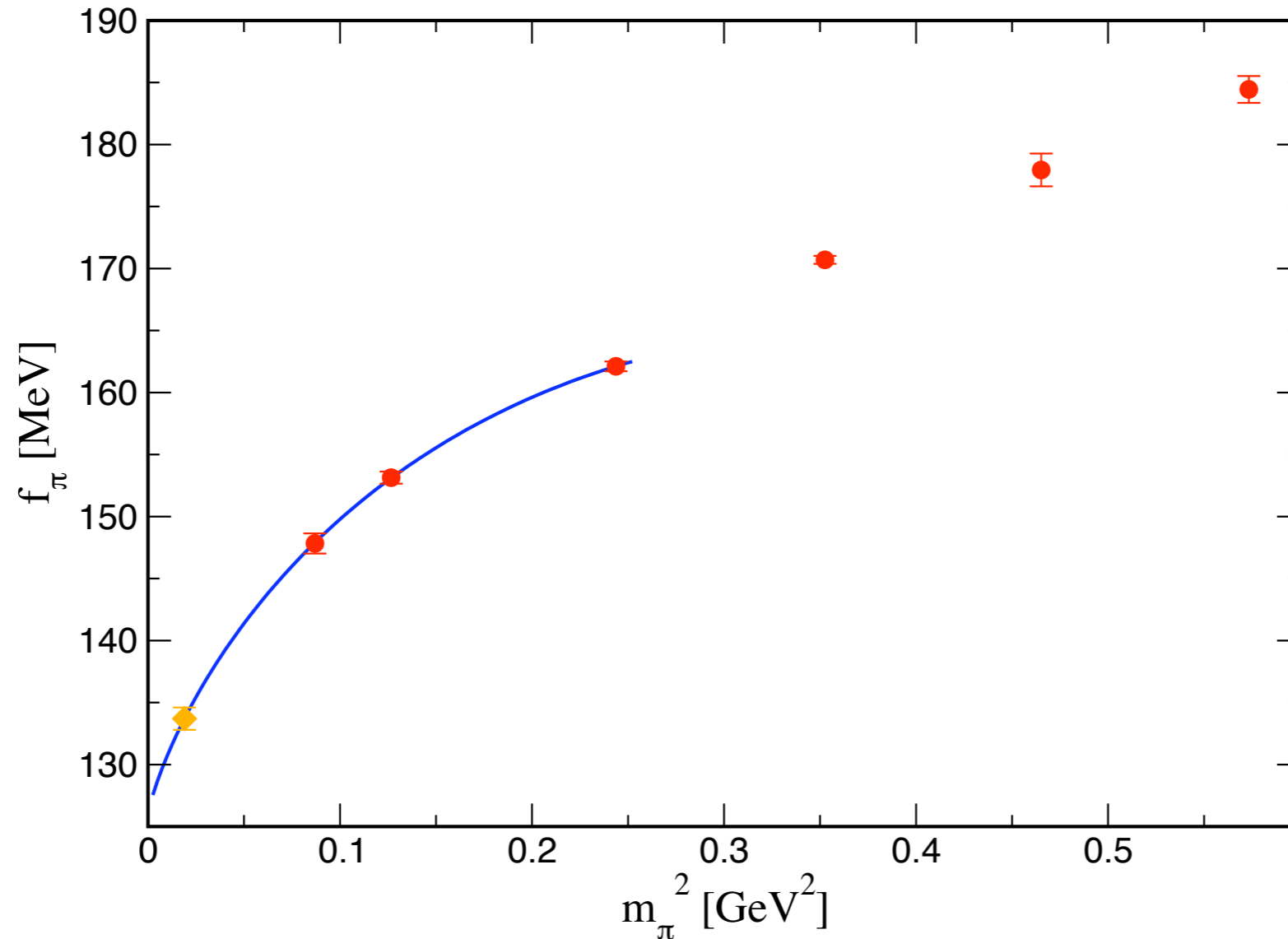




# Spectrum II



# Pion Decay constant



- Fit the lower 3 points

- One loop  $\chi$ PT extrapolation:  $133.7(9)(3.0)\text{MeV}$

- $\chi^2/\text{d.o.f.} \sim .5$

# $F_K/F_\pi$

Beane, Bedaque, KO, Savage hep-lat/0606023

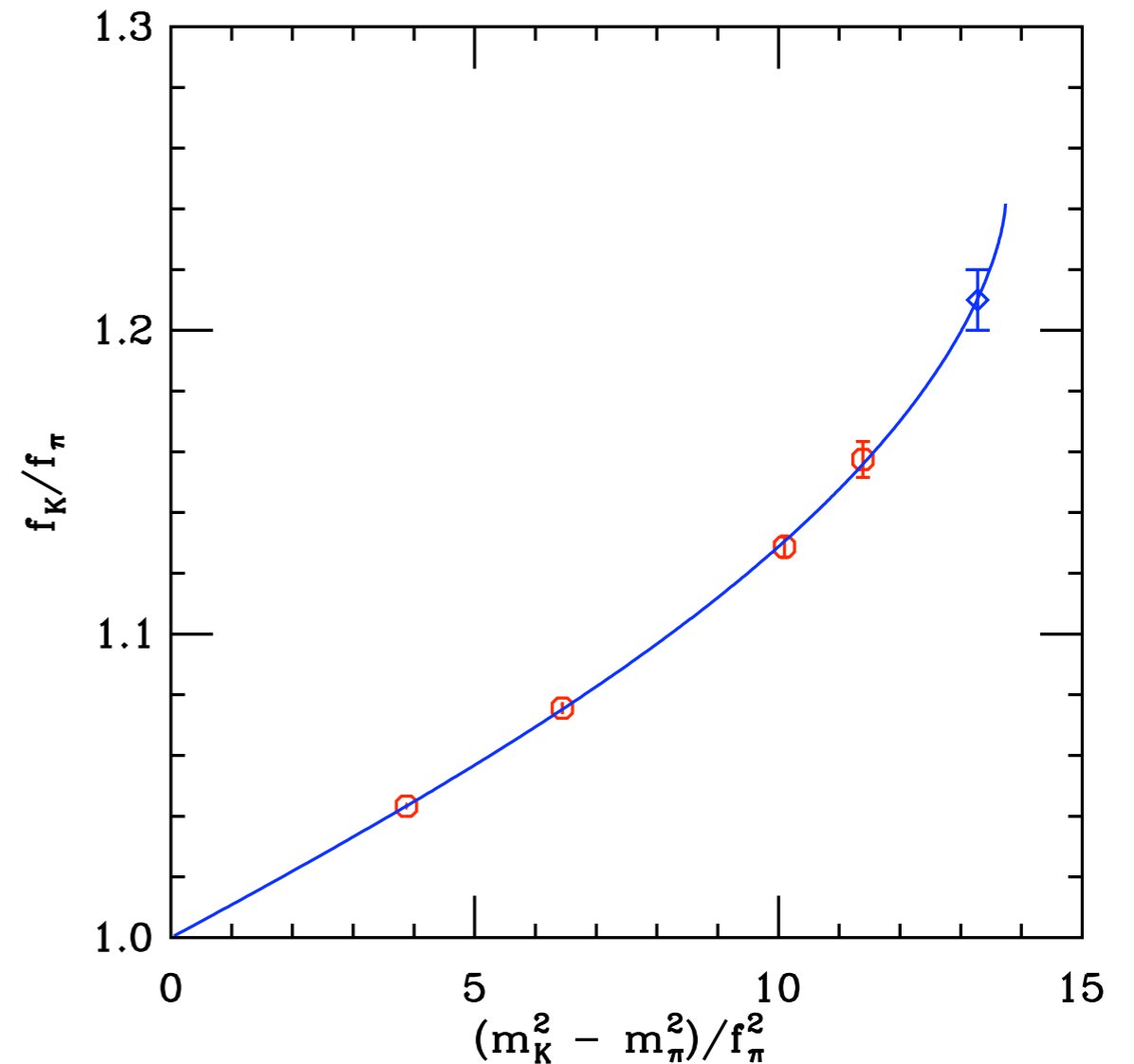
Gasser-Leutwyler:

$$\frac{f_K}{f_\pi} = 1 + \frac{5}{4}l_\pi(\mu) - \frac{1}{2}l_K(\mu) - \frac{3}{4}l_\eta(\mu) + \frac{8}{f^2} (m_K^2 - m_\pi^2) L_5(\mu)$$

$$l_i(\mu) = \frac{1}{16\pi^2} \frac{m_i^2}{f^2} \log\left(\frac{m_i^2}{\mu^2}\right)$$

$$f_K/f_\pi = 1.218 \pm 0.002 \begin{matrix} +0.011 \\ -0.024 \end{matrix}$$

$$\left. \frac{f_K}{f_\pi} \right|_{\text{exp.}} = 1.223(12)$$



Result comparable with MILC

$$\left. \frac{f_K}{f_\pi} \right|_{\text{MILC}} = 1.210(4)(13)$$

Need much higher precision to see effects of Mixed  $\chi$ PT Baer et.al.'05

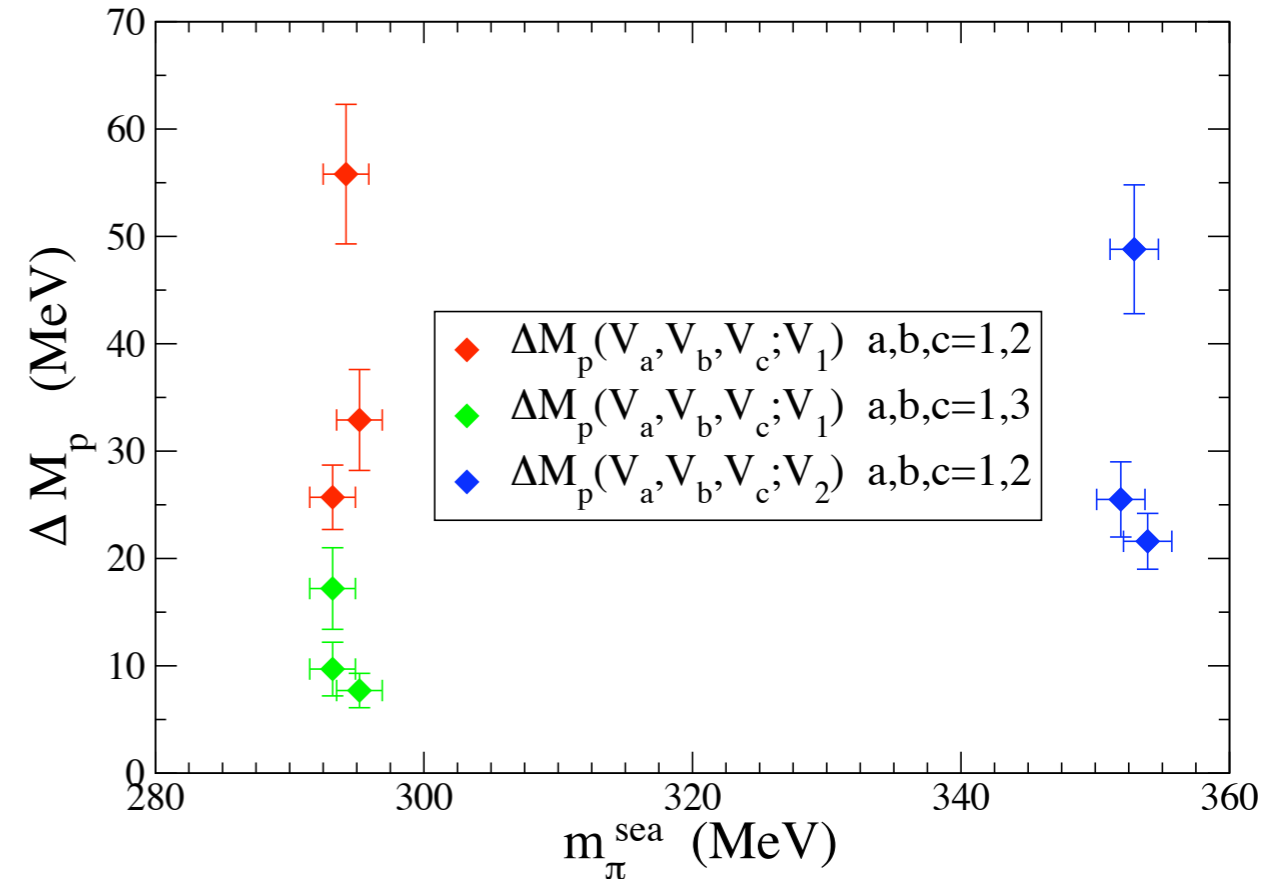
# Neutron-Proton Mass difference

Beane, KO, Savage hep-lat/0605015

$$M_n - M_p|^{d-u} = \frac{2}{3} (2\bar{\alpha} - \bar{\beta}) \left( \frac{1 - \eta}{1 + \eta} \right) m_\pi^2$$

MILC:  $\eta = m_u/m_d = 0.43(1)(8)$

Extraction	$M_n - M_p ^{d-u}$ (MeV) at $m_\pi^{\text{phys.}}$
LO $\mathcal{O}(m_q)$	$1.96 \pm 0.92 \pm 0.37$
NLO $\mathcal{O}(m_q^{3/2})$	$2.26 \pm 0.57 \pm 0.42$



Extraction	$\frac{1}{3} (2\bar{\alpha} - \bar{\beta})$ (l.u.)	$\bar{\alpha} + \bar{\beta}$ (l.u.)	$g_1$	$ g_{\Delta N} $	$\chi^2/\text{dof}$
LO $\mathcal{O}(m_q)$	$0.198 \pm 0.093$	$2.07 \pm 0.08$	---	---	0.56
NLO $\mathcal{O}(m_q^{3/2})$	$0.229 \pm 0.058$	$3.4 \pm 1.1$	$-0.10 \pm 0.35$	$0.60 \pm 0.66$	0.21

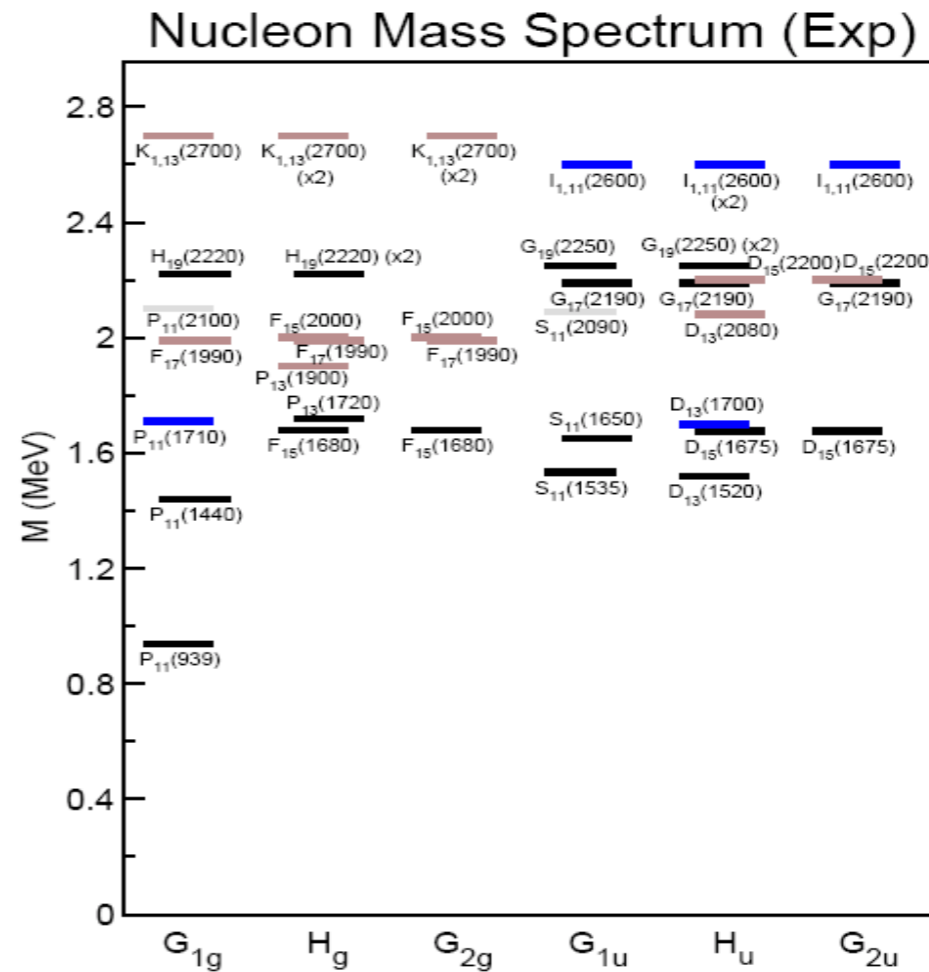
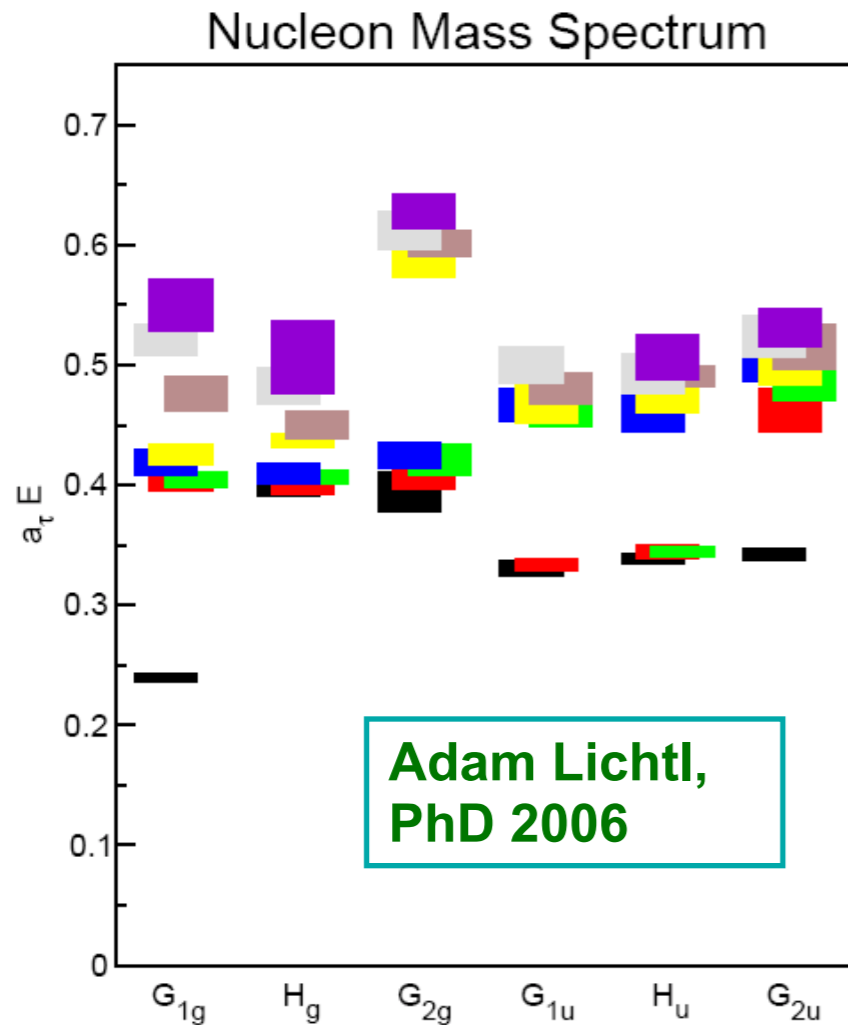
Exp. value:  $M_n - M_p = 1.2933317(5)$  MeV

minus EM part  
  
 Gasser Leutwyler '82

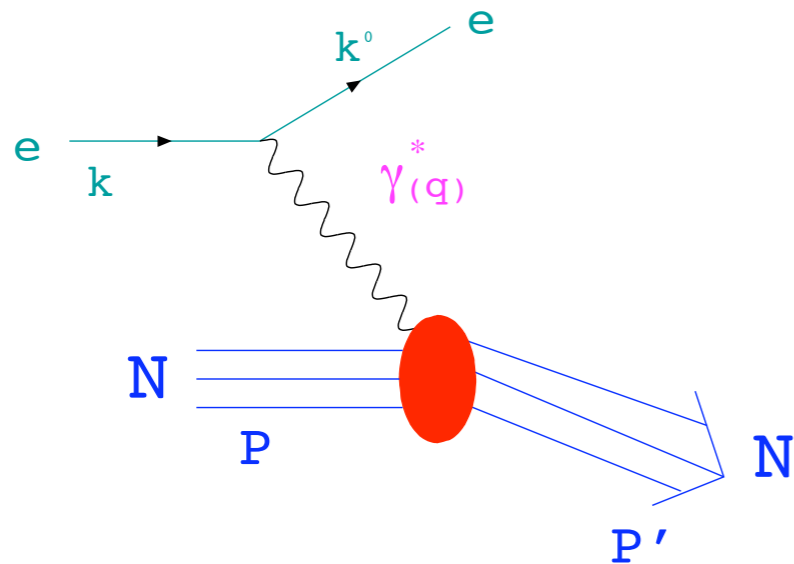
$M_n - M_p = 2.05(30)$  MeV

# Spectrum (Future)

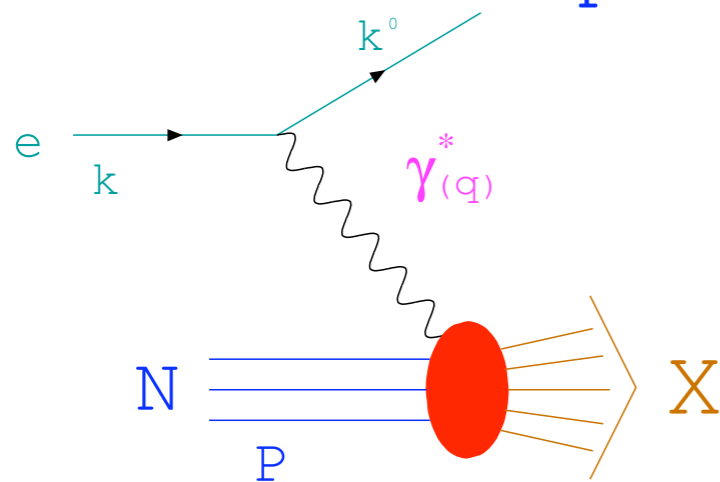
- Variational methods
- Classify states according to lattice representations
- Several excited states should be extracted



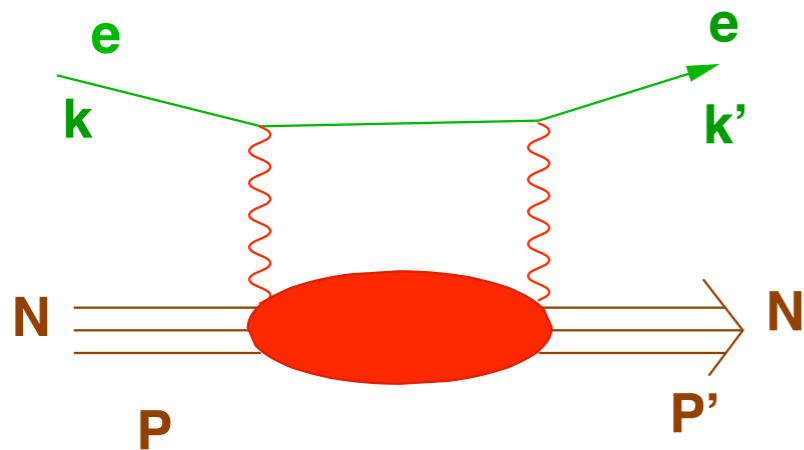
# Hadron Structure



Elastic scattering  
Form Factors

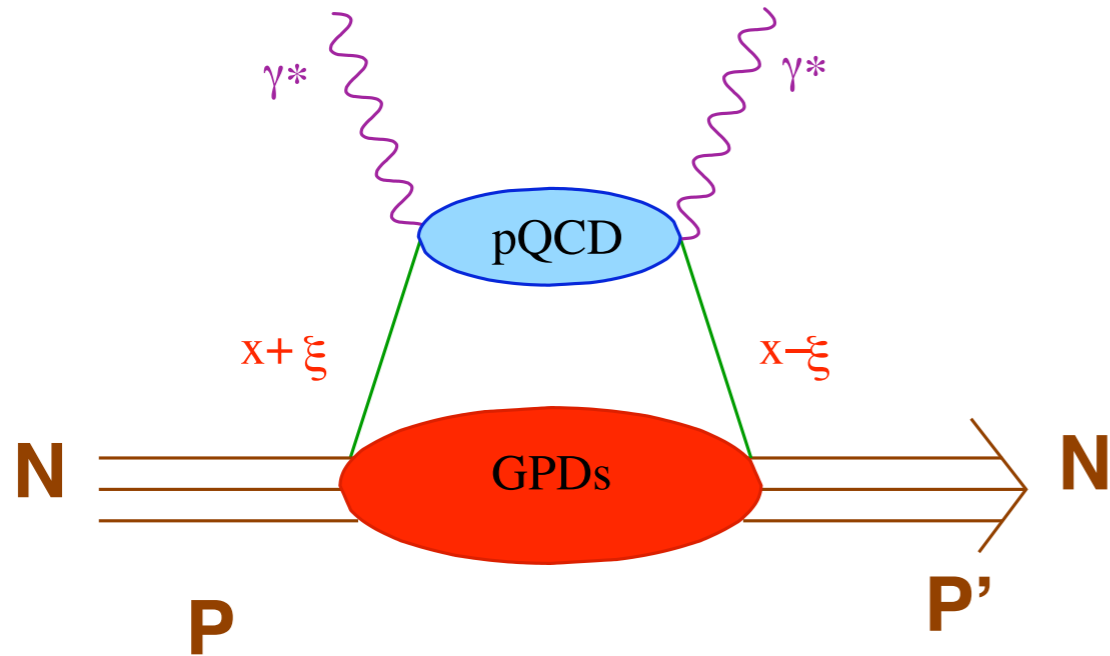


Deep Inelastic Scattering  
Structure functions



Deeply Virtual Compton Scattering  
Generalized Parton Distribution functions

# Generalized Parton Distributions



$$\mathcal{O}_\Gamma(x) = \int \frac{d\lambda}{4\pi} e^{i\lambda x} \bar{q}\left(\frac{-\lambda n}{2}\right) \Gamma \mathcal{P} e^{-ig \int_{-\lambda/2}^{\lambda/2} d\alpha n \cdot A(\alpha n)} q\left(\frac{\lambda n}{2}\right)$$

$$\Gamma = \not{n} \text{ or } \Gamma = \not{n}\gamma_5 \text{ or } \Gamma = n_\mu \sigma^{\mu\nu} \gamma_5$$

$$\Delta = P' - P \quad \xi = -n \cdot \Delta / 2 \quad t = \Delta^2$$

**Vector:**  $\langle P, s | \mathcal{O}_{\not{n}}(x) | P', s' \rangle = \bar{u}(p, s) \left[ \not{n} H(x, \xi, t) + \frac{n_\mu \Delta_\nu}{2m} i\sigma^{\mu\nu} E(x, \xi, t) \right] u(p', s')$




**Axial Vector:**  $\langle P, s | \mathcal{O}_{\not{n}\gamma_5}(x) | P', s' \rangle = \bar{u}(p, s) \left[ \not{n}\gamma_5 \tilde{H}(x, \xi, t) + \frac{n \cdot \Delta}{2m} \gamma_5 \tilde{E}(x, \xi, t) \right] u(p', s')$

**Tensor:**

$$\begin{aligned} \langle P, s | \mathcal{O}_{5T}(x) | P', s' \rangle &= \bar{u}(p, s) \left[ n_\mu \sigma^{\mu k} \gamma_5 \left( H_T(x, \xi, t) - \frac{t}{2m^2} \tilde{H}_T \right) + \frac{\epsilon^{\mu\nu\alpha\beta} \Delta_\alpha \gamma_\beta}{2m} \left( E_T(x, \xi, t) + 2\tilde{H}_T(x, \xi, t) \right) \right. \\ &+ \left. \frac{n_\mu \Delta^{[\mu} \sigma^{\nu]\alpha} \gamma_5 \Delta_\alpha}{2m^2} \tilde{H}_T(x, \xi, t) + \frac{\epsilon^{\mu\nu\alpha\beta} P_\alpha \gamma_\beta}{m} \tilde{E}_T(x, \xi, t) \right] u(p', s') \end{aligned}$$

# GPDs: Unified picture of hadronic structure

Forward limit:  $\Delta=0$

	$H(x, 0, 0) = q(x)$	
	$\tilde{H}(x, 0, 0) = \Delta q(x)$	
	$H_T(x, 0, 0) = \delta q(x)$	

Local limit

Vector	$\int dx H(x, \xi, t) = F_1(t)$	$\int dx E(x, \xi, t) = F_2(t)$
Axial Vector	$\int dx \tilde{H}(x, \xi, t) = g_A(t)$	$\int dx \tilde{E}(x, \xi, t) = g_P(t)$
Tensor	$\int dx H_T(x, \xi, t) = g_T(t)$	



# Moments of GPDs

## Operator Product Expansion

Off forward Matrix elements of local operators  $\langle P, S | \mathcal{O} | P', S' \rangle$

Unpolarized  $\mathcal{O}_{\{\mu_1 \mu_2 \dots \mu_n\}}^q = \bar{q} \left[ \left( \frac{i}{2} \right)^{n-1} \gamma_{\mu_1} \overleftrightarrow{D}_{\mu_2} \dots \overleftrightarrow{D}_{\mu_n} - \text{trace} \right] q$

Polarized  $\mathcal{O}_{\{\mu_1 \mu_2 \dots \mu_n\}}^{5q} = \bar{q} \left[ \left( \frac{i}{2} \right)^{n-1} \gamma_5 \gamma_{\mu_1} \overleftrightarrow{D}_{\mu_2} \dots \overleftrightarrow{D}_{\mu_n} - \text{trace} \right] q$

Transversity  $\mathcal{O}_{\rho\nu\{\mu_1 \mu_2 \dots \mu_n\}}^{\sigma q} = \bar{q} \left[ \left( \frac{i}{2} \right)^n \gamma_5 \sigma_{\rho\nu} \overleftrightarrow{D}_{\mu_1} \dots \overleftrightarrow{D}_{\mu_n} - \text{traces} \right] q$

- Generalized form factors:  $A_{nk}(t)$   $B_{nk}(t)$   $C_{nk}(t)$
- Moments of GPDs are polynomials in  $\xi$  with coefficients the generalized form factors.

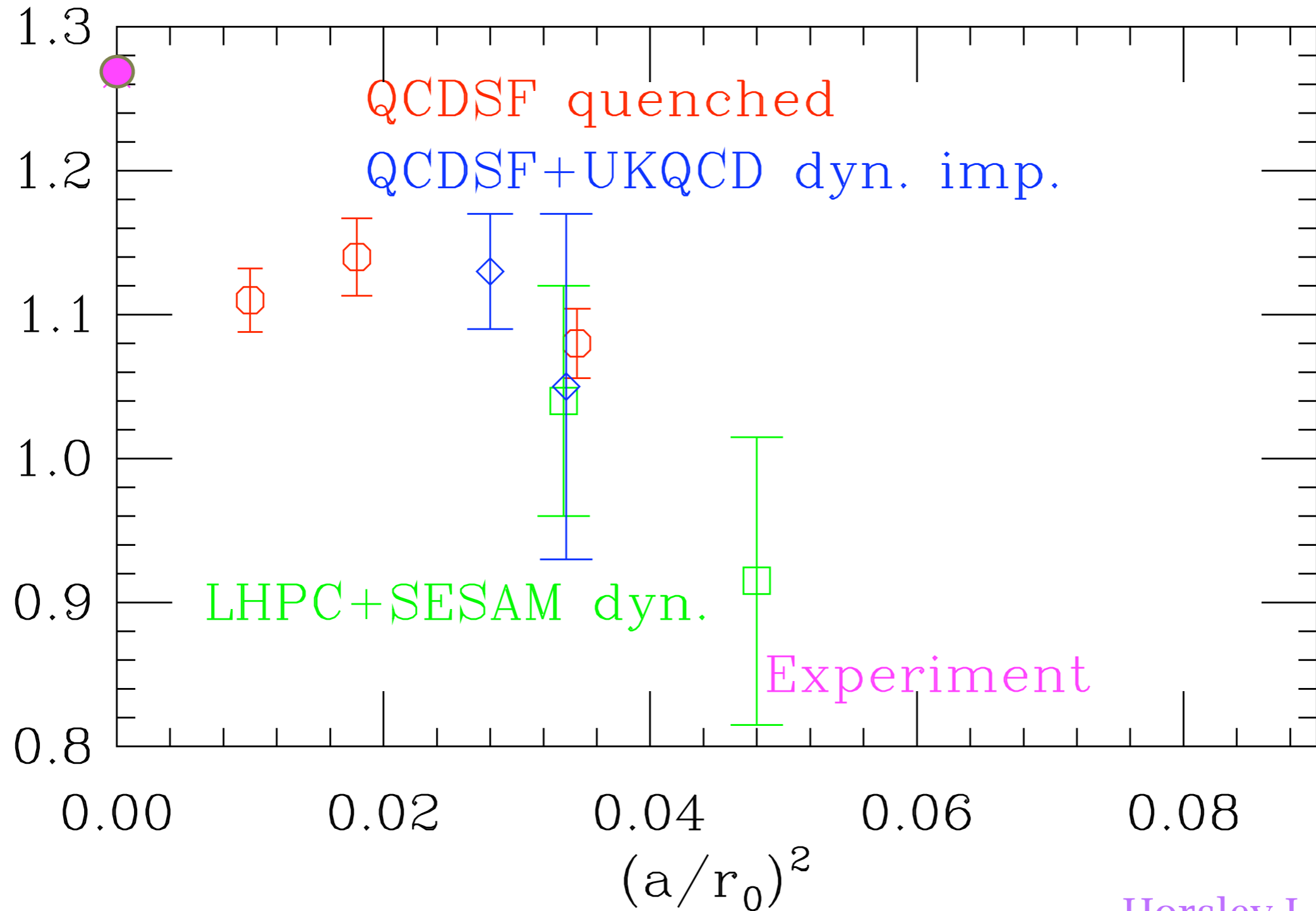
# The Axial coupling

- Accurately known (neutron beta decay)

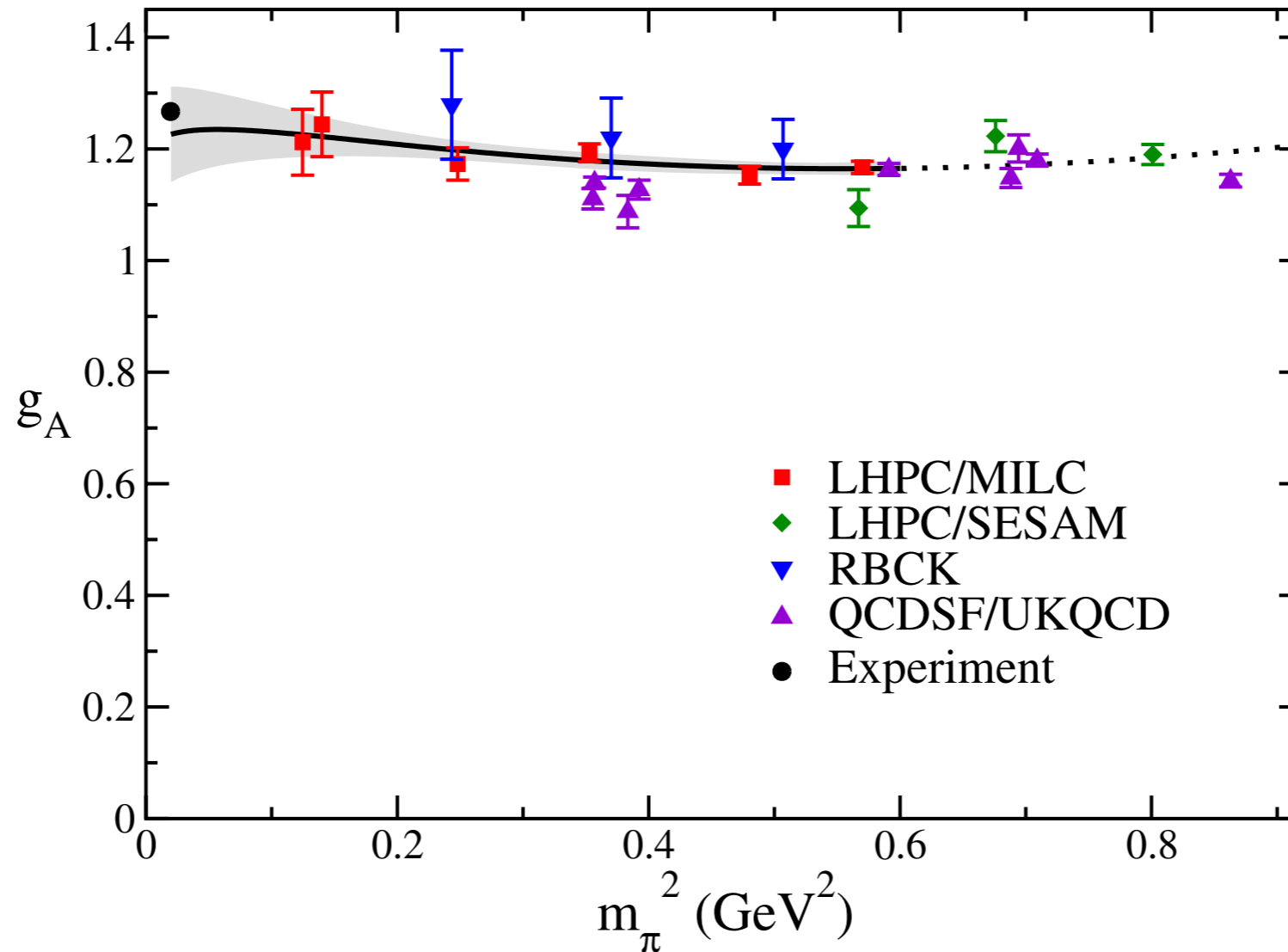
$$g_A / g_V = 1.2695(29) \quad [\text{PDG2006}]$$

- Lattice calculations had trouble computing it
- Charge symmetry breaking effects not taken into account
- ChiPT results:
  - Finite volume: [Bean, Savage '04]
  - Small Scale expansion: [T. R. Hemmert, M. Procura, and W. Weise '03]
  - Partial NNLO: [Bernard, Veronique and Meissner' 06]

# Axial Coupling (past)



# Axial Coupling (present)



- Large volumes

Cost: ~ 1Tflop-year

- Lighter pion masses

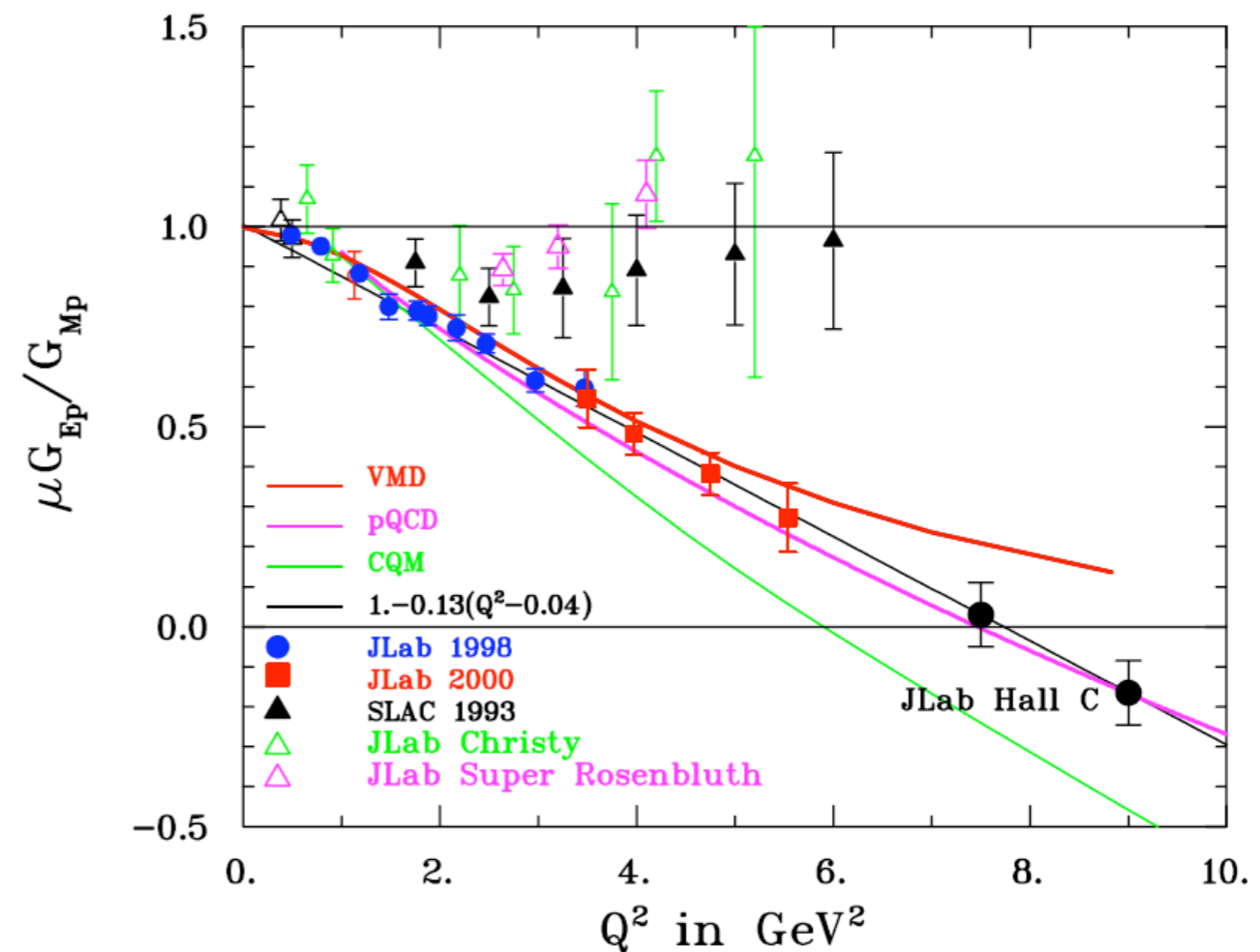
- $g_A(m_\pi=140\text{MeV}) = 1.23(8)$

# Axial Coupling (future)

- Continuum extrapolation
- Lighter pion masses
- Study the behavior of chiral extrapolation and reduce systematics from the extrapolation
- Include charge symmetry breaking effects
- Future: Expect few percent accuracy both statistical and systematic

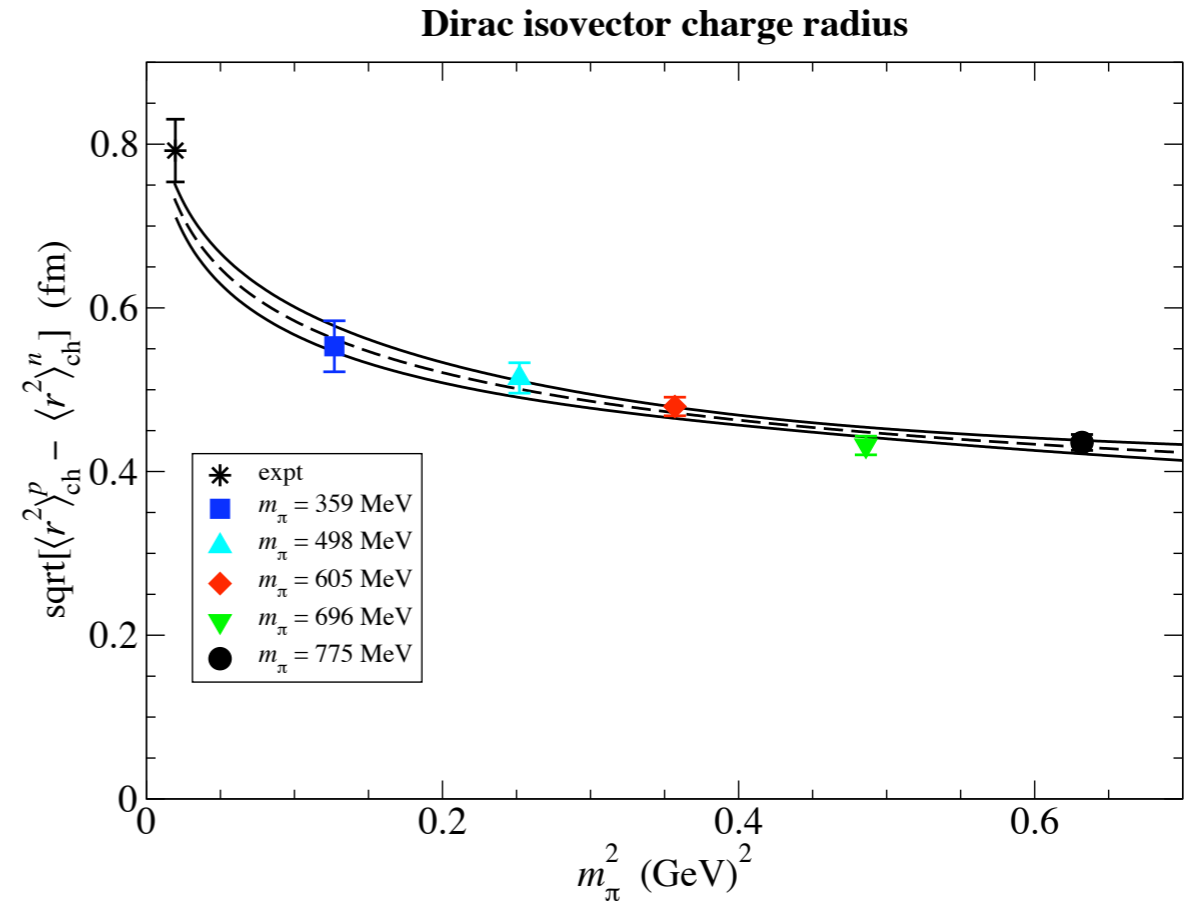
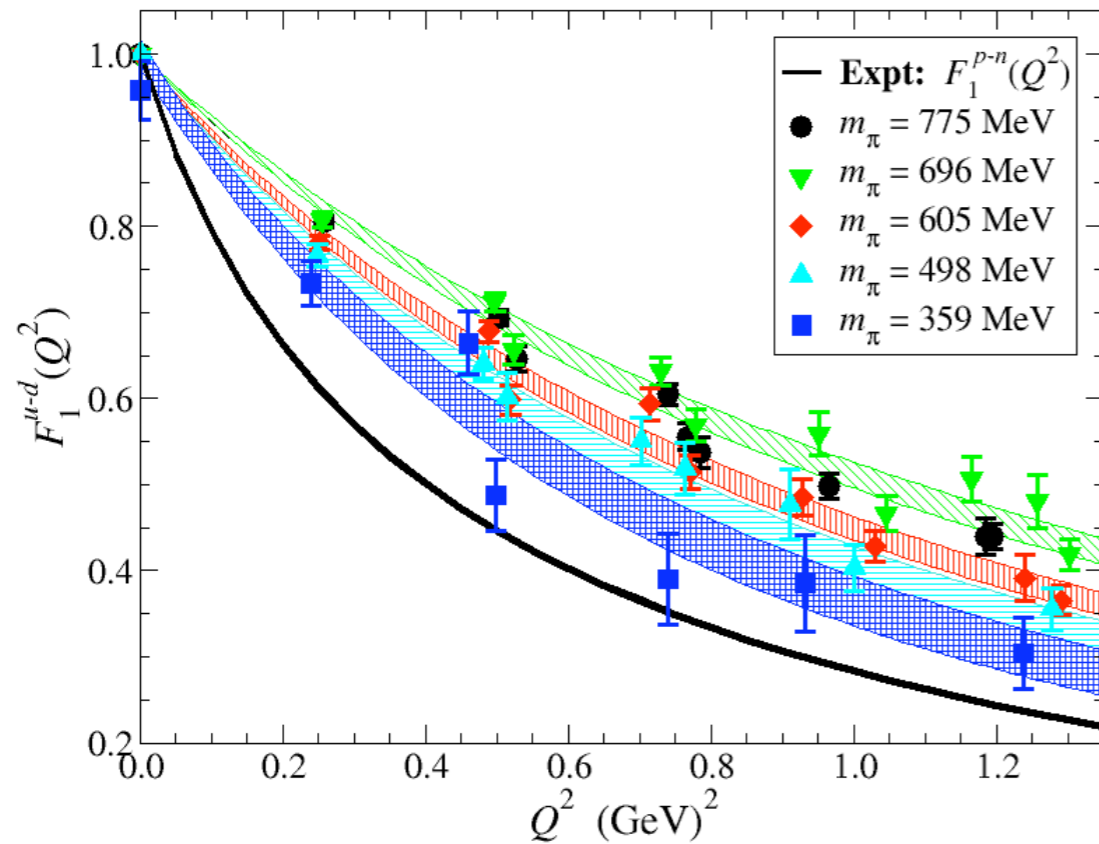
# Proton ElectroMagnetic Form Factors

- Rosenbluth separation disagrees with Polarization transfer
- Two photon effects
- What does the lattice predict for the ratio?



# Vector Isovector form factor

[LHPC]

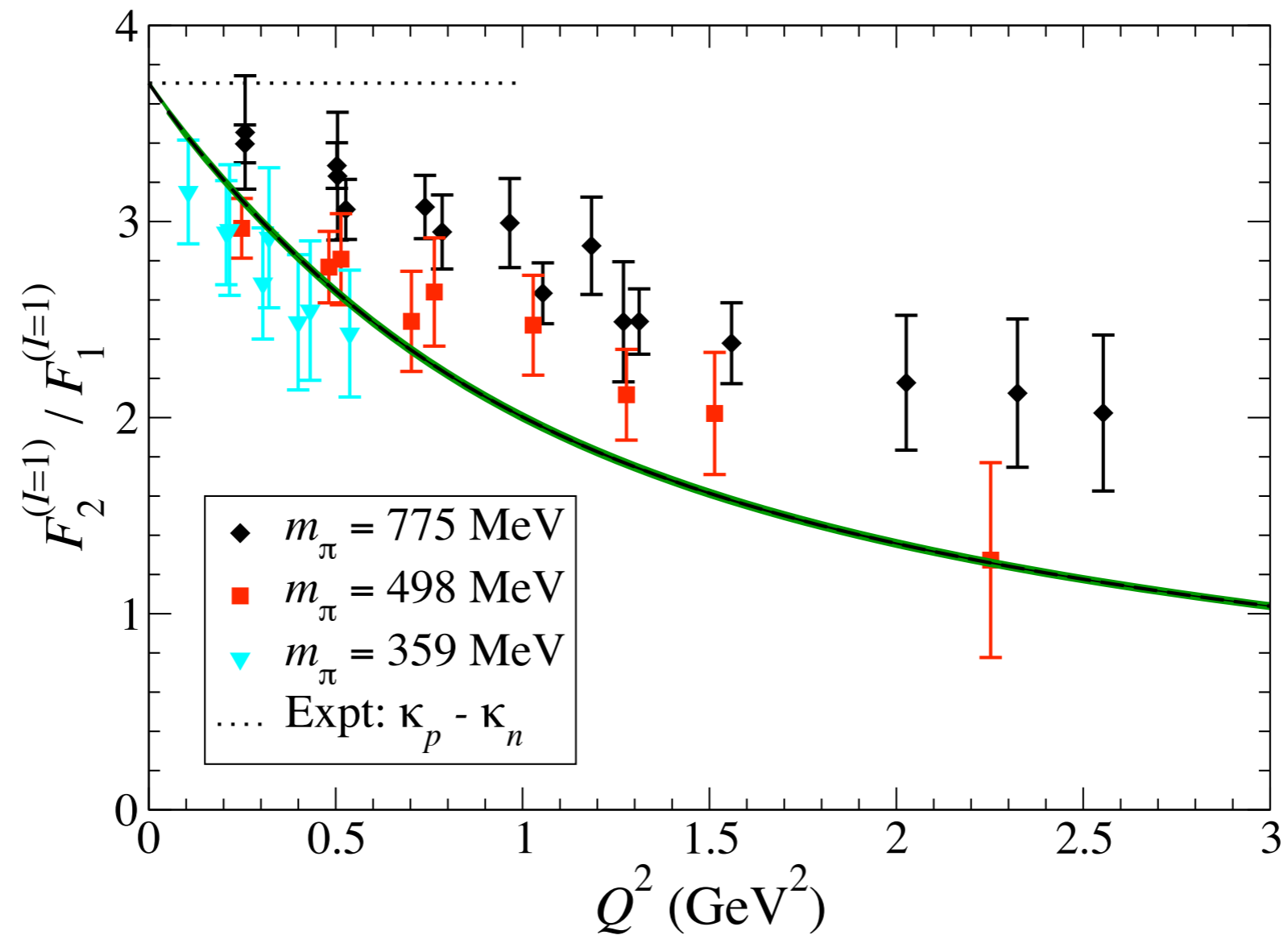


- Light pion masses: Lattice approaches experiment
- Chiral fit using leading order ChiPT [Leinweber et.al. '01 ]
- Nucleon size grows as quarks become lighter

[G. T. Fleming]

# Vector Isovector form factor ratio

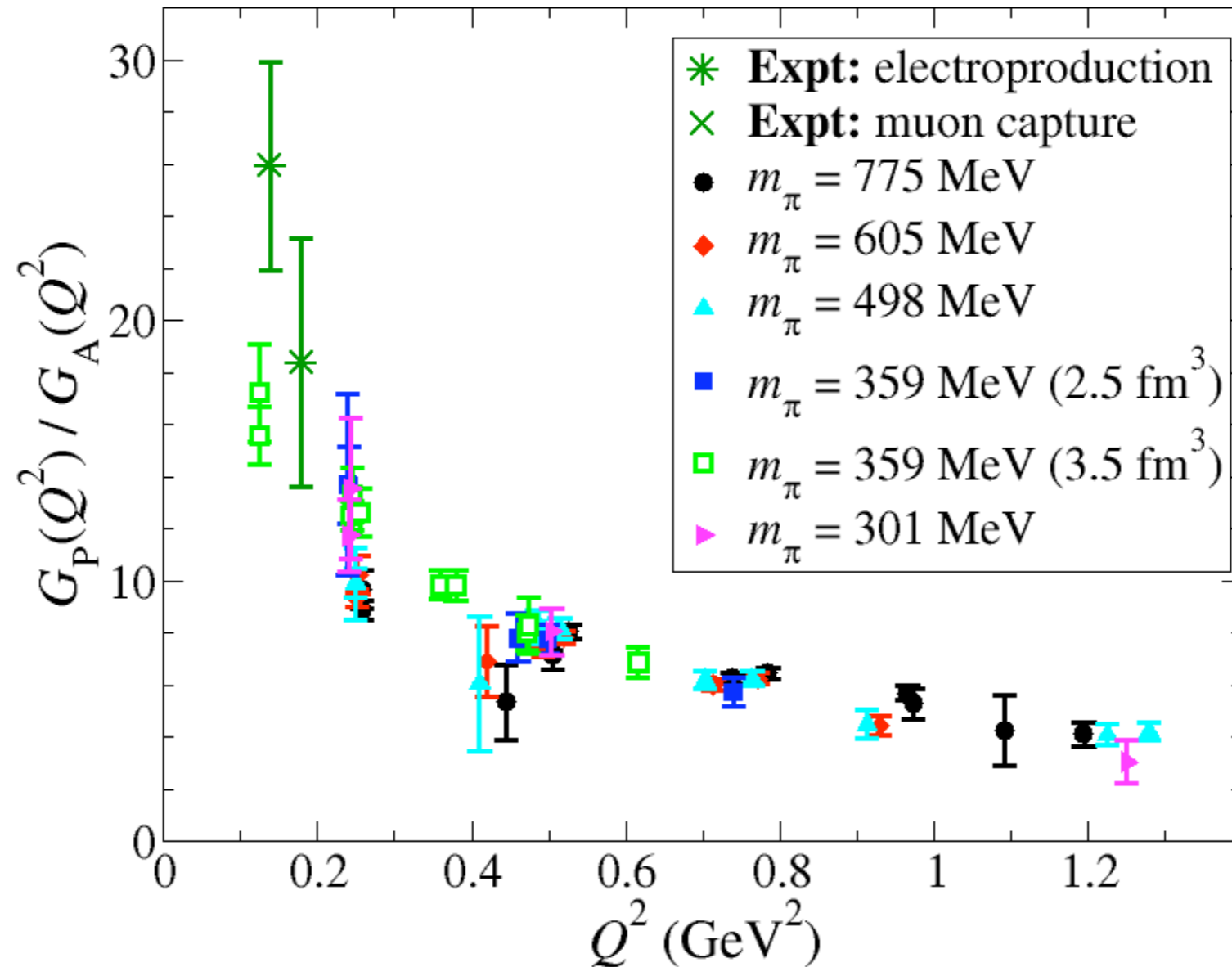
[LHPC]



- Lattice results approach experiment as quark mass is lowered



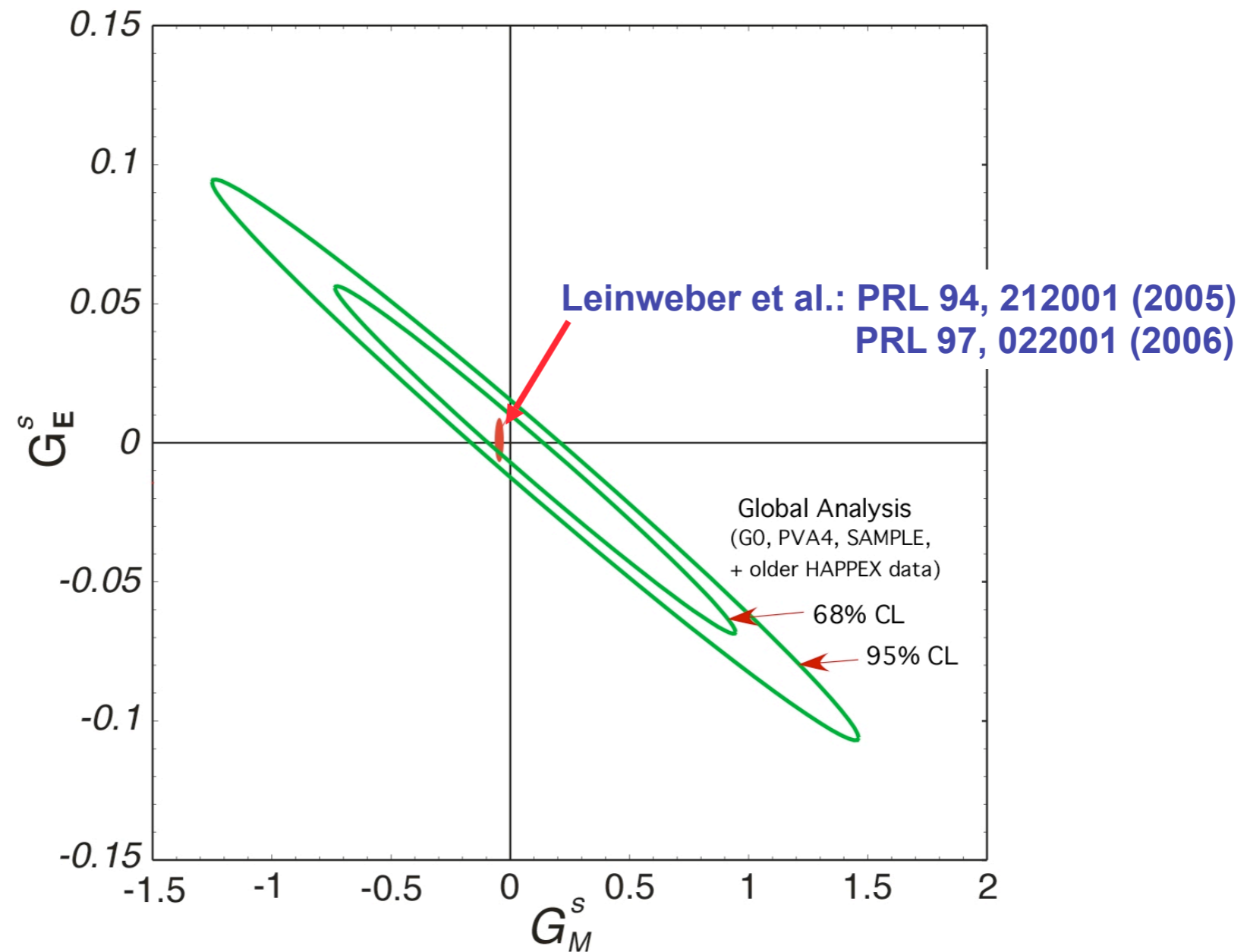
# Axial Isovector Form Factor



# Electromagnetic Structure of Octet Baryons

- Magnetic moments and charge radii of the octet baryons in the quenched approximation [Boinepalli et. al. '06]
- Magnetic moments of baryon octet and decuplet using the background field method in the quenched approximation [Lee et. al. '05].

# Strange Form Factors



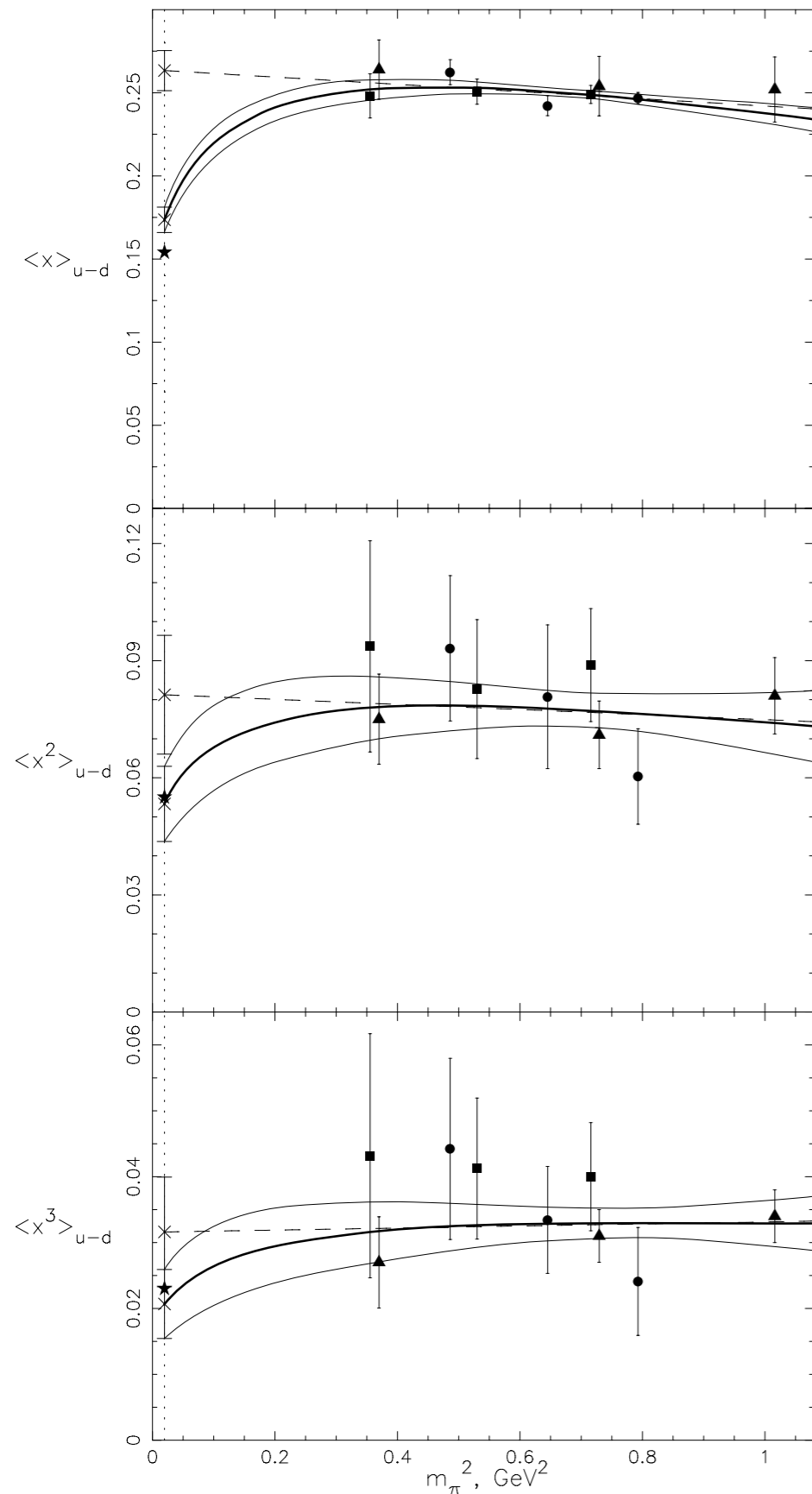
Slide contributed by A. Thomas (Young et.al. Phys.Rev.Lett. 97, '06)

# Form Factors (future)

- Understand continuum and chiral extrapolations
- Low  $Q^2$ : Comparison with experiment provides a benchmark
- Predict the High  $Q^2$  behavior
- Computation of flavor singlet form factors (proton and neutron)
  - This requires the next generation of computational resources
  - Exploratory studies can be done now
  - New algorithmic developments could provide further aid
- Form factors of resonances (Decouplet baryons, Roper etc.)
- Transition form factors
  - N- Delta already done in quenched and heavy dynamical quarks

# Unpolarized moments of Structure Functions

(year 2002)



LHPC-SESAM:

diamonds - quenched,  
squares - dynamical

QCDSF:

quenched - triangles

[[hep-lat/0201021](#)]

$$\langle x \rangle_{u-d} \sim a_1 \left[ 1 - \frac{(3g_A^2 + 1)m_\pi^2}{(4\pi f_\pi)^2} \ln \left( \frac{m_\pi^2}{m_\pi^2 + \mu^2} \right) \right] + b_1 m_\pi^2.$$

Where  $\mu = 550 \text{ MeV}$

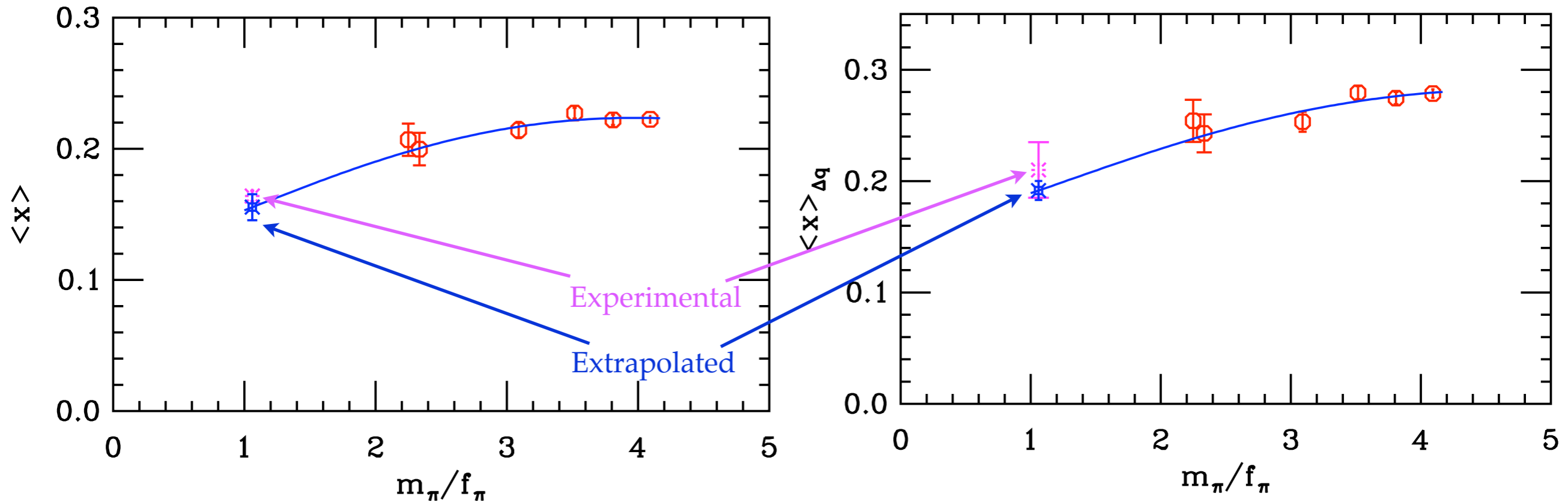
The log coefficient is valid for full QCD

[[Detmold et.al. Phys.Rev.D87 2001](#)]

# First Moments of Structure functions (present) [LHPC]

Domain Wall Valence, Staggered Sea (MILC)

$\mu = 2 \text{ GeV}$



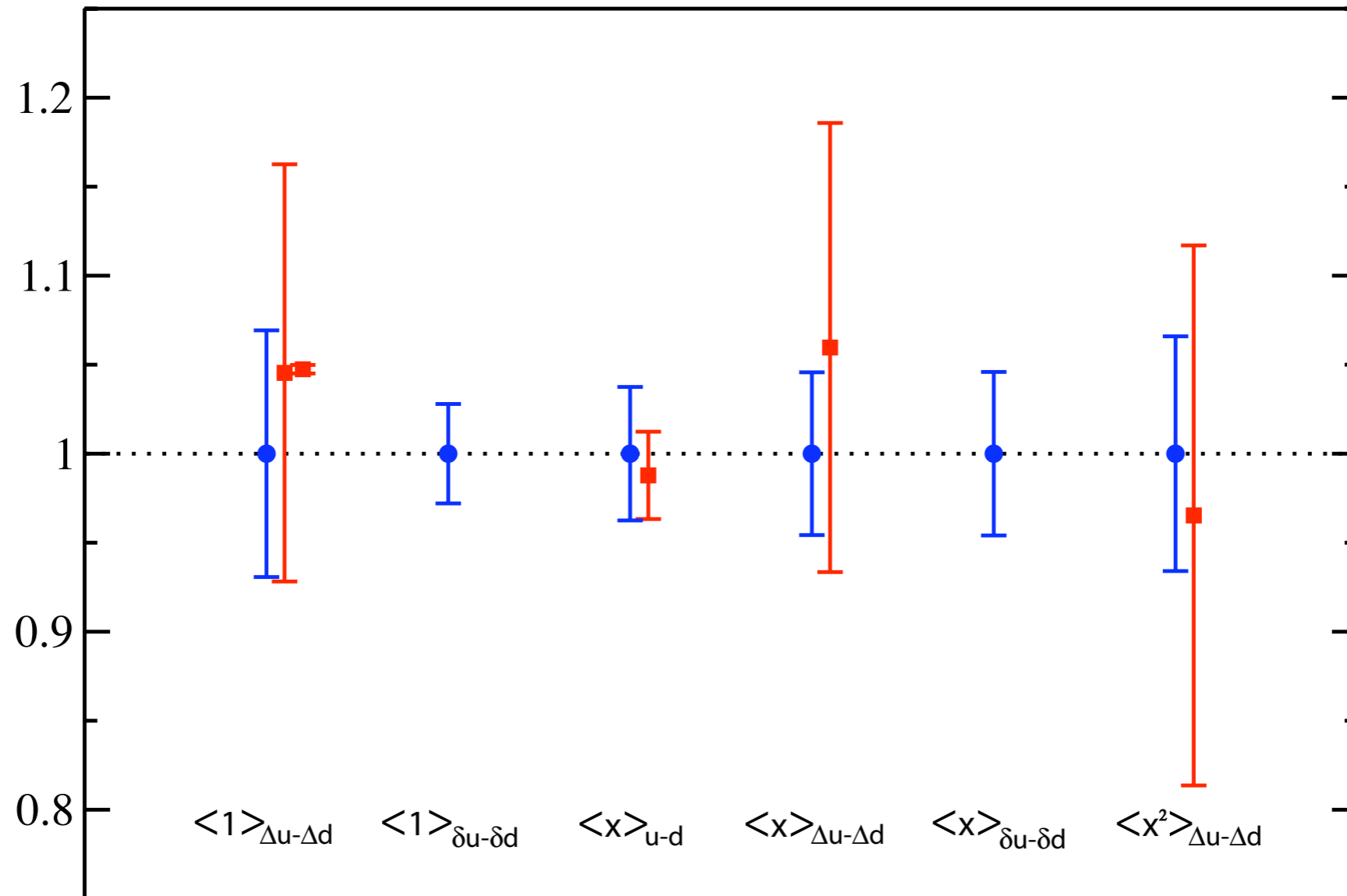
- Hint of curvature just below 400MeV
- Isovector moments only
- Fit to leading ChiPT keeping the mass dependence of  $g_A$
- Perturbative renormalization [Bistrovic '05 (thesis)]

[Renner Lattice '06]

$$\langle x \rangle_{u-d} = a \left[ 1 - \frac{3g_A^2 + 1}{8\pi^2} \left( \frac{m_\pi^2}{f_\pi^2} \right) \ln \left( \frac{m_\pi^2}{f_\pi^2} \right) \right] + c \frac{m_\pi^2}{f_\pi^2}$$

$$\langle x \rangle_{\Delta u - \Delta d} = a' \left[ 1 - \frac{2g_A^2 + 1}{8\pi^2} \left( \frac{m_\pi^2}{f_\pi^2} \right) \ln \left( \frac{m_\pi^2}{f_\pi^2} \right) \right] + c' \frac{m_\pi^2}{f_\pi^2}$$

# Moments of Structure functions Experiment vs LQCD



Need to include the Delta in the fits [Arndt and Savage, '02]

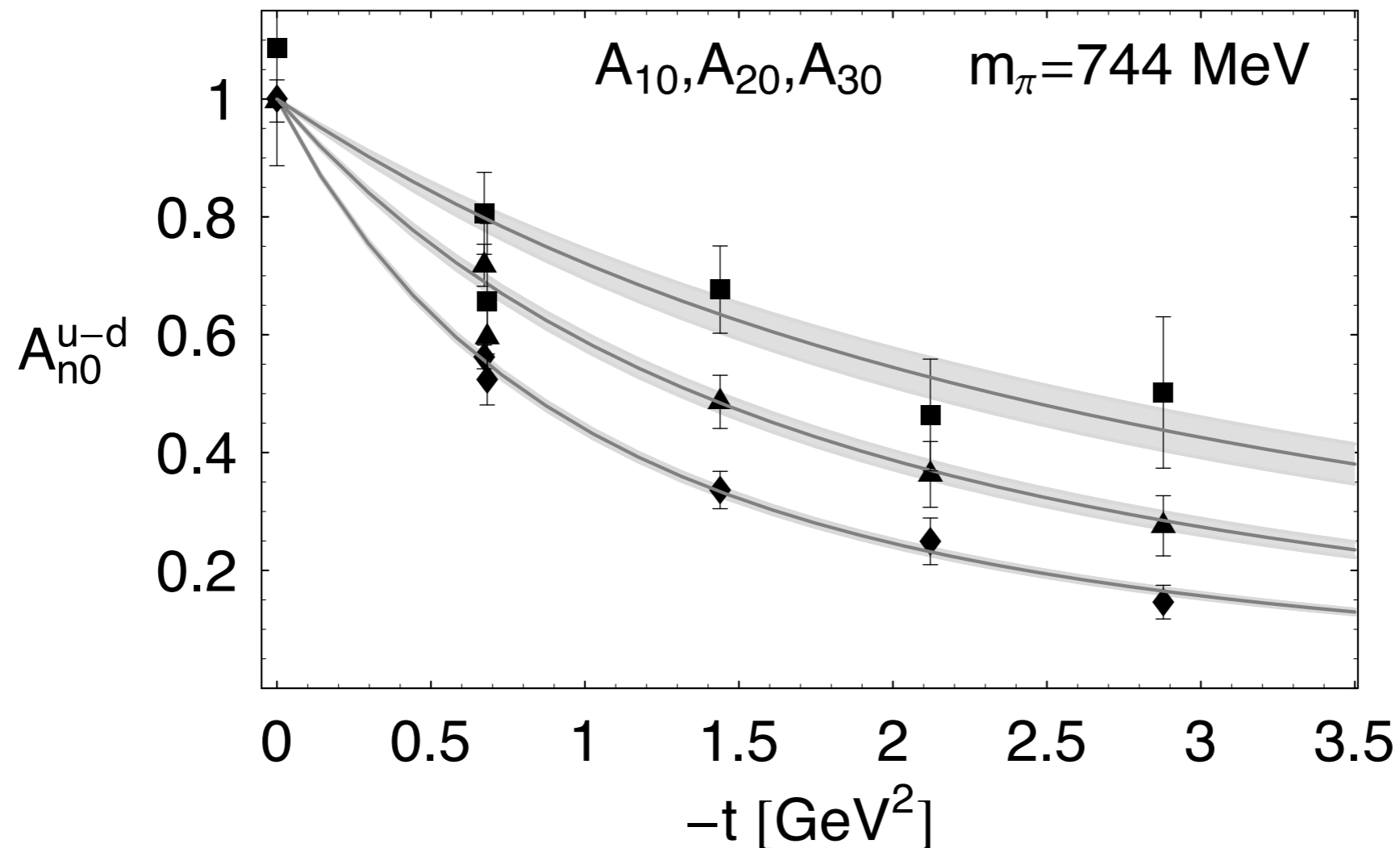
[Renner Lattice '06]

# Moments of Structure functions (future)

- Study systematics from chiral extrapolations
- Continuum Limit
  - Currently one lattice spacing ( $a=0.125\text{fm}$ )
  - Plan to do in the next few years two more ( $a=0.09\text{fm}$  and  $a=0.06\text{fm}$ )  
Cost: ~ 5-6 Tflop-years
- Compute flavor singlet moments.
  - Next generation of resources (Cost: ~ 10 Tflop-years)
  - Exploratory studies near future
- New ideas
  - Go beyond the first few moments [**Detmold and Lin '05**]



# Moments of Generalized Parton Distributions [LHPC 2003]



- Heavy dynamical quarks
- Slope at small  $t$  decreases as we go to higher moments
- Higher moments dominated by higher  $x$

# Transverse Structure

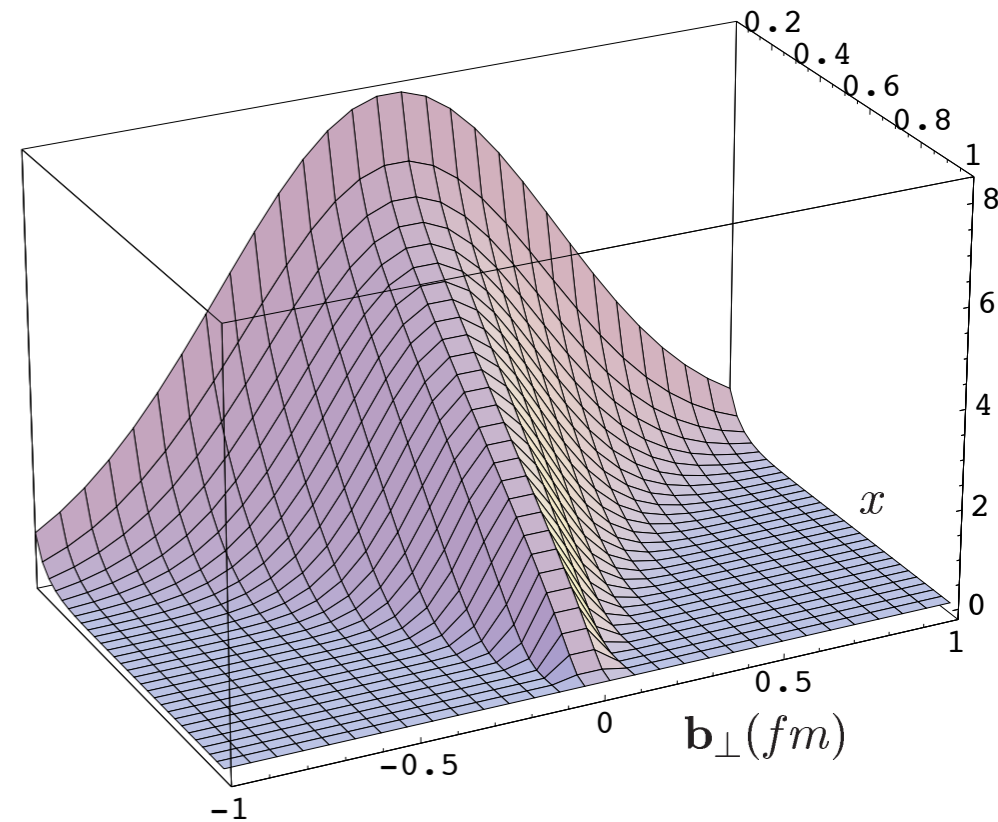
$\xi=0$  limit

$$H(x, 0, t)$$

- The generalized form factors have simple interpretation

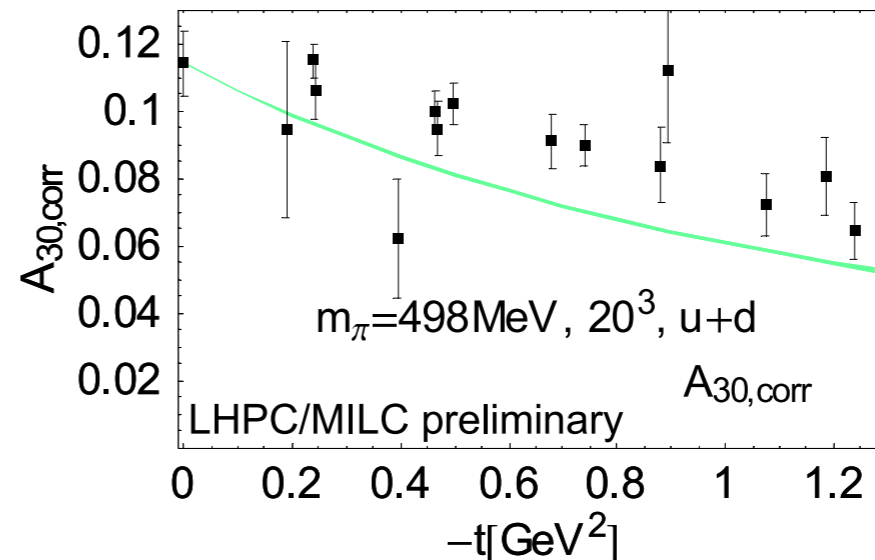
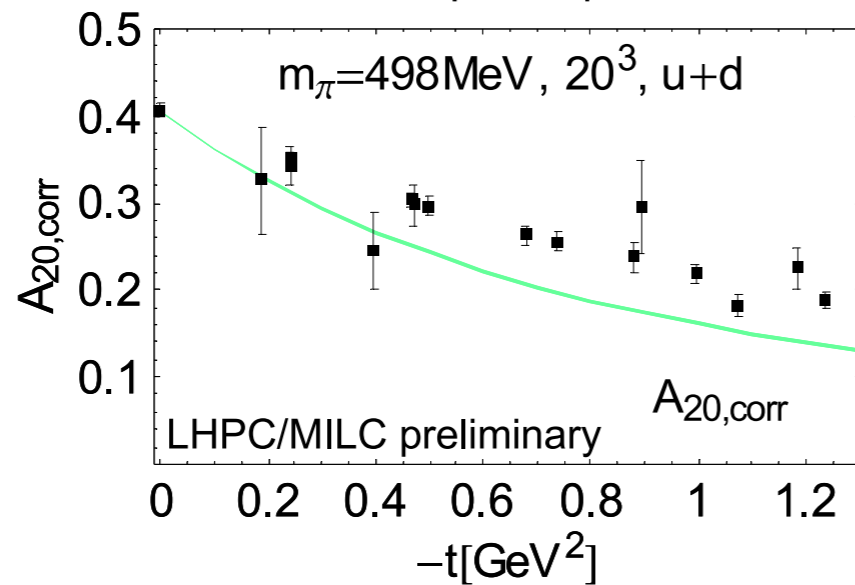
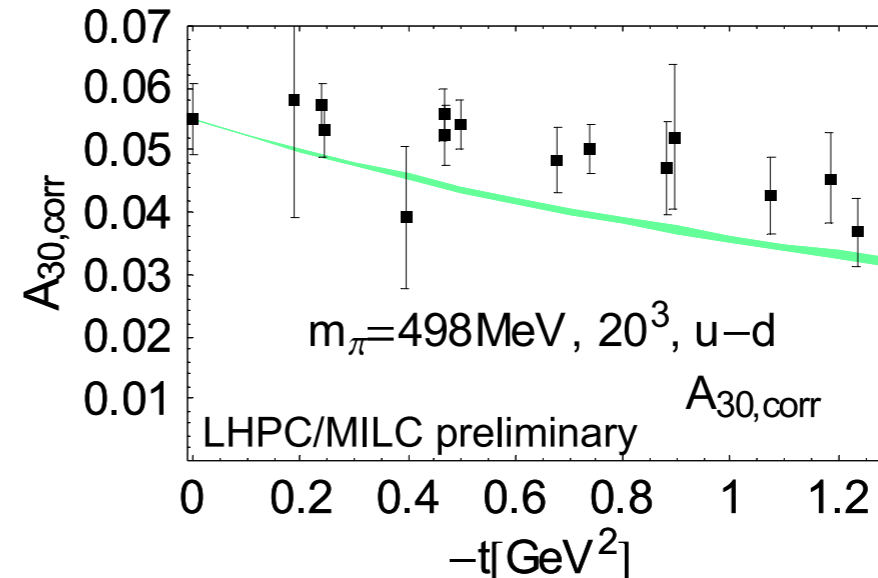
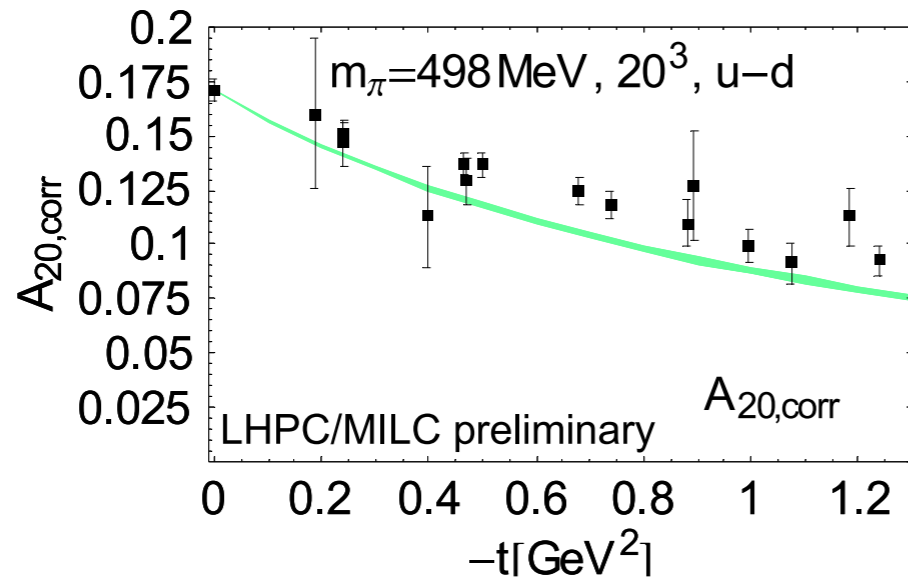
$$\int \frac{d^2 \Delta_T}{(2\pi)^2} e^{-i\Delta_T \cdot b} \longrightarrow \rho(x, b)$$

- $x \longrightarrow 1$   $\rho$  is a delta function



[Burkardt hep-ph/0207047]

# Moments of Generalized Parton Distributions (present)



- Lighter pion masses are attainable
- Green band is a phenomenological parameterization using Form factor data, CTEQ parton distributions, and Regge Ansatz as input [Deihl et.al.]

# The Proton Spin

- What is the contribution of the quark spin to the spin of the proton?
  - EMC (1988)  $Q^2 = 10 \text{ GeV}^2$   $\Delta\Sigma = 0.00(24)$
  - SMC (1998)  $Q^2 = 5 \text{ GeV}^2$   $\Delta\Sigma = 0.13(17)$
- Quarks contribute nothing to the spin of the proton!
- Spin crisis

$$\Delta\Sigma = \Delta u + \Delta d + \Delta s$$

# The Proton Spin

$$\frac{1}{2} = \frac{1}{2}\Delta\Sigma + \Delta g + L_z \quad \text{or} \quad \frac{1}{2} = \frac{1}{2}\Delta\Sigma + L_z^q + J_z^g$$

$$\Delta\Sigma = \Delta u + \Delta d + \Delta s$$

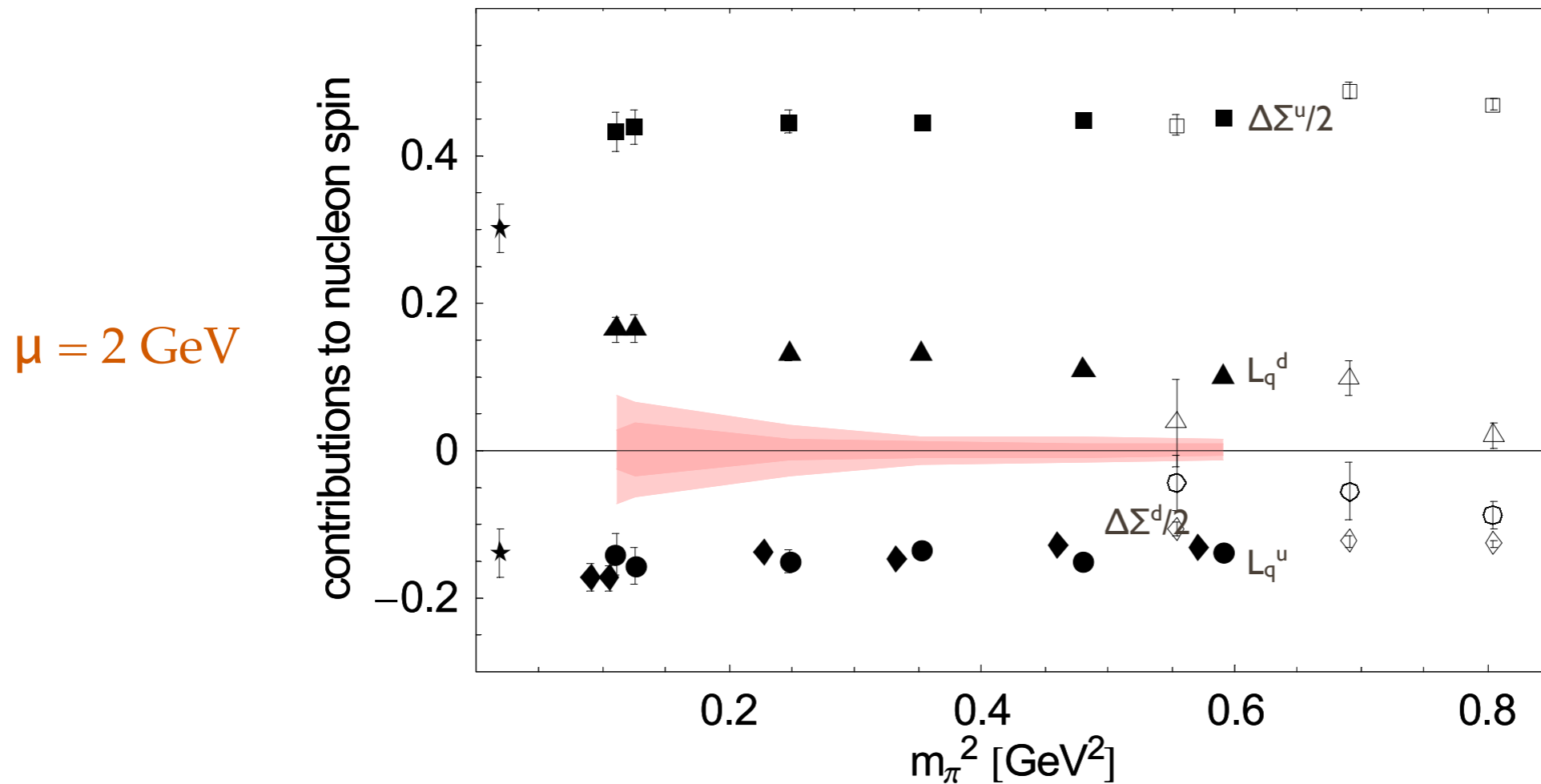
- The quark angular momentum can be computed on the lattice

- $J_z^q = \frac{1}{2} [A_{20}(0) + B_{20}(0)]$  [Ji,'98]

- A and B are the generalized form factors of

$$\mathcal{O}_{\mu\nu} = \bar{q}\gamma_{\{\mu}\overleftrightarrow{D}_{\nu\}}q = T_{\mu\nu}$$

# Proton SPIN



- Quark orbital angular momentum almost zero due to cancelation of the up and down contributions
- Disconnected diagrams are missing

# GPDs (future)

- Study systematics from chiral extrapolations
- Continuum Limit
  - Currently one lattice spacing ( $a=0.125\text{fm}$ )
  - Plan to do in the next few years two more ( $a=0.09\text{fm}$  and  $a=0.06\text{fm}$ )  
Cost: ~ 5-6 Tflop-years
- Compute flavor singlet moments.
  - Next generation of resources (Cost: ~ 10 Tflop-years)
  - Exploratory studies near future
- New ideas
  - Go beyond the first few moments [**Detmold and Lin '05**]

# Hadronic Interactions


- Effective field theory description of few nucleon systems
- Use lattice QCD to extract the low energy constants needed
  - Decay constants:  $f_\pi, f_K$
  - Axial couplings:  $g_A, g_{N\Delta}, g_{\Sigma\Sigma}, g_{\Xi\Xi}, g_{\Sigma\Lambda}, \dots$
  - Scattering lengths: **NPLQCD**
- Lattice Nuclear physics [[Lee et al.](#), [Borasoy et al.](#)]
- Lattice offers flexibility!
  - Study quark mass dependence
  - Compute experimentally inaccessible quantities (Hyperons)



# Hadronic Interactions

- Scattering processes from Lattice QCD are not straight forward
- Miani-Testa **no-go** theorem ('90) [and C. Michael '89]

- Infinite Volume:

Euclidean  Minkowski

- Finite volume: **discrete spectrum**
  - Avoids Miani-Testa no-go theorem [M. Luscher]

# Lüscher Formula

Energy level shift in finite volume:

$$\Delta E_n \equiv E_n - 2m = 2 \sqrt{p_n^2 + m^2} - 2m$$

$p_n$  solutions of:

$$p \cot \delta(p) = \frac{1}{\pi L} \mathbf{S} \left( \frac{p^2 L^2}{4\pi^2} \right)$$

$$\mathbf{S}(\eta) \equiv \sum_{|\mathbf{j}| < \Lambda} \frac{1}{|\mathbf{j}|^2 - \eta} - 4\pi\Lambda$$

$$p_n \cot \delta(p_n) = \frac{1}{a} + \dots$$

$$\frac{1}{a} = \frac{1}{\pi L} \mathbf{S} \left( \frac{p_0^2 L^2}{4\pi^2} \right) + \dots$$

Expansion at  $p \sim 0$  :

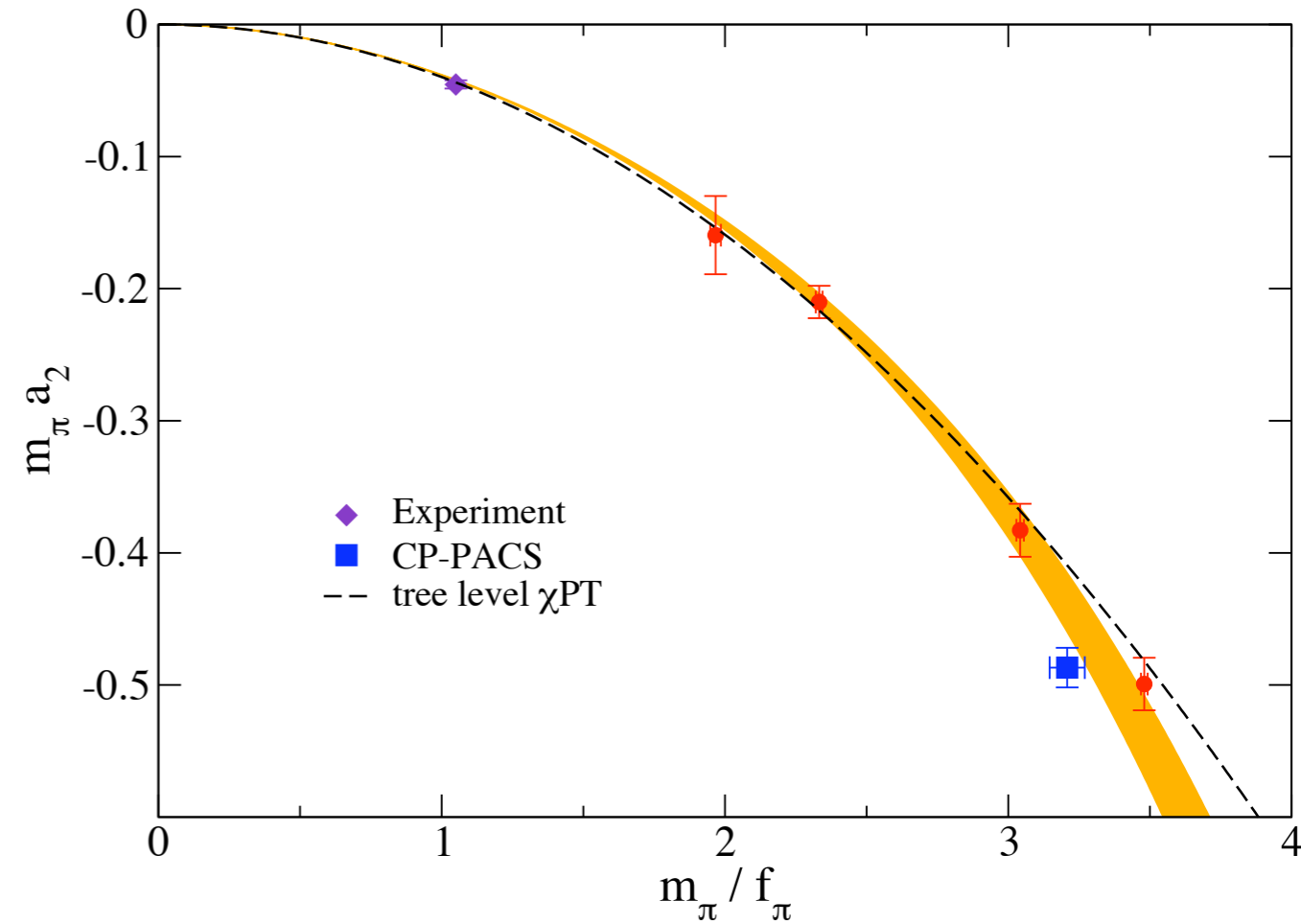
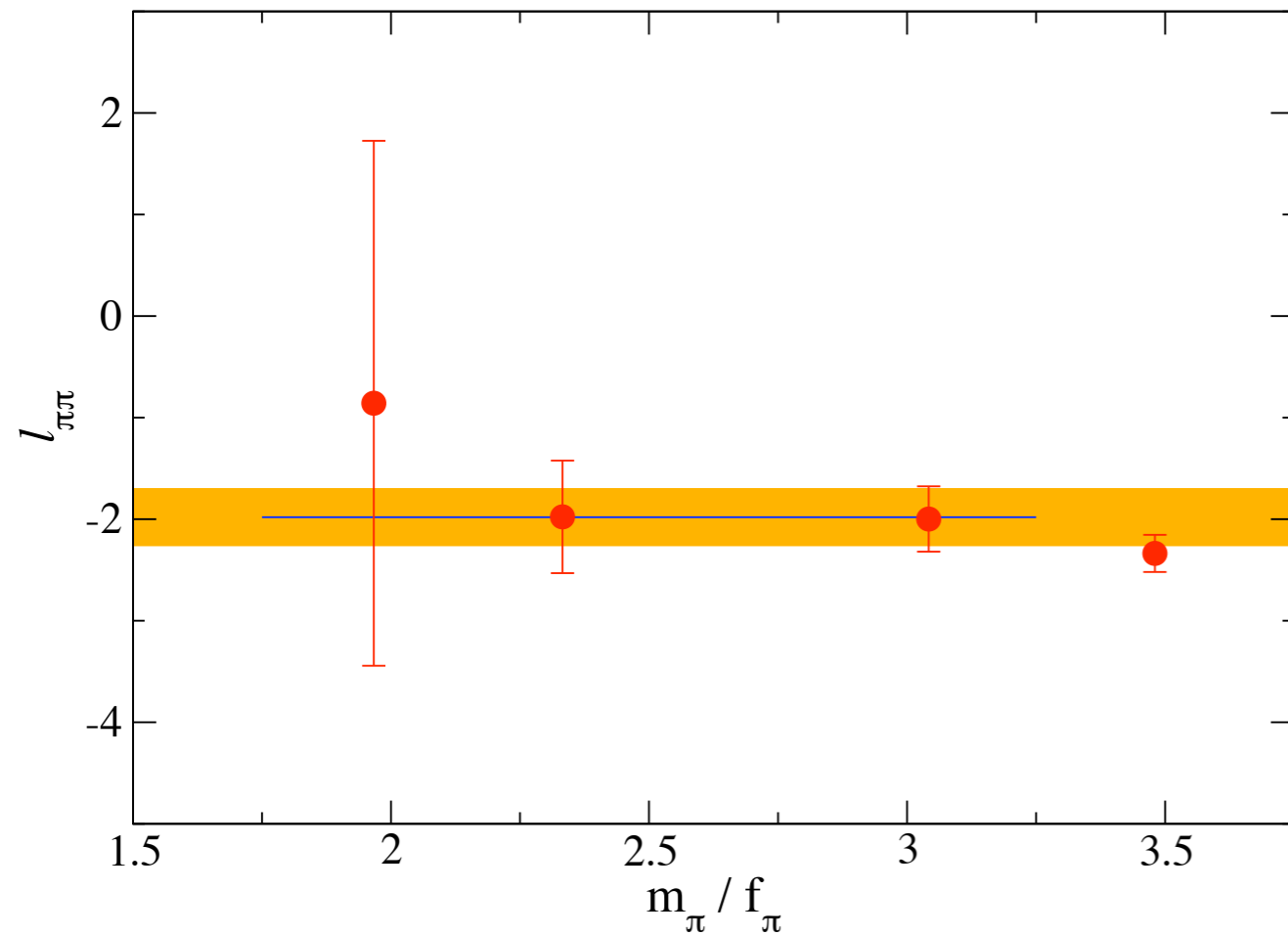
$$\Delta E_0 = -\frac{4\pi a}{mL^3} \left[ 1 + c_1 \frac{a}{L} + c_2 \left( \frac{a}{L} \right)^2 \right] + \mathcal{O} \left( \frac{1}{L^6} \right)$$

$a$  is the scattering length

$c_1$  and  $c_2$  are universal constants

# I=2 Pion Scattering

NPLQCD



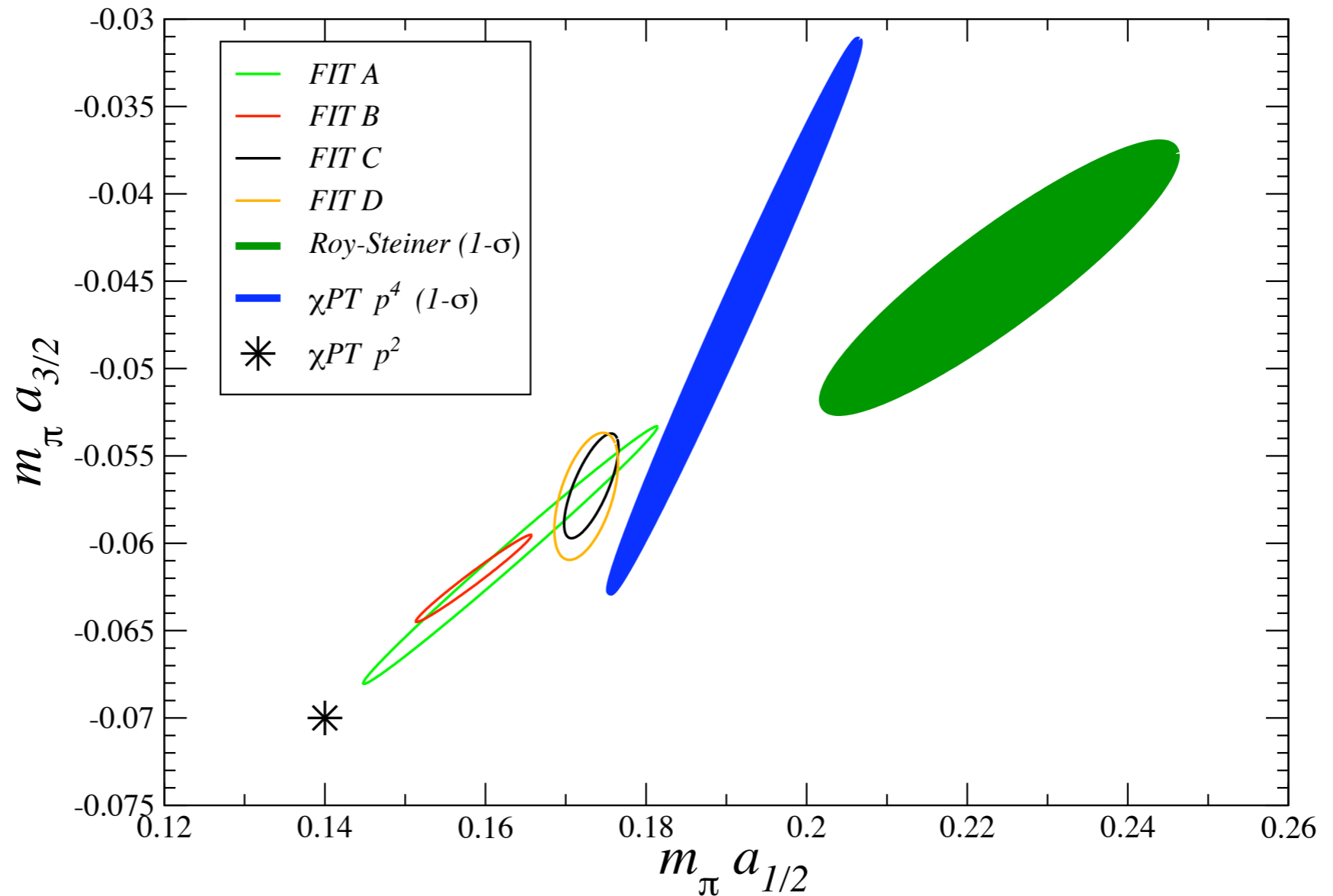
$$m_\pi a_2 = -\frac{m_\pi^2}{8\pi f_\pi^2} \left[ 1 + \frac{3m_\pi^2}{16\pi^2 f_\pi^2} \left( \log \frac{m_\pi^2}{\mu^2} + l_{\pi\pi}(\mu) \right) \right]$$

[Gasser-Leutwyler '84]  
[Colangelo et al. '01]

- $m_\pi a_2 = -0.0422(3)(18)$
- Experiment:  $m_\pi a_2 = -0.0454(31)$
- $S_\chi$ PT has insignificant effect to the result [Chen et al. '05]

# Kaon Pion Scattering Lengths

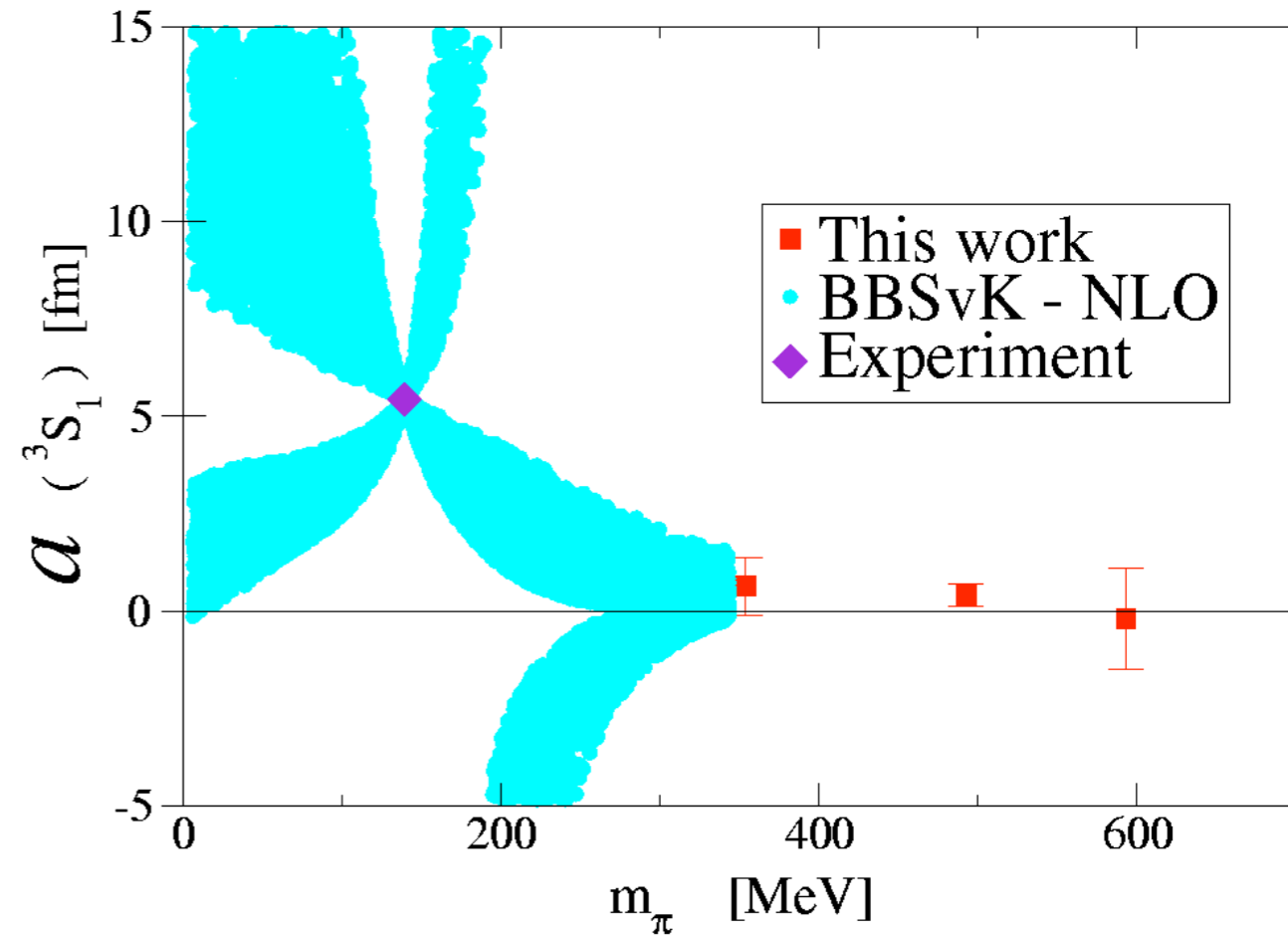
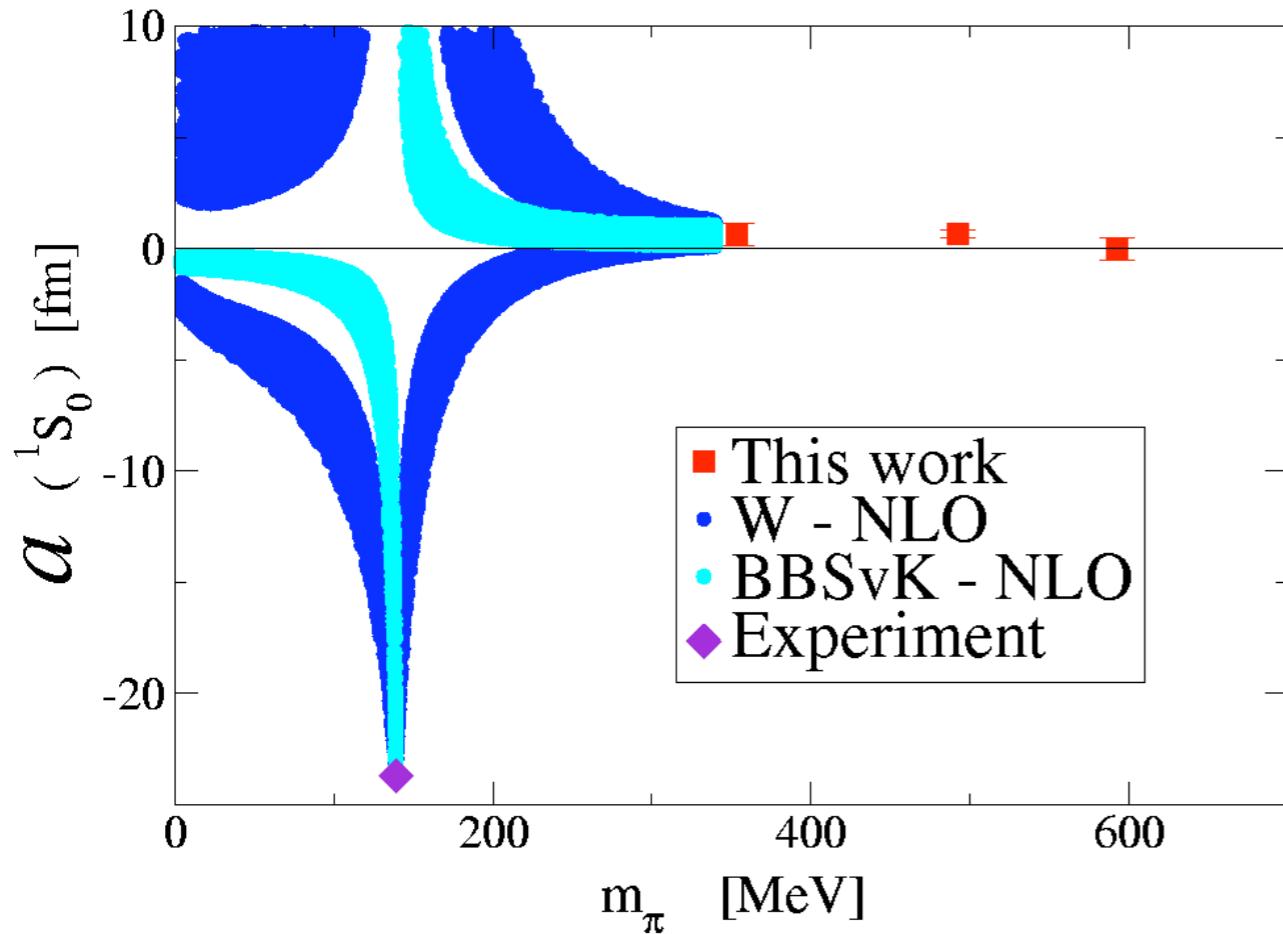
NPLQCD



- Upcoming experiments on Kaon - pion molecules (DIRAC collab.)
- Continuum extrapolation still needed

# Nucleon-Nucleon

NPLQCD: *Phys.Rev.Lett.*97 2006

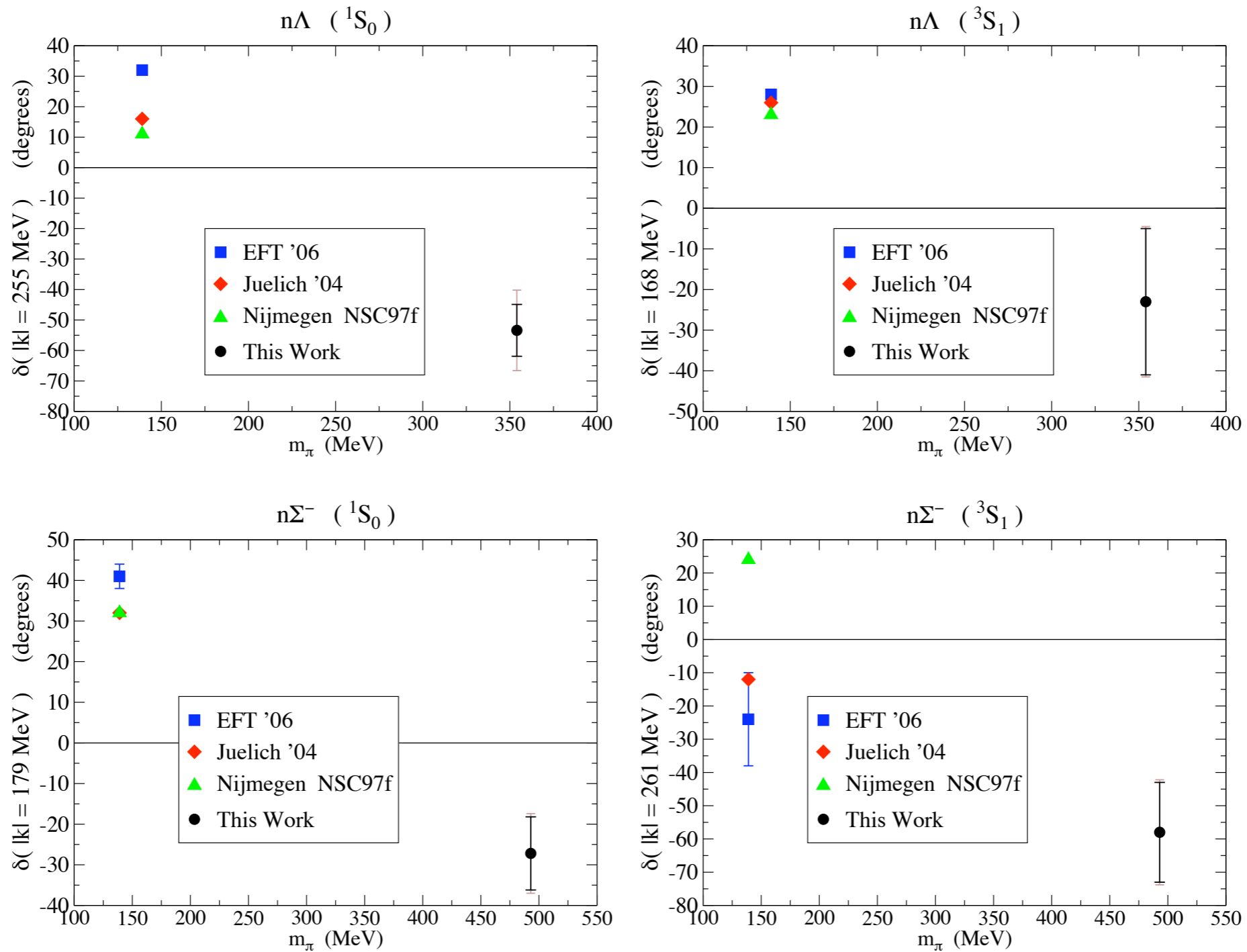


BBSvK: Beane Bedaque Savage van Kolck '02  
W: Weinberg '90; Weingberg '91; Ordonez et.al '95

Fukugita et al. '95: Quenched heavy pions

# Nucleon-Hyperon

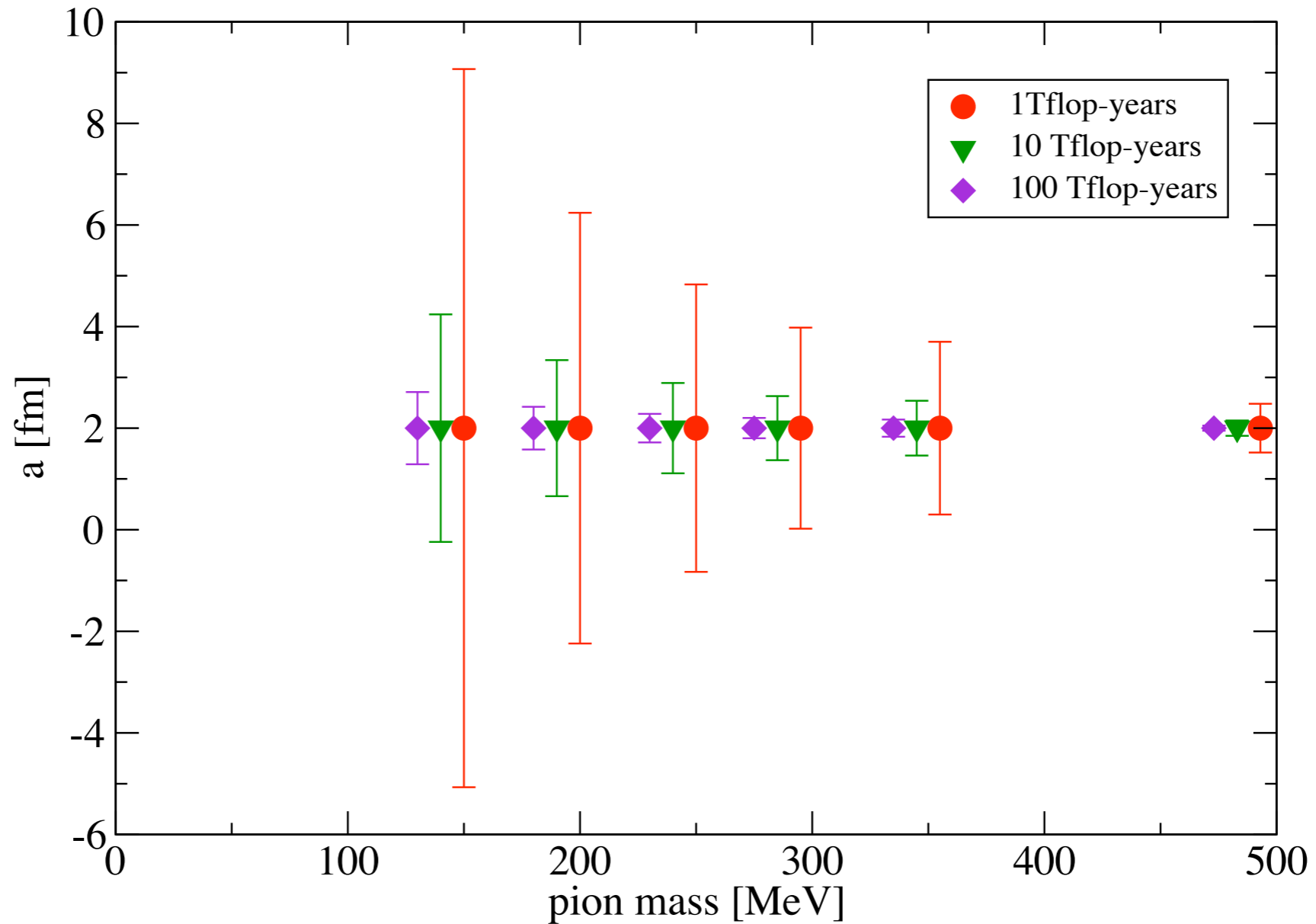
NPLQCD: [hep-lat/0612026](#)



# Hadronic interactions (Future)

- These calculations are the beginning of the beginning!
- Need lighter pion masses, multiple volume sizes, and lattice spacings
  - Determine if we see scattering states
- Meson baryon channels: (K-n, K- $\Sigma$  ...) ----- Neutron stars
- Hyperon-Hyperon and Hyperon-Nucleon channels [[NPLQCD: hep-lat/0612026](#)]
  - Hyper-nuclear physics and Neutron stars
- Need to make lattices designed for this project
- Higher statistics: (JLAB spectrum program -- INCITE recent award)

# Hadron Interactions: Projected errors



- Errors on scattering nucleon-nucleon scattering length as function of computational resources
- Only cost for correlation function calculation presented



# Conclusions

- Lattice QCD is a mature field
  - Direct comparison with experiment is now possible for several observables
  - Predictions are now emerging
- Extraction of GPDs: Synergy between experiment, Lattice and phenomenology
- Petaflop computing is around the corner
  - Will allow us to perform precision calculations for spectrum, form factors and GPDs
  - Will take us long ways in understanding the nuclear force

# Polarizabilities

- Compute the response of the hadron in external electric or magnetic field
- Use the external field method
- Electric polarizabilities of neutral hadrons [Christensen, Wilcox, Lee '04 ]
- Magnetic polarizabilities of hadrons [Lee, Zhou, Wilcox, Christensen '05 ]
- Spin polarizabilities and electric polarizabilities of charged particles proposed to be measured [Detmold, Tiburzi, Walker-Loud '06]