Computational QCD

J.W. Negele

QCD and Hadron Physics Town Meeting

Rutgers January 13, 2007

Lattice QCD has come of age

- Entering era of solving full QCD in chiral regime
- Unprecedented opportunities:
  - Impact National experimental nuclear physics program
  - Fundamental understanding of how QCD works
- Confluence of 3 developments:
  - Lattice field theory
    - Wilson, Kaplan, ...
  - Computer technology
    - Optimized clusters, QCDOC, Blue Gene, ...
  - Investment in frontier resources
- US has played leadership role
- 37 senior members of USLQCD working on nuclear physics

Resources

- US
  - DOE NP, HEP, ASCR Partnership: 8 sustained Tflop
  - NERSC, ORNL, ANL, LLNL
  - NSF centers
  - SciDAC infrastructure: software + prototype hardware
  - Significant investments by BNL, Fermilab, JLab
- 2006 world sustained Teraflops for lattice
  - USLQCD 8
  - Europe + UK 20 - 25
  - Japan 14 - 18

Physics Goals

- Quantitative calculation of nuclear physics observables from first principles
  - Agreement with experiment
  - Credibility for predictions and guiding experiment
- Insight into how QCD works
  - Mechanisms, role of instantons, diquarks, N_c, N_f, m_q ...
- Two nuclear physics foci:
  - QCD at finite temperature and density
  - Spectrum, structure, and interaction of hadrons
- Synergy with high energy physics study of weak decays
  - Investigate same hadronic structure and physics issues
  - Share common dynamical configurations - MILC and DW

Physics Goals

- QCD Thermodynamics RHIC, LHC, ...
  - Equation of state, T_c : Basic input to models
  - Search for critical point at finite chemical potential
    - First order regime? Location of transition
  - In-medium properties of hadrons
    - Quarkonium, light mesons, thermal dileptons & photons
  - Transport coefficients
- Hadron spectroscopy JLab 12 GeV upgrade
  - What are the low energy degrees of freedom of QCD?
  - Spectrum of low-lying mesons and baryons
    - Exotics
    - Widths, transition form factors

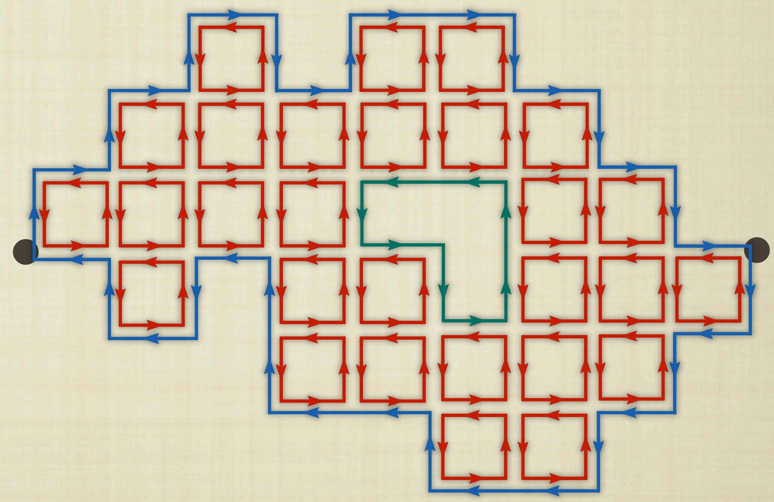
Physics Goals

- Hadron structure JLab, RHIC-spin, EIC,...
  - Vector and axial form factors
    - Distribution of charge, current, strange quark content; onset of scaling
  - Moments of quark density, spin and transversity distributions
  - Moments of gluon distributions
  - Moments of generalized parton distributions
    - Origin of nucleon spin
    - Transverse structure of nucleon
  - Diquark correlations, variational wave functions, ...
- Hadron interactions
  - Hadron scattering lengths and phase shifts
    - Mesons, nucleons, hyperons
  - Use effective field theory to connect with nuclei

Lattice QCD - summing over paths

$$\langle T\, e^{-\beta H} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \rangle = \prod_n \int dU_n \frac{1}{Z} \det M(U) e^{-S(U)} \sum M^{-1}(U) M^{-1}(U) \cdots M^{-1}(U)$$

- $M^{-1} = (1 + \kappa U)^{-1}$ connects Ψ's with line of U's
  Sum over valence quark paths
- det M generates closed loops of U's
  Sum over sea quark excitations
- S(U) tiles with plaquettes
  → Sum over all gluons
- $32^3 \times 64$ lattices → 10^8 gluon variables



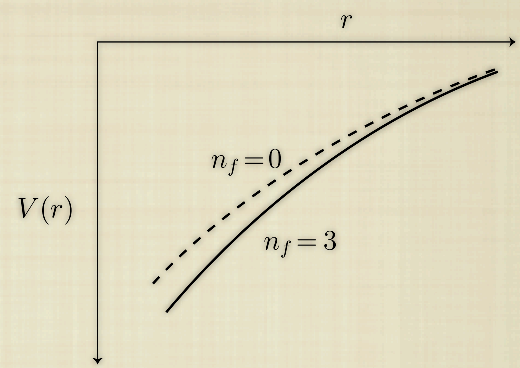
Computational Issues

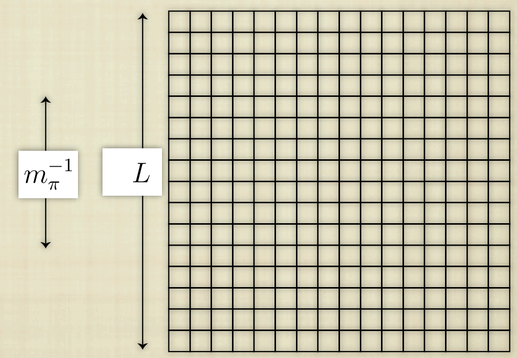
- Fermion determinant - Full QCD
- Chiral symmetry
- Small lattice spacing
- Small quark mass
- Large lattice volume

$$\frac{1}{m_\pi} \leq \frac{L}{4}$$

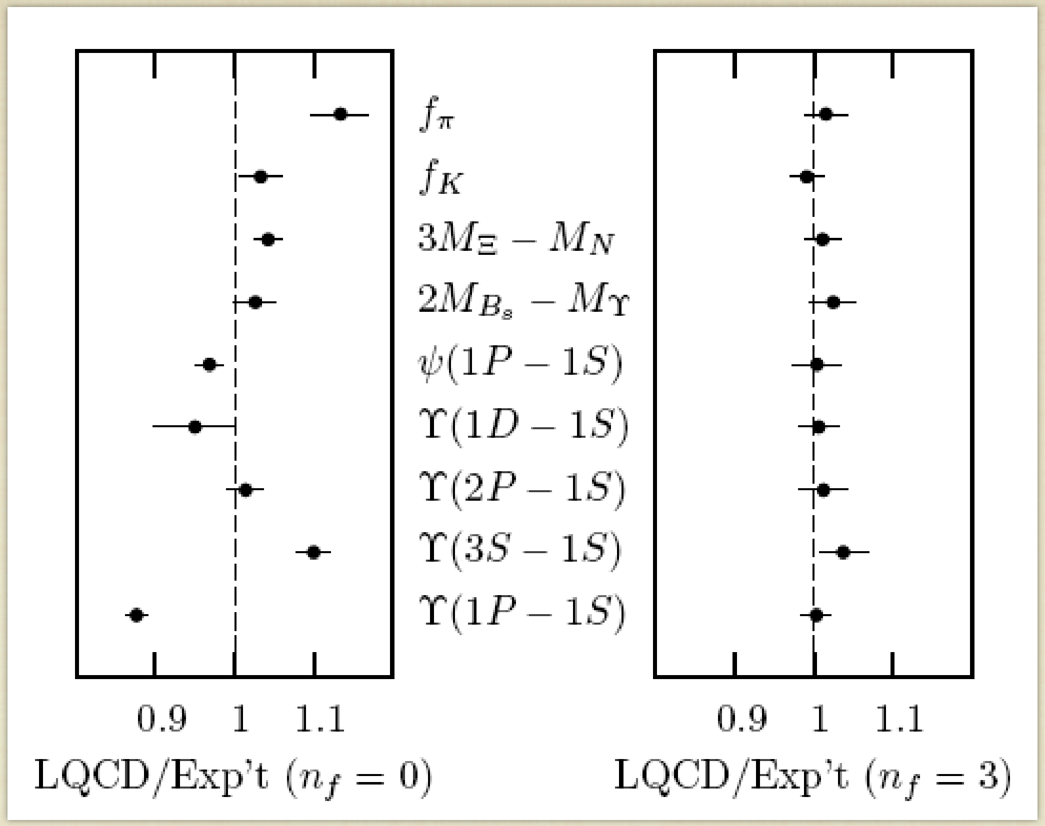
L(fm)	m_π (Mev)
1.6	500
4.0	200
5.7	140

- Cost ~ $(m_\pi)^{-7}$ - $(m_\pi)^{-9}$



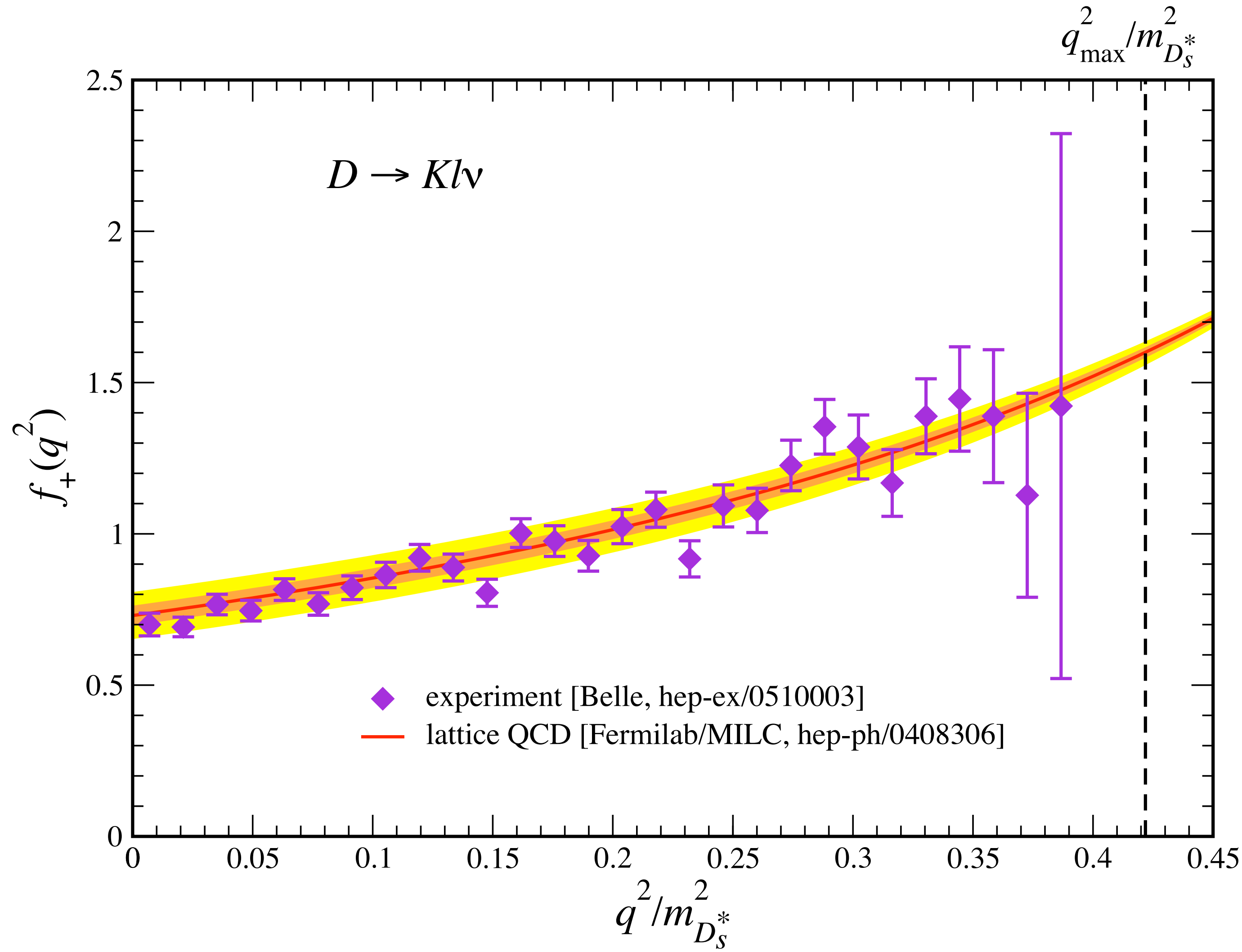


Precision agreement in heavy quark systems



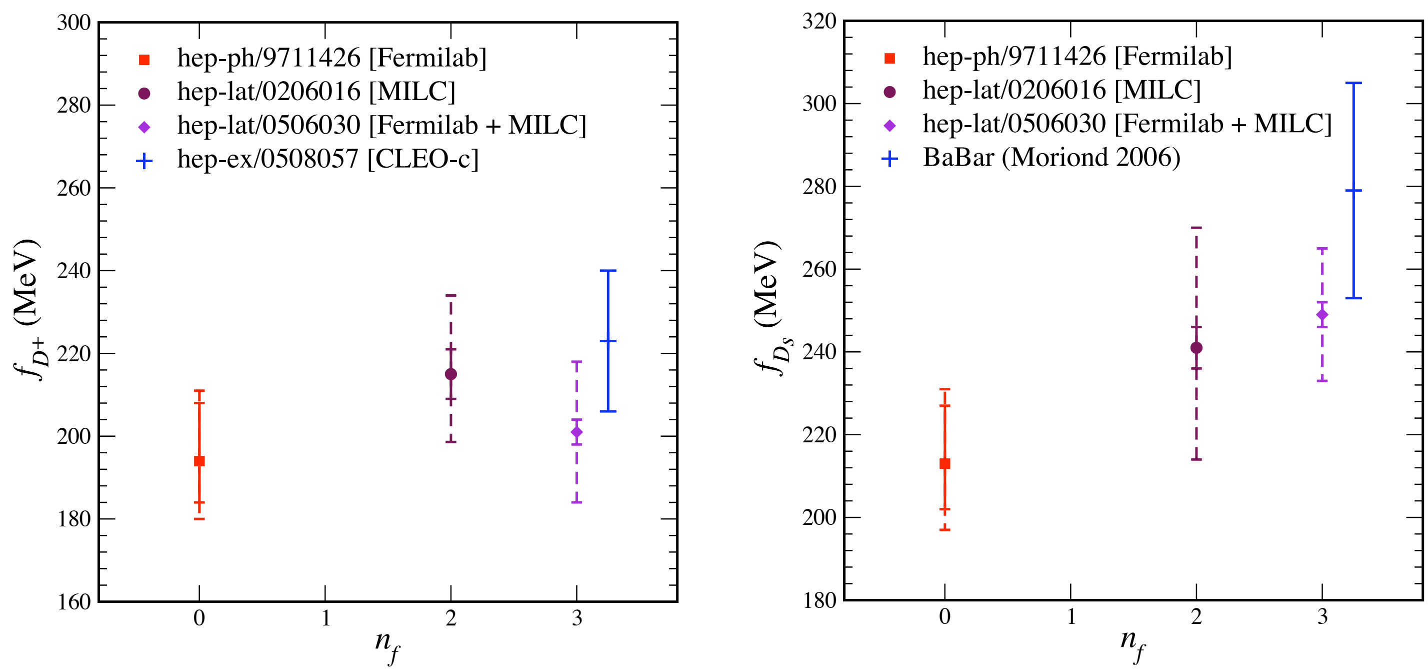
- "Gold Plated Observables" (Davies et. al. hep-lat/0304004)
  - Staggered quarks
  - Asqtad improved action
  - a = 0.13, 0.09 fm
  - Errors ~ 3%

Lattice QCD Predictions



Lattice QCD Predictions

D meson decay constants



$$\frac{\sqrt{m_D} f_D}{\sqrt{m_{D_s}} f_{D_s}} = 0.786 \pm 0.042 \quad \text{lattice}$$

$$= 0.779 \pm 0.093 \quad \text{CLEO/BaBar}$$

Mass of B_c meson

Highlights of Accomplishments

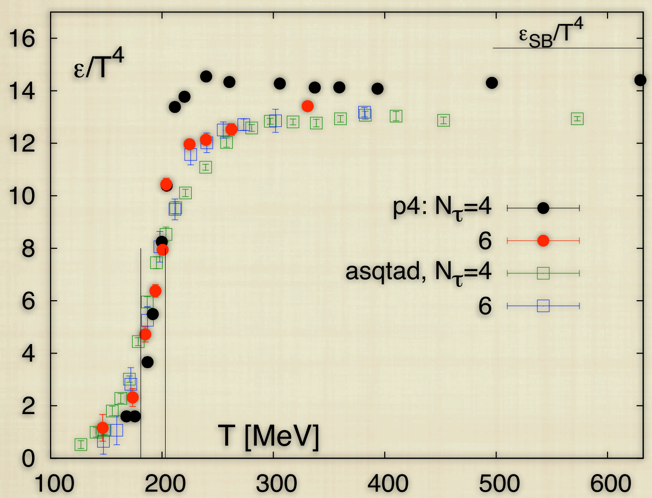
Lattice QCD at Finite Temperature and Density

See Talk by F. Karsch

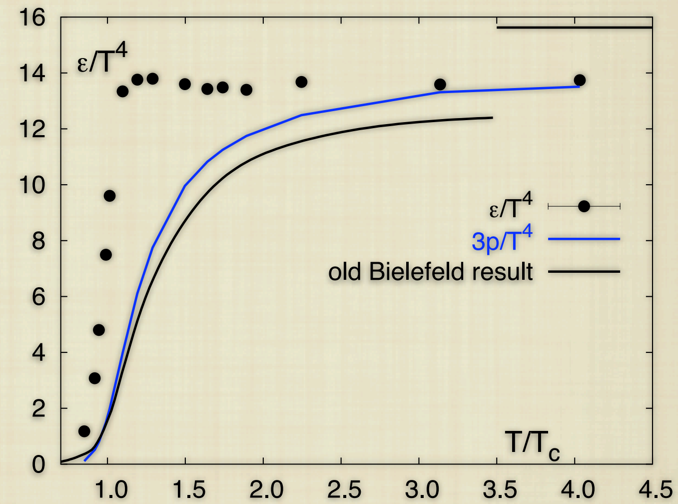
Phases of QCD Matter meeting, Sunday, 9:40

Energy density and pressure

- RBC-Bielefeld vs. MILC: overall good agreement for $N_\tau = 4,\ 6$
- detailed quantitative analysis at low as well as high T requires significantly more CPU time
- towards the chiral limit: want to establish the interplay of deconfinement and chiral symmetry breaking in the vicinity of T_c



band marks $T = (192 \pm 11)$ MeV
RBC-Bielefeld, preliminary



pressure increased slightly with smaller quark mass

F. Karsch – p.7/21

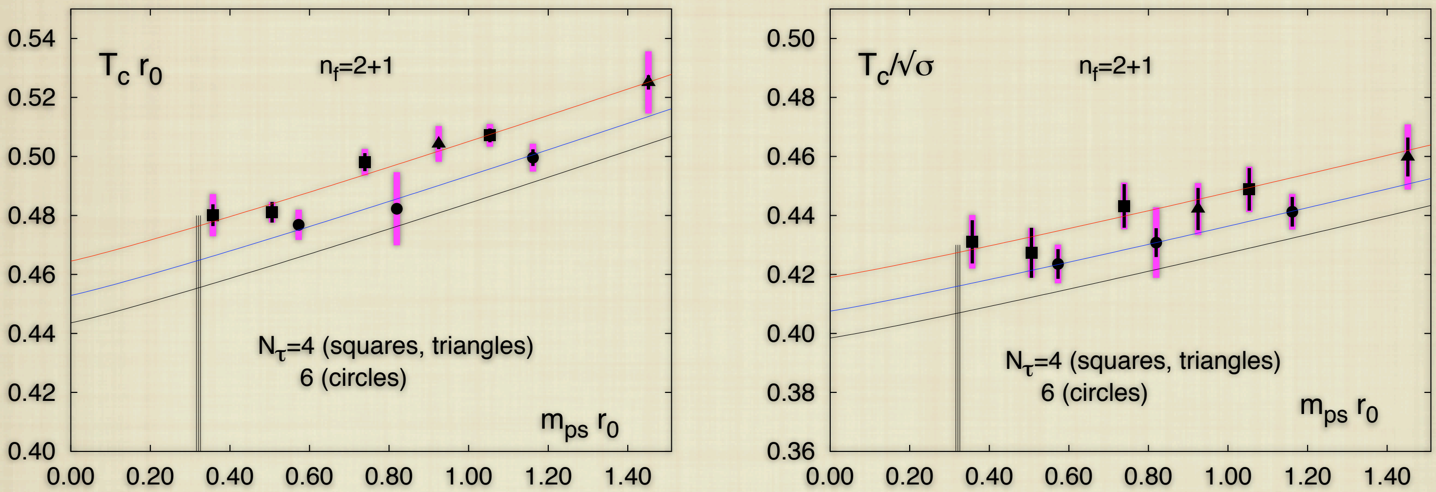
Transition temperature in QCD

N. H. Christ et al. (RBC-Bielefeld collaboration), Phys. Rev. D74, 054507 (2006)

extrapolation to chiral and continuum limit

$$(r_0 T_c)_{N_\tau} = (r_0 T_c)_{cont.} + b\,(m_{PS} r_0)^d + c/N_\tau^2$$

(d=1.08 (O(4), 2nd ord.), d=2 (1st ord.))



$\Rightarrow \quad r_0 T_c = 0.456(7)^{+3}_{-1} \quad , \quad T_c/\sqrt{\sigma} = 0.408(7)^{+3}_{-1}$ at phys. point

$\Rightarrow T_c = 192(7)(4)$ MeV

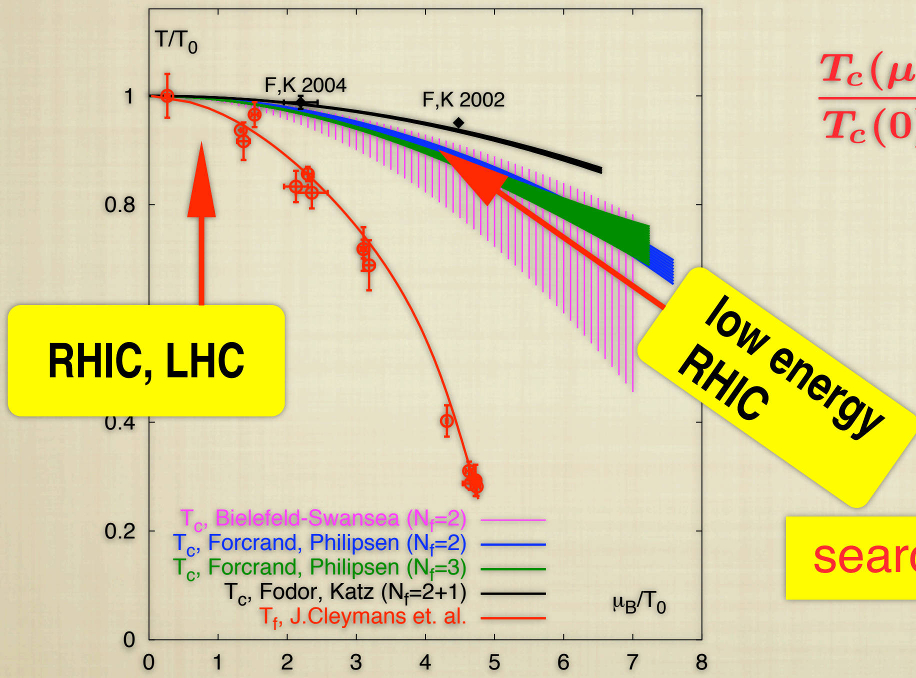
(1st error: stat. error on β_c and r_0; 2nd error: N_τ^{-2} extrapolation)

F. Karsch – p.9/21

Phase diagram at non-zero chemical potential

non-zero baryon number density: $\mu > 0$

$$Z(V,T,\mu) = \int \mathcal{D}A\mathcal{D}\psi\mathcal{D}\bar{\psi}\ \mathrm{e}^{-S_E(V,T,\mu)}$$
$$= \int \mathcal{D}A\mathcal{D}\ \det M(\mu)\ \mathrm{e}^{-S_E(V,T)}$$



$\frac{T_c(\mu)}{T_c(0)}$: $1 - 0.0056(4)(\mu_B/T)^2$

deForcrand, Philipsen (imag. μ)

$1 - 0.0078(38)(\mu_B/T)^2$

Bielefeld-Swansea

($\mathcal{O}(\mu^2)$ reweighting)

search for critical point

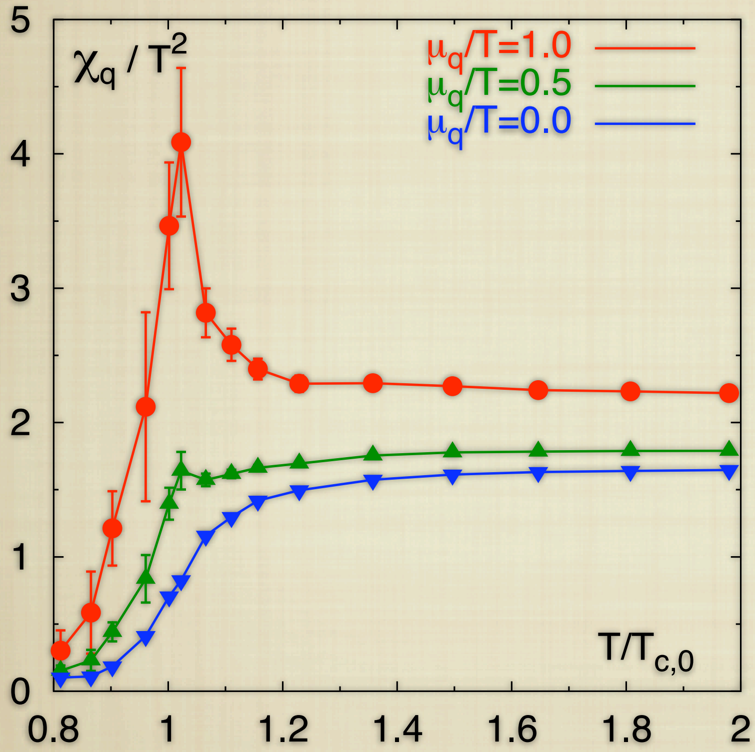
F. Karsch – p.13/21

Fluctuations in baryon number density

baryon number density fluctuations:

(Bielefeld-Swansea, PRD68 (2003) 014507)

$\mu \geq 0, n_f = 2$



$$\frac{\chi_q}{T^3} = \left(\frac{d^2}{d(\mu/T)^2} \frac{p}{T^4} \right)_{T \text{ fixed}}$$

$$= \frac{9\,T}{V} \left(\langle N_B^2 \rangle - \langle N_B \rangle^2 \right)$$

susceptibilities

to be studied in event-by-event fluctuations

recent papers:

V. Koch, E.M. Majumder, J. Randrup, nucl-th/0505052

S. Ejiri, FK, K. Redlich, hep-ph/05090521

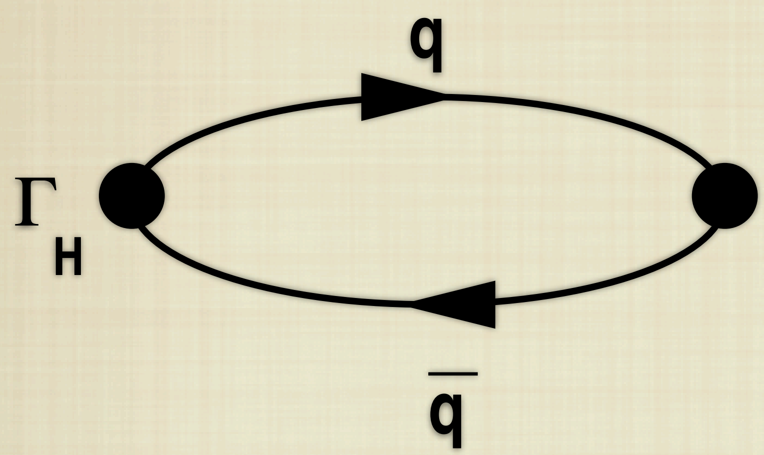
R.V. Gavai, S. Gupta, hep-lat/0510044

F. Karsch – p.14/21

Thermal meson correlation functions

Thermal correlation functions: 2-point functions which describe propagation of a $\bar{q}q$-pair

spectral representation of correlator ⇒ dilepton and photon rates



spectral representation of
thermal photon rate: $\omega = |\vec{p}|$

$$\omega \frac{d^3 R^\gamma}{d^3 p} = \frac{5\alpha}{6\pi^2} \frac{\sigma_V(\omega, \vec{p}, T)}{\omega^2 (e^{\omega/T} - 1)}$$

spectral representation of
thermal dilepton rate

$$\frac{d^4 W}{d\omega d^3 p} = \frac{5\alpha^2}{27\pi^2} \frac{\sigma_V(\omega, \vec{p}, T)}{\omega^2 (e^{\omega/T} - 1)}$$

spectral representation of
Euclidean correlation functions

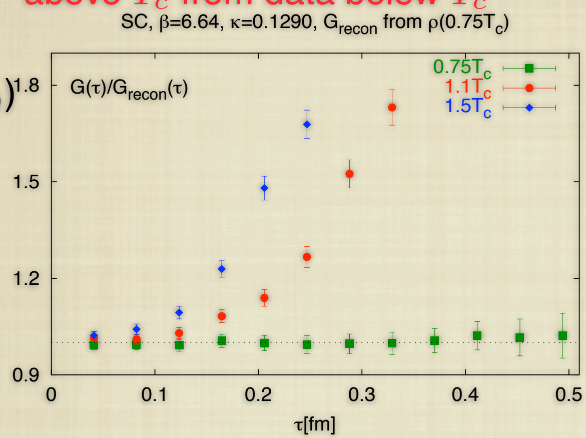
$$G_H^\beta(\tau, \vec{r}) = \int_0^\infty d\omega \int \frac{d^3\vec{p}}{(2\pi)^3} \sigma_H(\omega, \vec{p}, T)\, e^{i\vec{p}\vec{r}} \frac{\cosh(\omega(\tau - 1/2T))}{\sinh(\omega/2T)}$$

F. Karsch – p.16/21

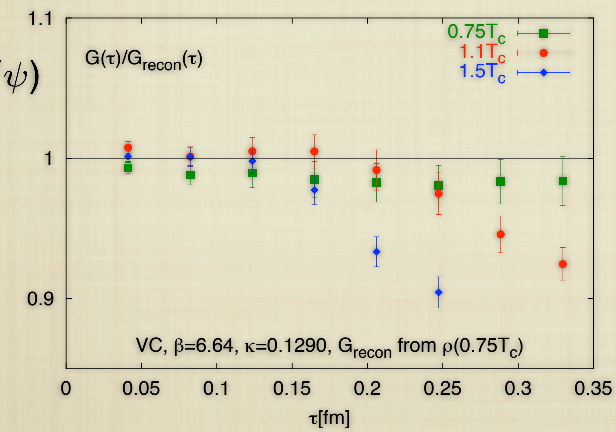
Charmonium spectral functions

reconstructed correlation functions
above T_c from data below T_c

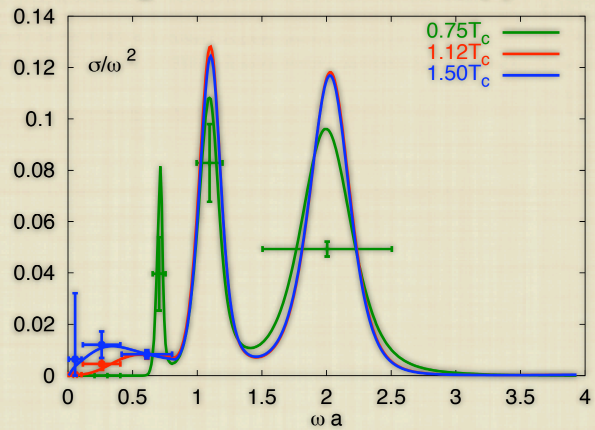
(χ_{c0})

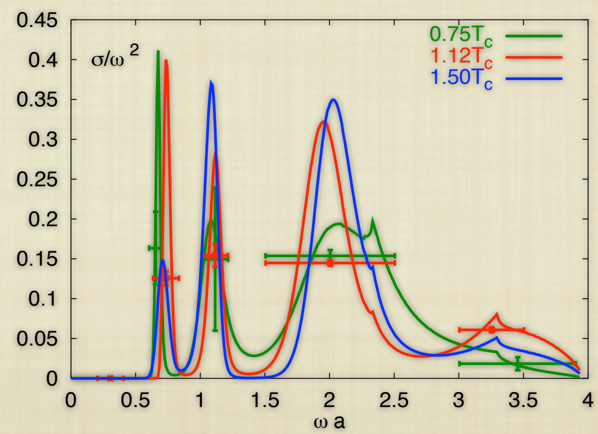


(J/ψ)



reconstructed spectral functions
using the Maximum Entropy Method





F. Karsch – p.18/21

Highlights of Accomplishments

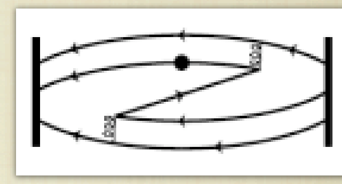
Spectrum, Structure and Interactions of Hadrons

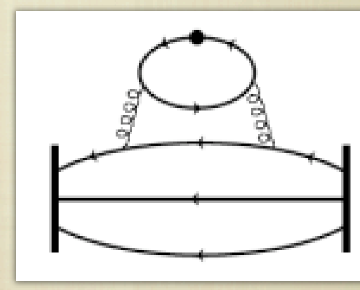
See Talk by K. Orginos

QCD and Hadron Physics meeting, Sunday, 1:50 pm

Hadron structure we can calculate now

- Domain wall quarks on improved staggered sea (MILC collab.)
- Masses
- Matrix elements of twist 2 operators
  - Note - omit disconnected diagrams, so only isovector exact
  - Form factors: em, transition
  - Moments of structure functions
  - Moments of GPD's - generalized form factors
    - Spin structure, transverse structure
- hadron scattering lengths



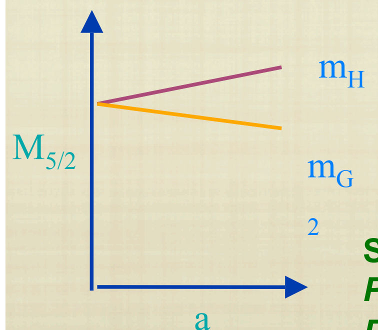


Lattice Spectroscopy

- Develop special technology for excited states
  - Diagonalize in large basis of hadron states
  - Anisotropic lattice for short times
  - Hypercubic symmetry must be related to continuum

J	$n^J_{G_1}$	$n^J_{G_2}$	n^J_H
$\frac{1}{2}$	1	0	0
$\frac{3}{2}$	0	0	1
$\frac{5}{2}$	0	1	1
$\frac{7}{2}$	1	1	1
$\frac{9}{2}$	1	0	2
$\frac{11}{2}$	1	1	2
$\frac{13}{2}$	1	2	2
$\frac{15}{2}$	1	1	3
$\frac{17}{2}$	2	1	3

Note that states with $J >= 5/2$ lie in representations with lower spins.

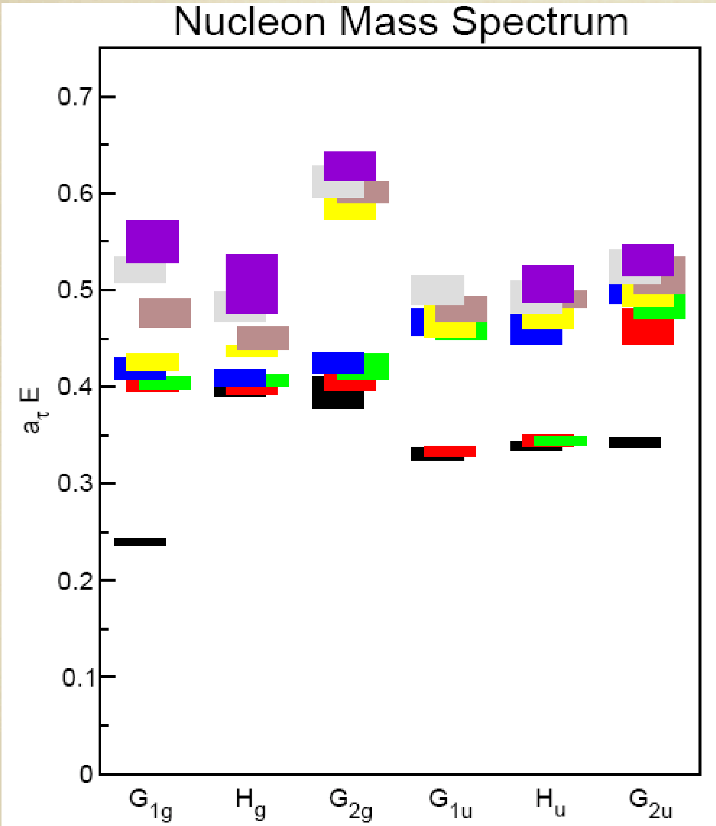


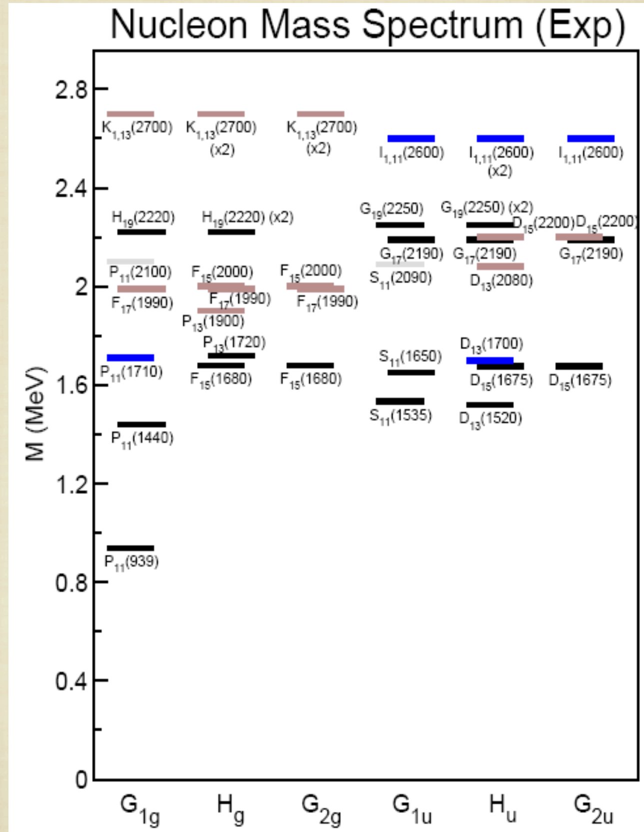
Spins identified from degeneracies in contiuum limit

S. Basak *et al.*,
PRD72:074501,2005
PRD72:094506,2005

Nucleon spectrum

Quenched nucleon spectrum compared with expt.





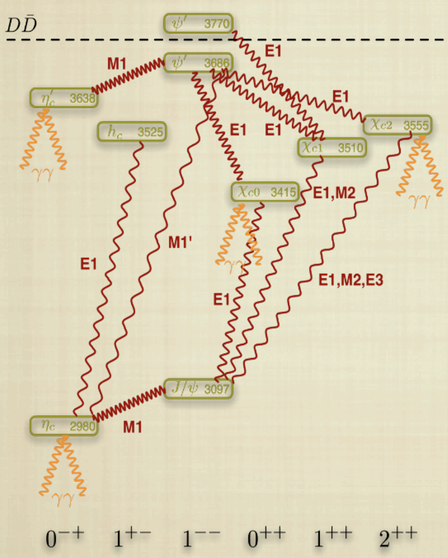
Adam Lichtl PhD 2006

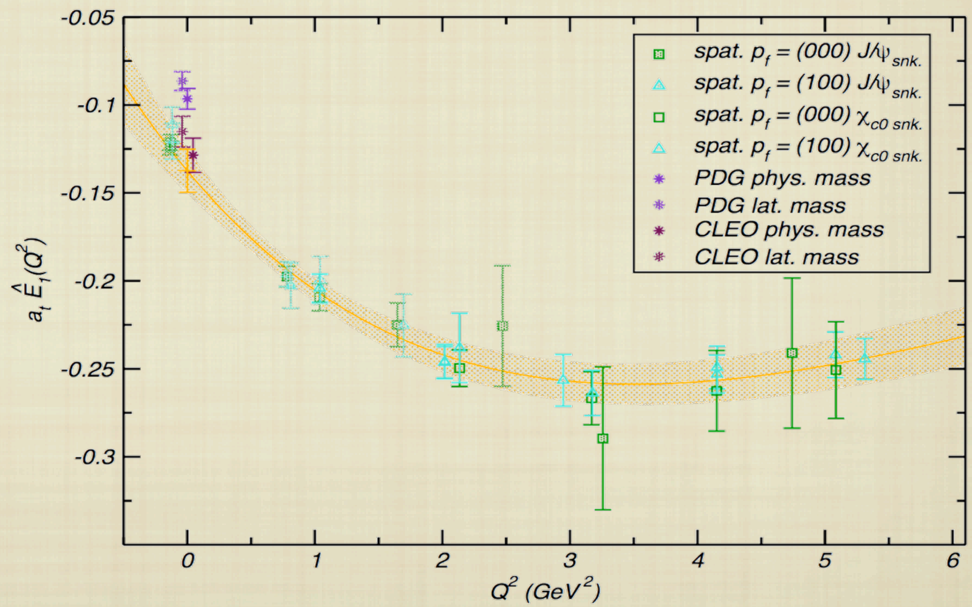
Photocouplings

Calculate photocouplings to predict hybrid meson production

Test methodology on charmonium decay

$$\Gamma(\chi_{c0} \to J/\psi\,\gamma) = \frac{1}{8\pi}\frac{|\vec{q}\,|}{m_S^2}\,2\,(2e_c)^2\,|\,E_1(0)\,|^2$$





Dudek et al, PRD73, 074507

Moments of parton distributions

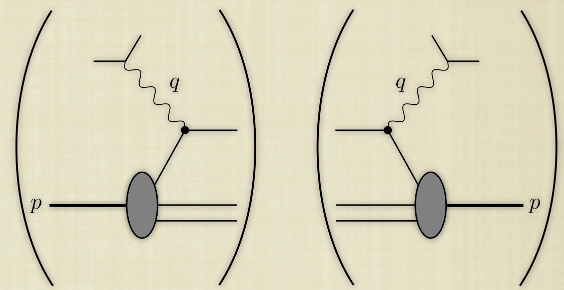
Expansion of $\mathcal{O}(x) = \int \frac{d\lambda}{4\pi} e^{i\lambda x} \bar{\psi}(-\frac{\lambda}{2}n) \not{n} \mathcal{P} e^{-ig\int_{-\lambda/2}^{\lambda/2} d\alpha n\cdot A(\alpha n)} \psi(\frac{\lambda}{2}n)$

Generates tower of twist-2 operators

$$\mathcal{O}_q^{\{\mu_1\mu_2\ldots\mu_n\}} = \overline{\psi}_q \gamma^{\{\mu_1} iD^{\mu_2} \ldots iD^{\mu_n\}} \psi_q$$

Diagonal matrix element

$$\langle P|\mathcal{O}_q^{\{\mu_1\mu_2\ldots\mu_n\}}|P\rangle \sim \int dx\, x^{n-1} q(x)$$



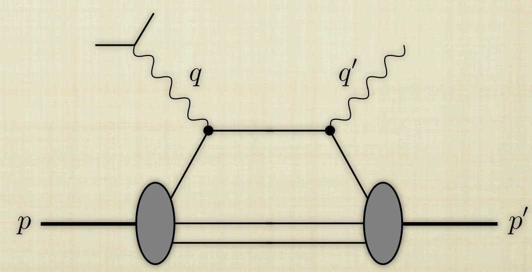
Off-diagonal matrix element

$$\langle P'|\mathcal{O}_q^{\{\mu_1\mu_2\ldots\mu_n\}}|P\rangle \to A_{ni}(t), B_{ni}(t), C_{n0}(t)$$

$$\int dx\, x^{n-1} H(x,\xi,t) \sim \sum \xi^i A_{ni}(t) + \xi^n C_{n0}(t)$$

$$\int dx\, x^{n-1} E(x,\xi,t) \sim \sum \xi^i B_{ni}(t) - \xi^n C_{n0}(t)$$

$[\not{n} \to \not{n}\gamma_5 : \quad \tilde{A}_{ni}(t), \tilde{B}_{ni}(t)]$



Nucleon axial charge g_A $\langle 1 \rangle_{\Delta q}^{u-d}$

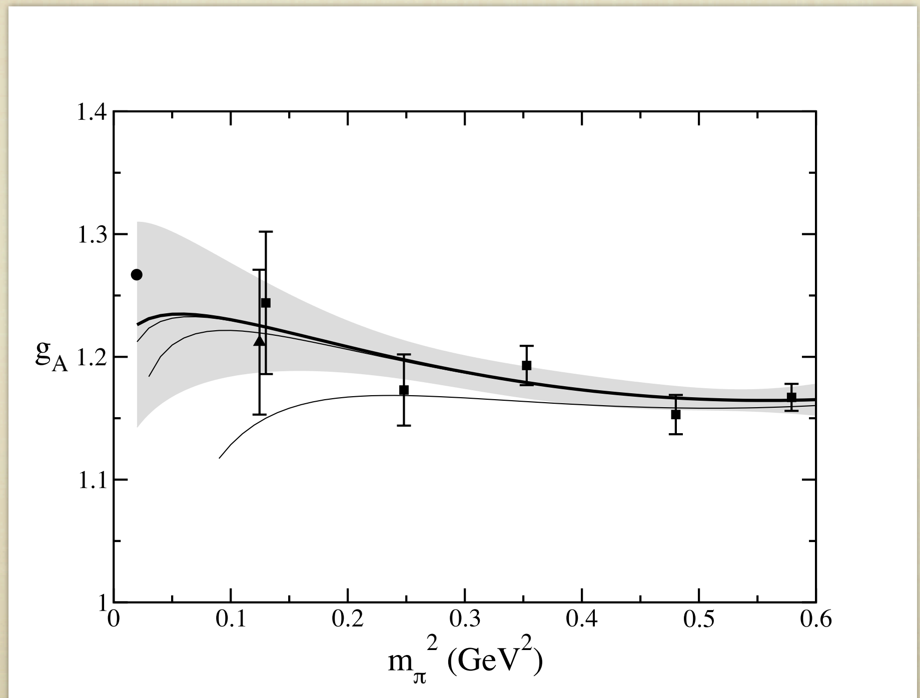
Example of application of chiral perturbation theory

6 low energy parameters describe m_π and L dependence

Measure 3 from other lattice observables

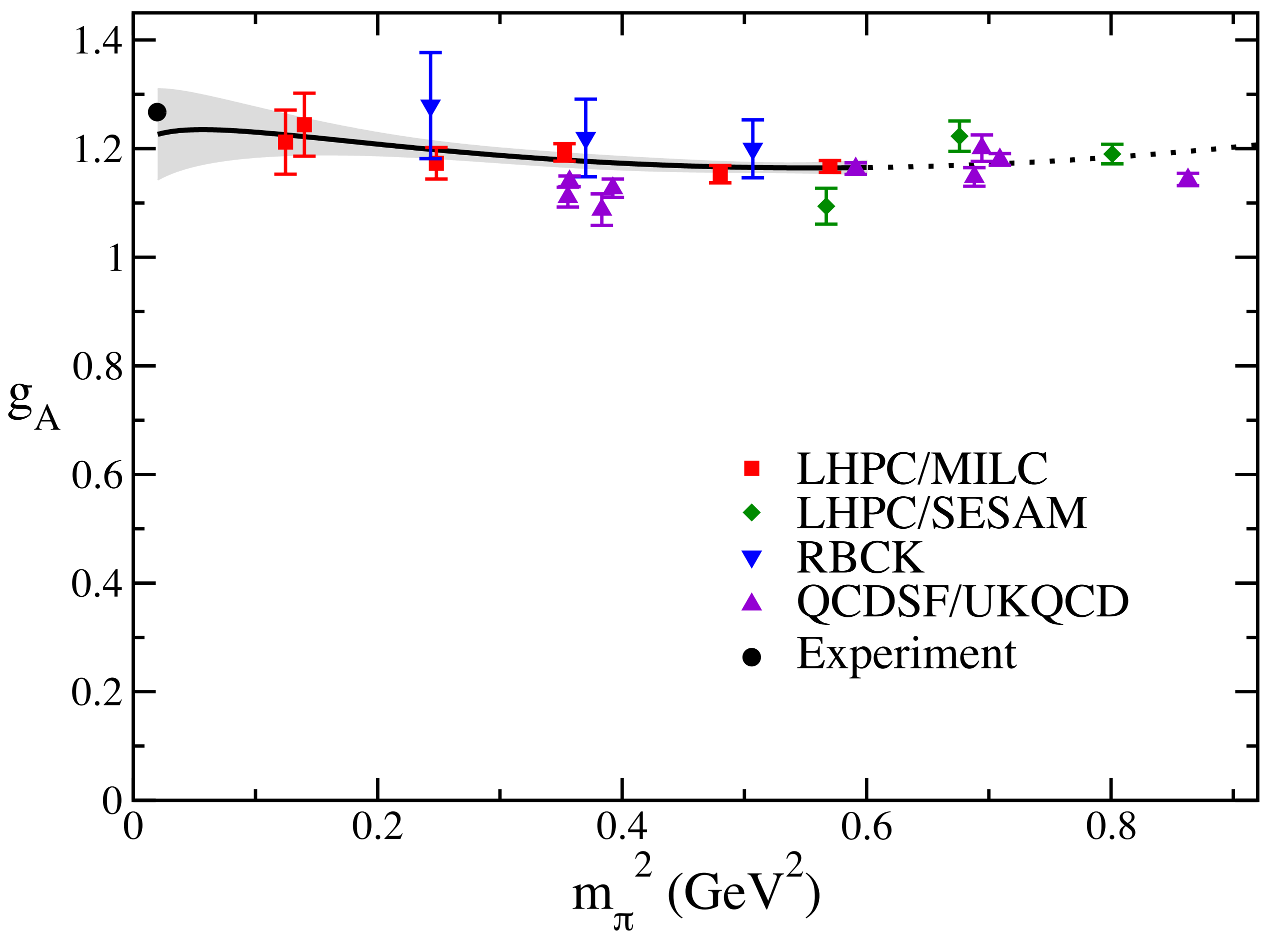
Fit 3 to this data

Extrapolate to physical m_π and L



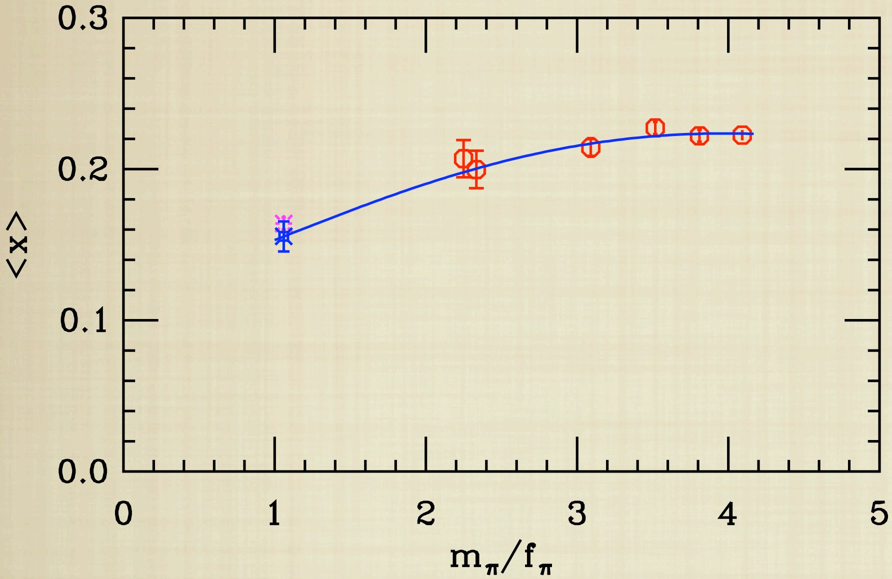
LHPC hep-lat/0510062

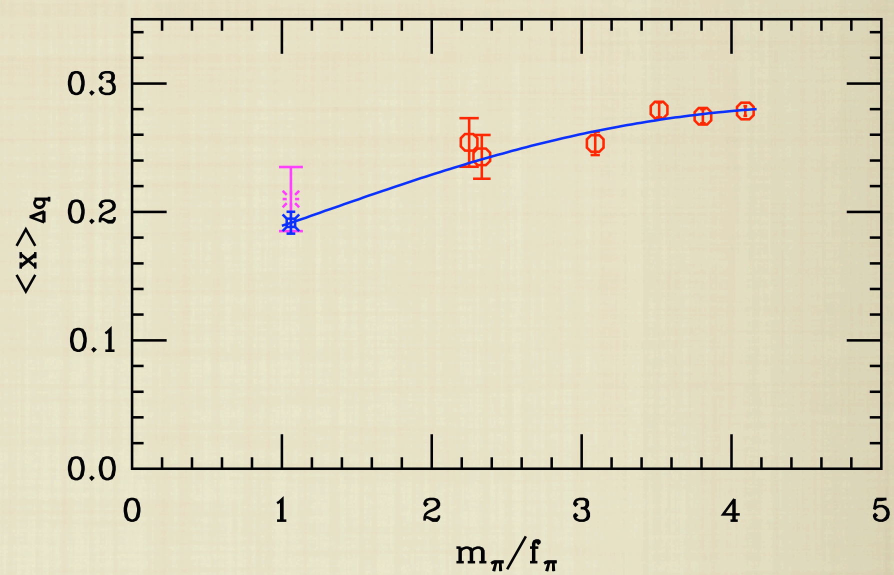
Nucleon axial charge g_A $\langle 1 \rangle_{\Delta q}^{u-d}$



LHPC hep-lat/0510062

Moments of structure functions



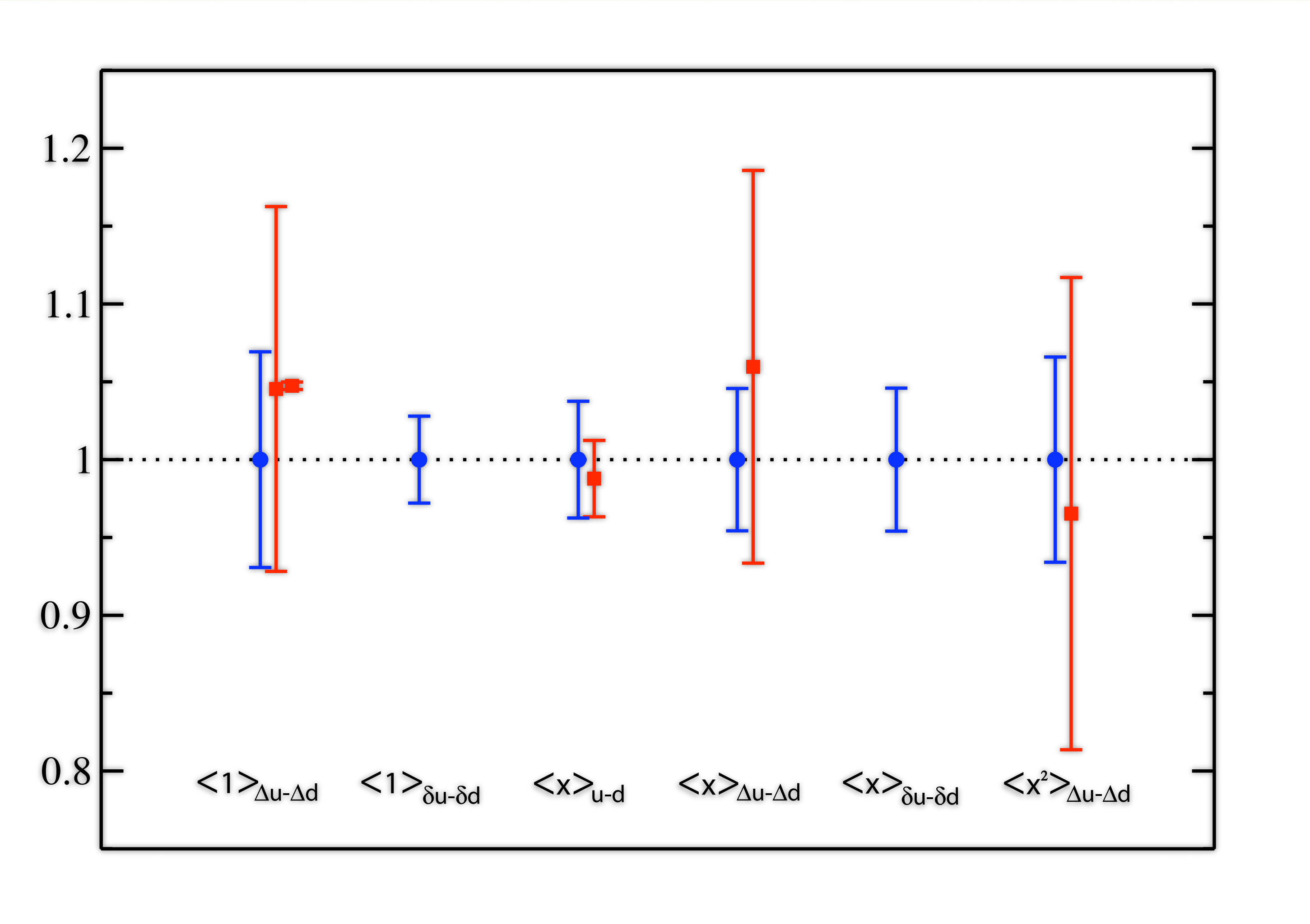


$$\langle x\rangle_{u-d} = a\left[1 - \frac{3g_A^2+1}{8\pi^2}\left(\frac{m_\pi^2}{f_\pi^2}\right)\ln\left(\frac{m_\pi^2}{f_\pi^2}\right)\right] + c\frac{m_\pi^2}{f_\pi^2}$$

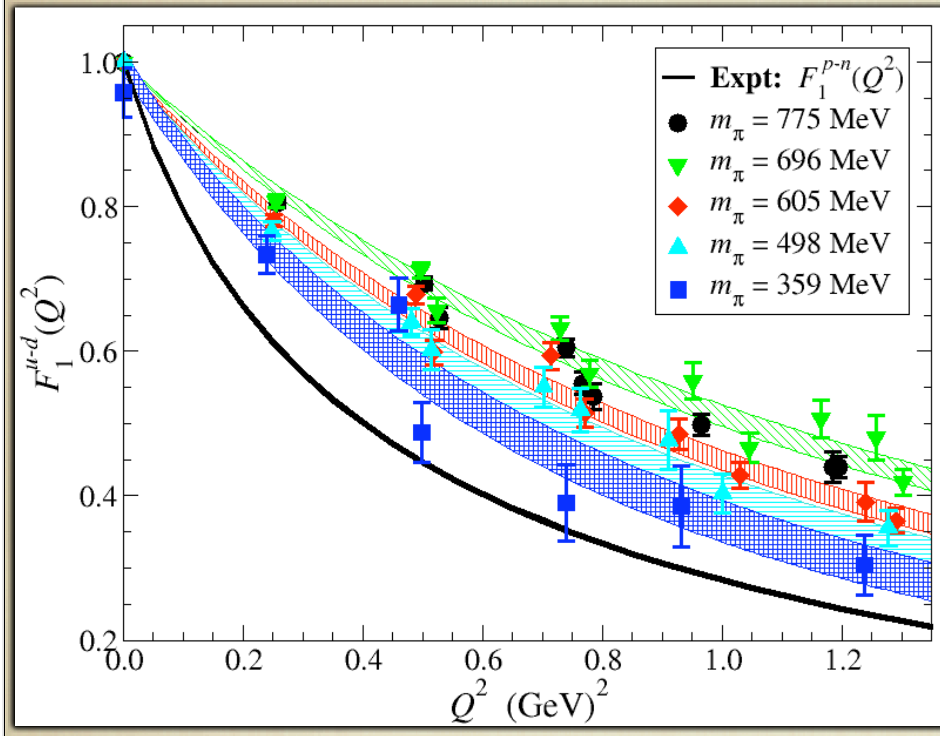
$$\langle x\rangle_{\Delta u-\Delta d} = a'\left[1 - \frac{2g_A^2+1}{8\pi^2}\left(\frac{m_\pi^2}{f_\pi^2}\right)\ln\left(\frac{m_\pi^2}{f_\pi^2}\right)\right] + c'\frac{m_\pi^2}{f_\pi^2}$$

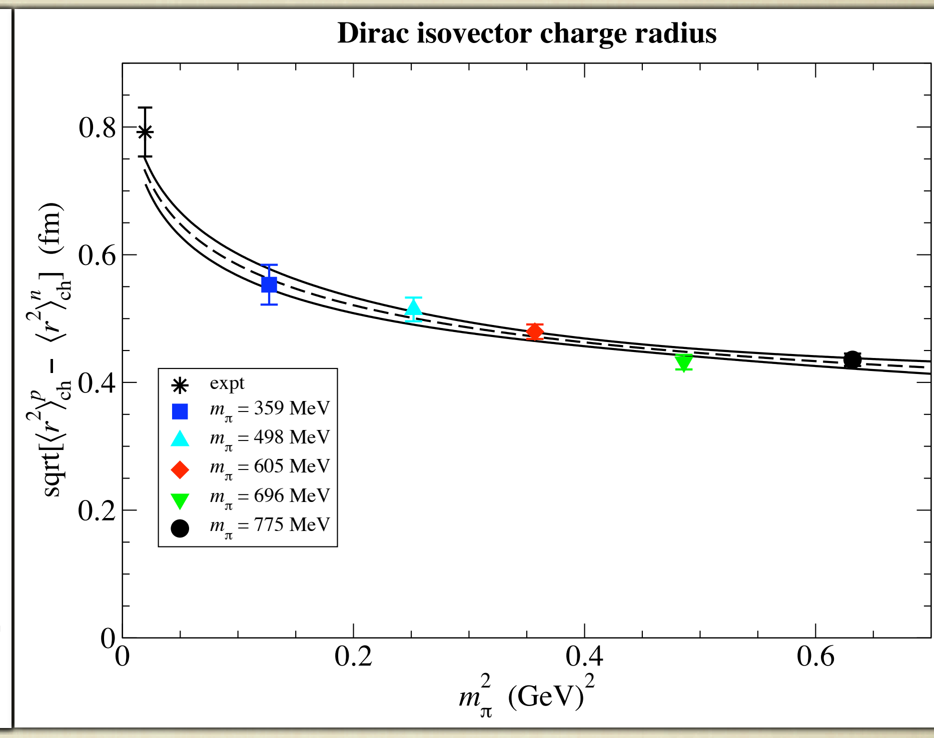
LHPC hep-lat/0607008

Chiral Extrapolation of Moments



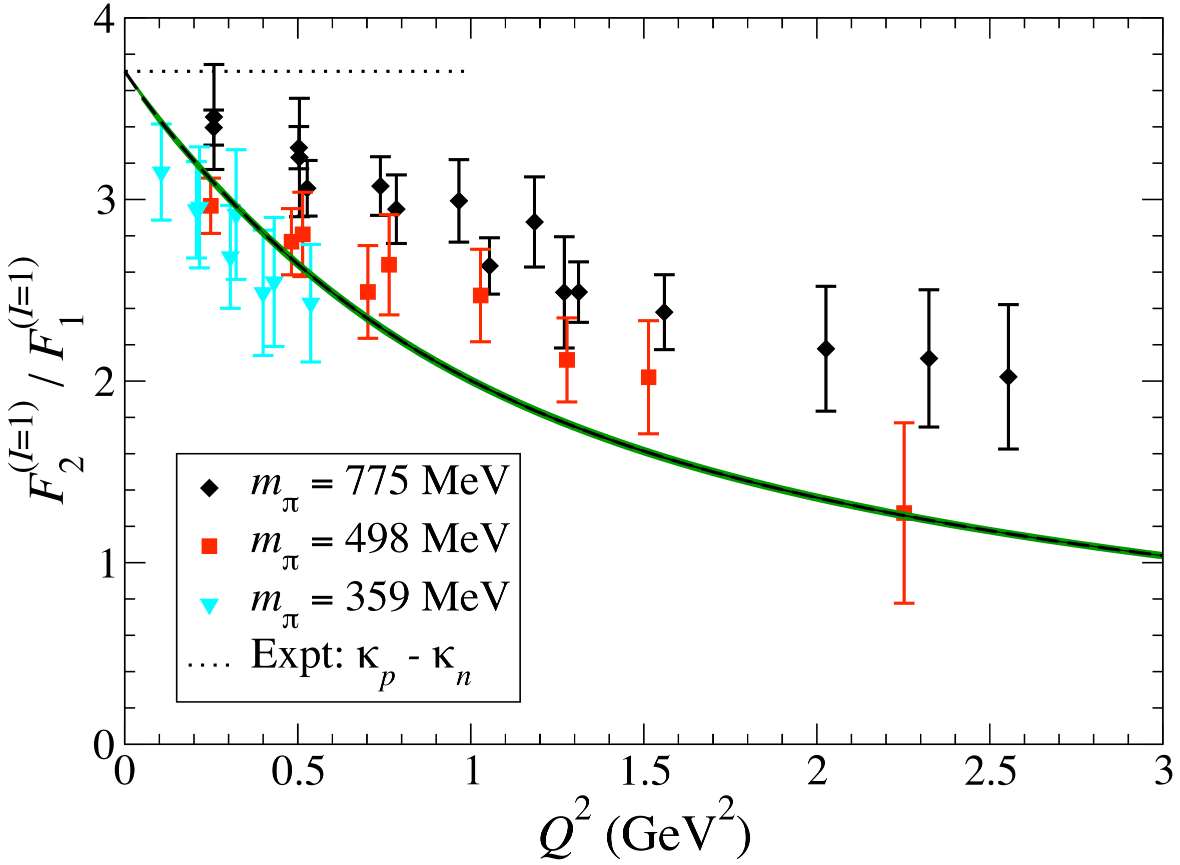
F_1 Isovector Form Factor





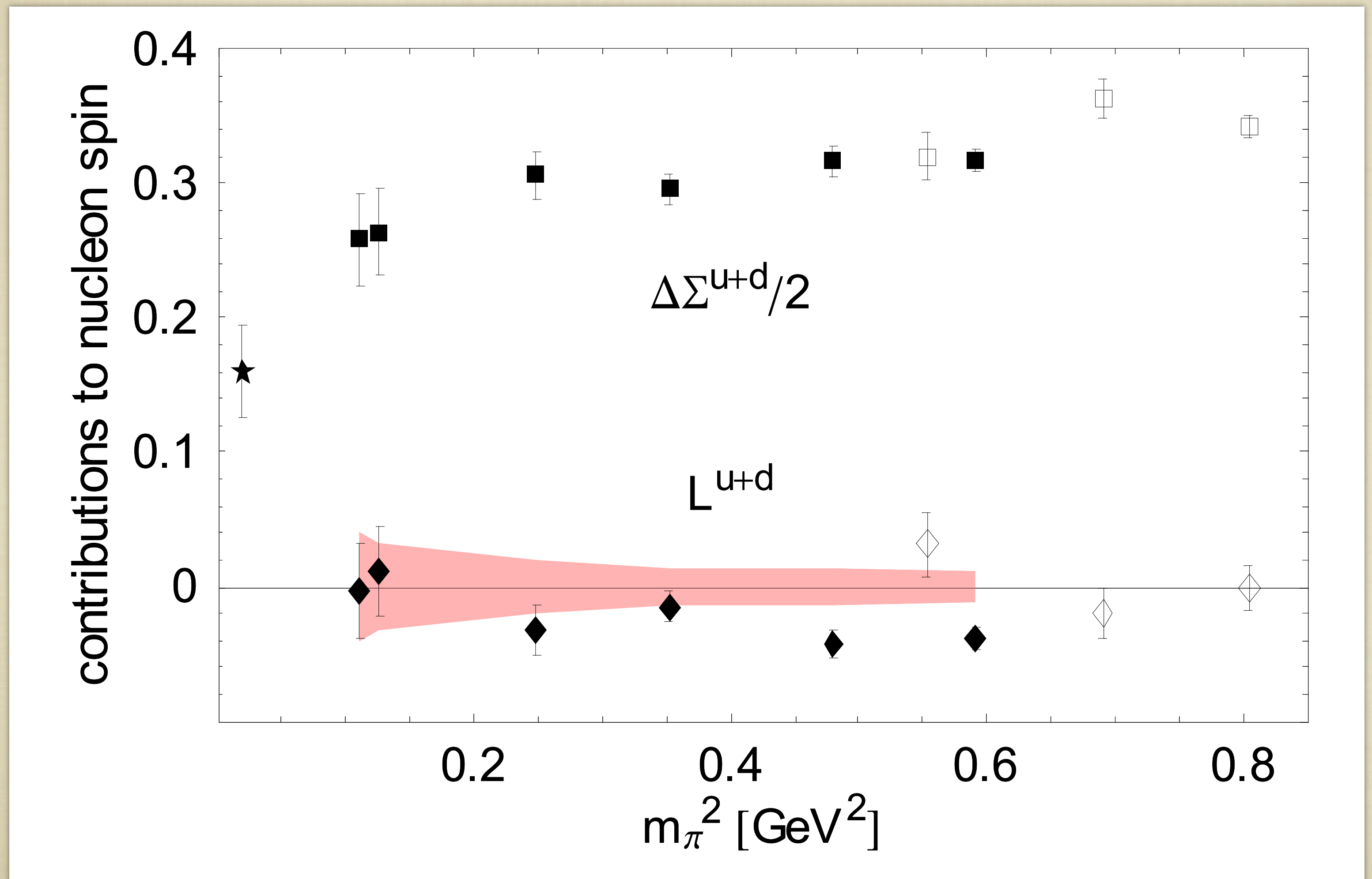
$$\langle r^2 \rangle^{u-d} = a_0 - \frac{(1+5g_A^2)}{(4\pi f_\pi)^2} \log\left(\frac{m_\pi^2}{m_\pi^2+\Lambda^2}\right)$$

Form factor ratio: F_2 / F_1



Nucleon spin decomposition

Connected contribution of quark spin and orbital angular momentum



Nucleon spin decomposition

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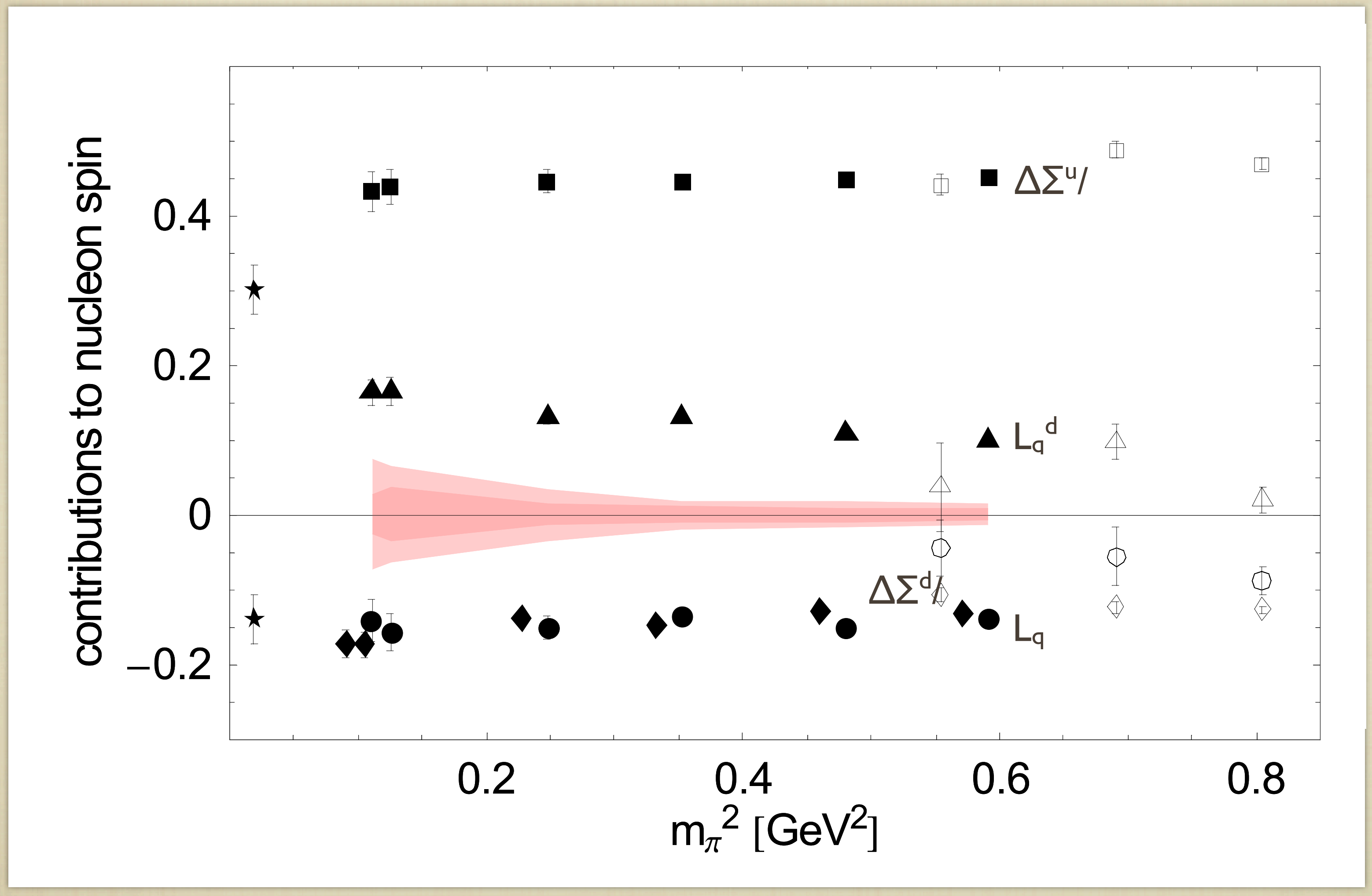
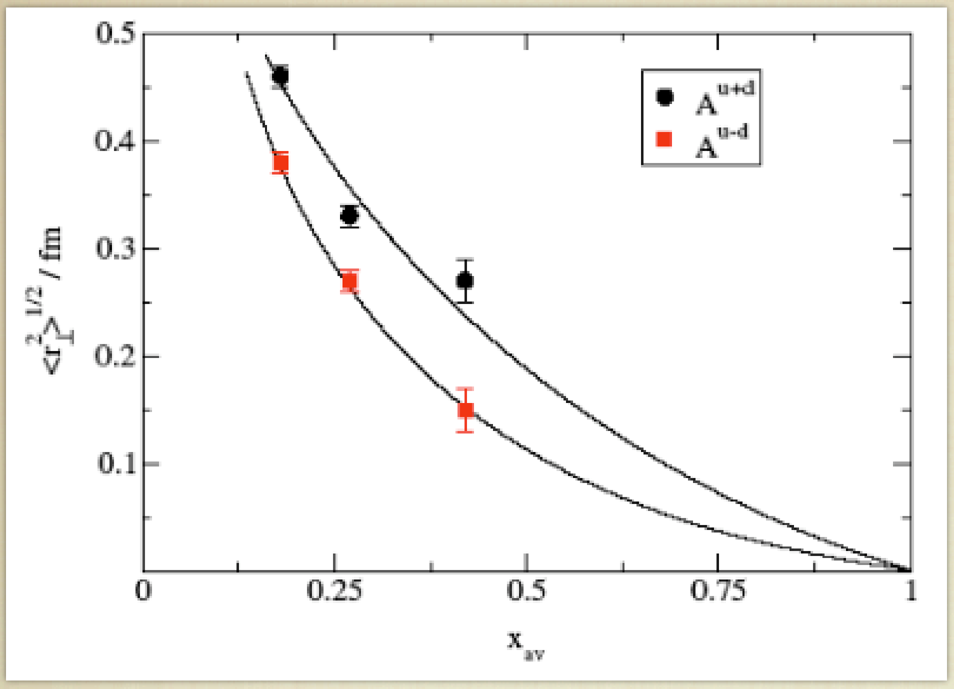
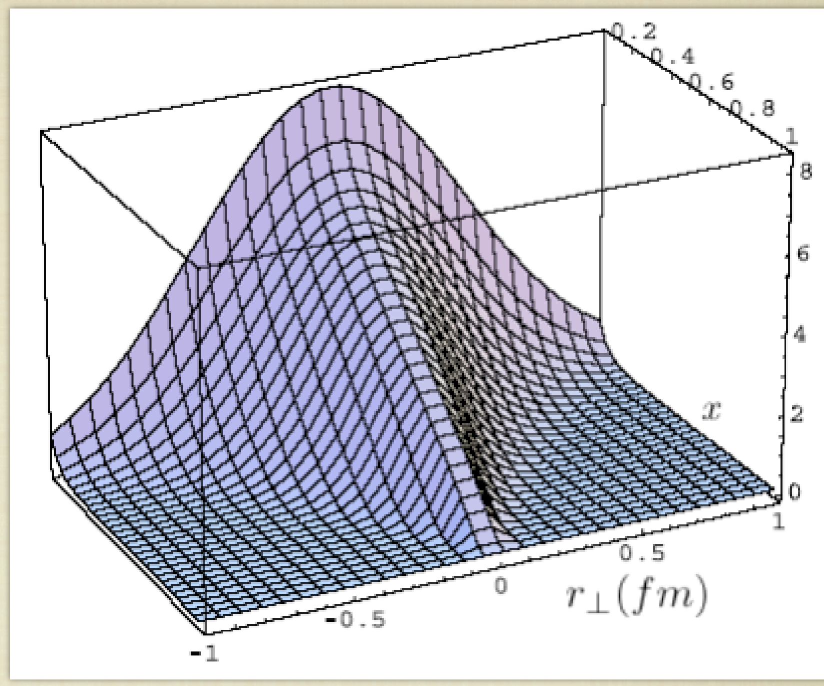


Transverse size of light-cone wave function

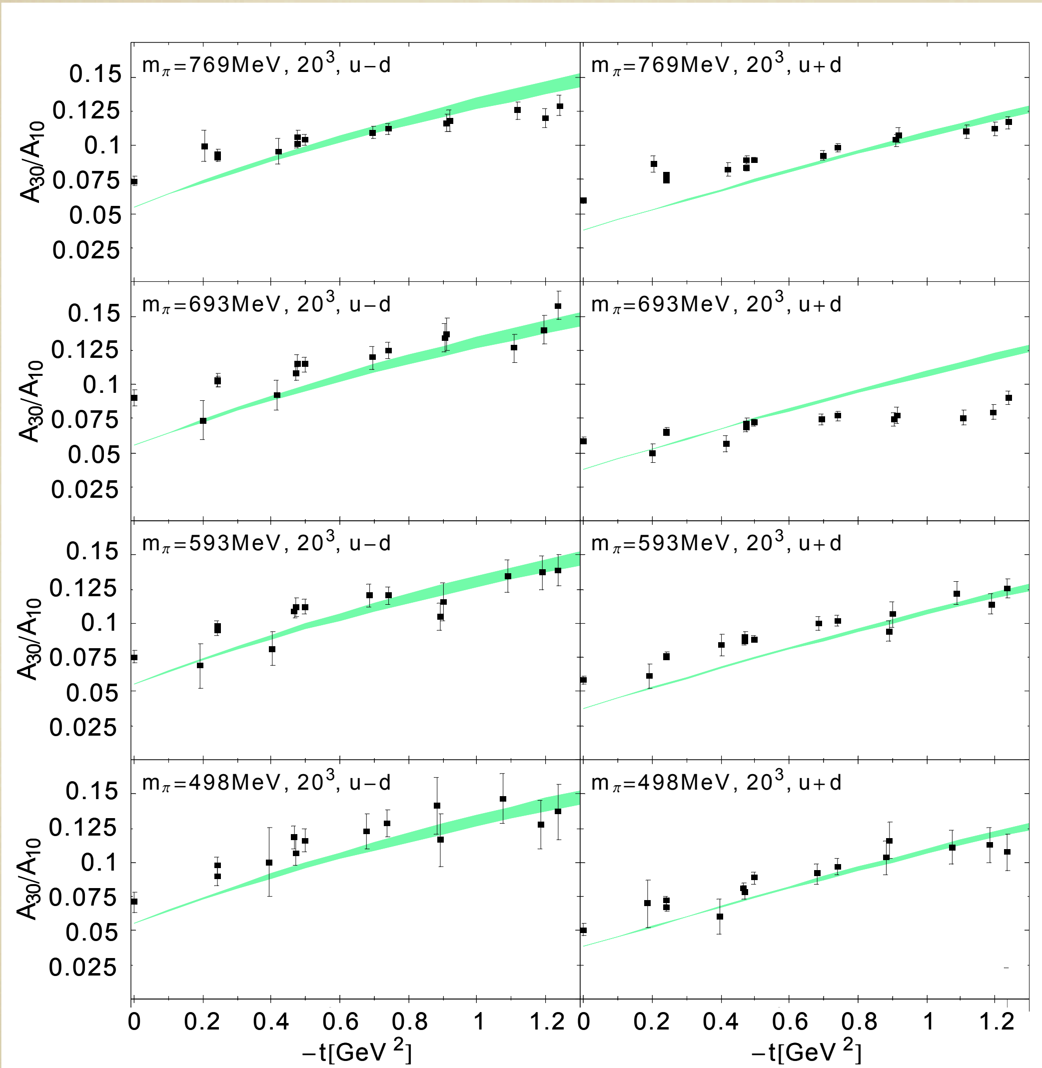




$$x_{\mathrm{av}}^n = \frac{\int d^2 r_\perp \int dx\, x \cdot x^{n-1} q(x, \vec{r}_\perp)}{\int d^2 r_\perp \int dx x^{n-1} q(x, \vec{r}_\perp)}$$

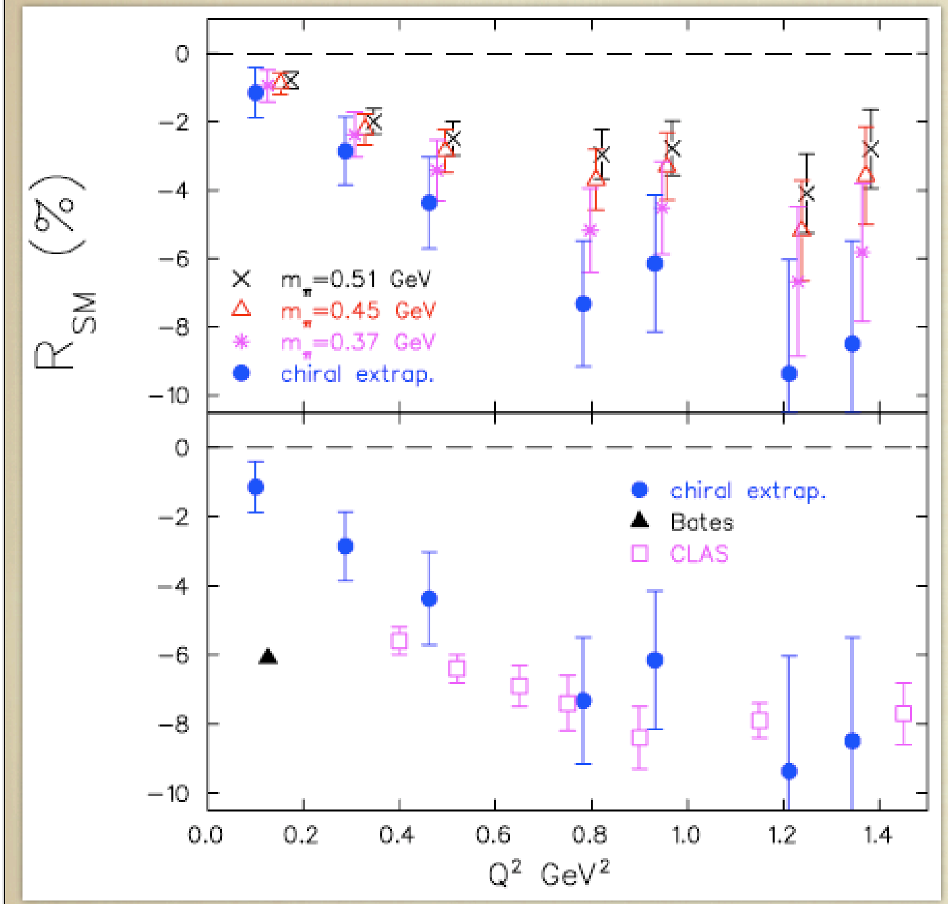
$q(x, \vec{r}_\perp)$ model (Burkardt hep-ph/0207047)

Comparison with Phenomenology

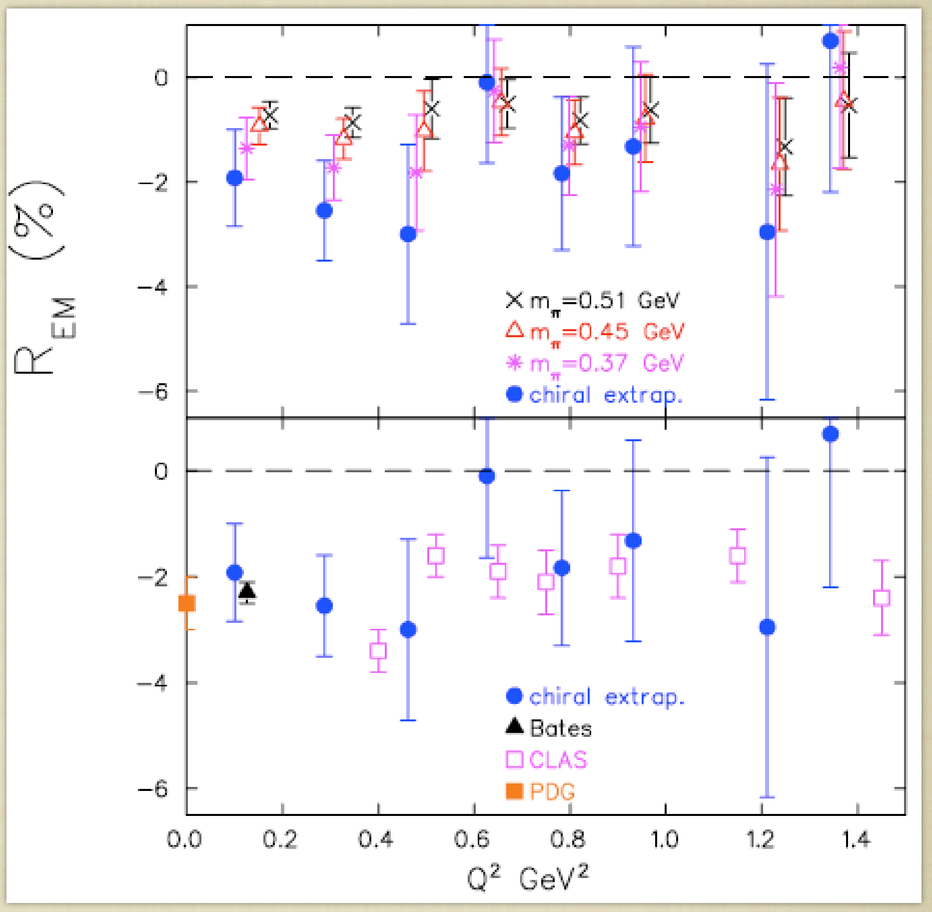


Diehl, Feldmann, Jakob, Kroll EPJC 2005

N-Delta transition form factor



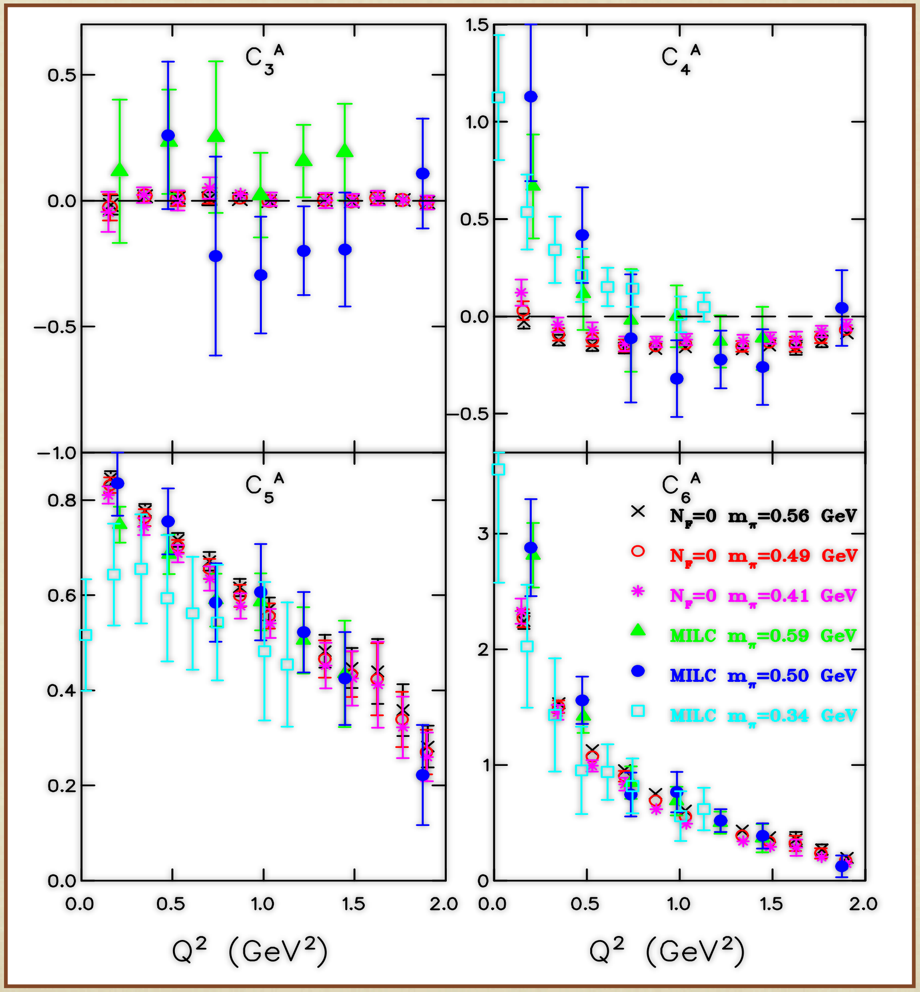
C2/M1



E2/M1

Axial N-Delta transition form factors

$$\langle\Delta(p',s')|A_\mu|N(p,s)\rangle \propto \bar{u}^\lambda(p',s')\left[\left(\frac{C_3^A(q^2)}{M}\gamma^\nu + \frac{C_4^A(q^2)}{M^2}p'^\nu\right)(g_{\lambda\mu}g_{\rho\nu} - g_{\lambda\rho}g_{\mu\nu})q^\rho + C_5^A(q^2)g_{\lambda\mu} + \frac{C_6^A(q^2)}{M^2}q_\lambda q_\mu\right]u(p,s)$$

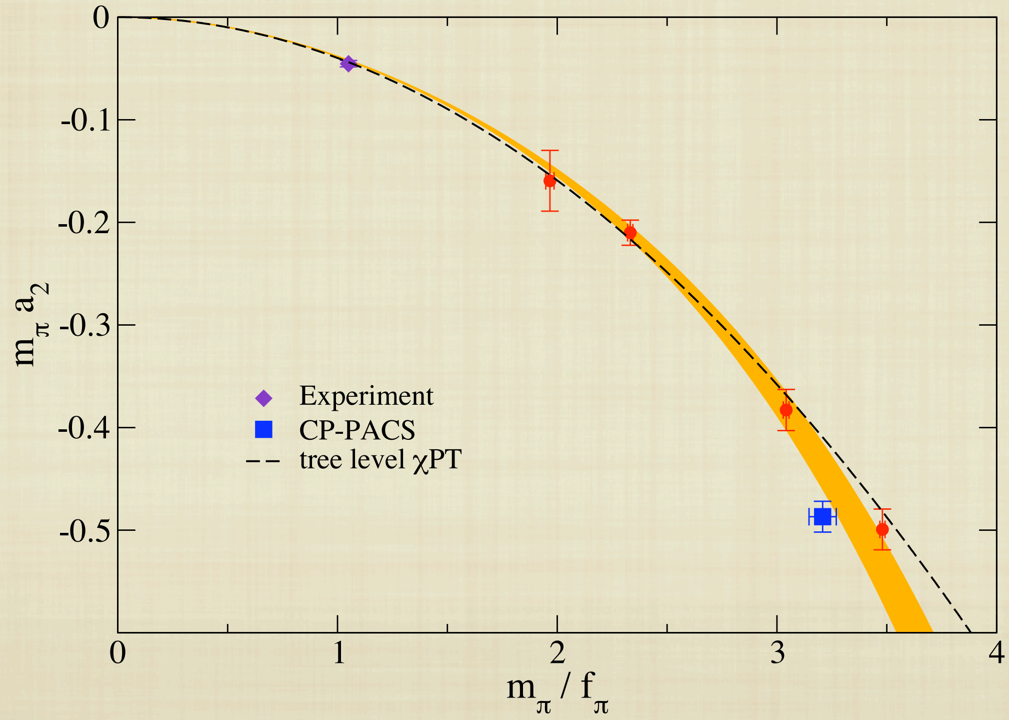


Alexandrou, Leontiou, Tsapalis, JN

I = 2 Pion scattering length

Calculate scattering length from energy variation with volume

Extrapolate with chiral perturbation theory

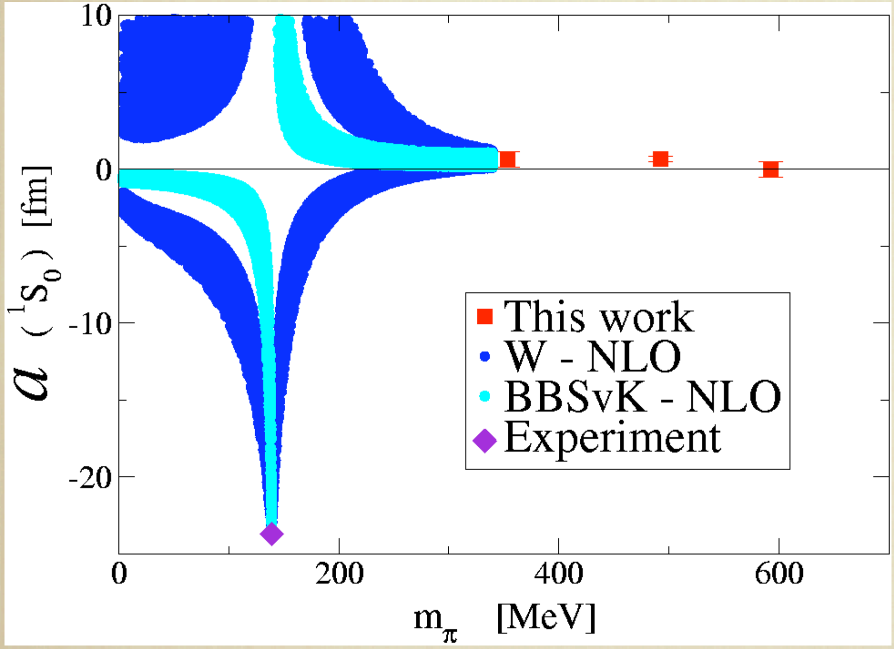


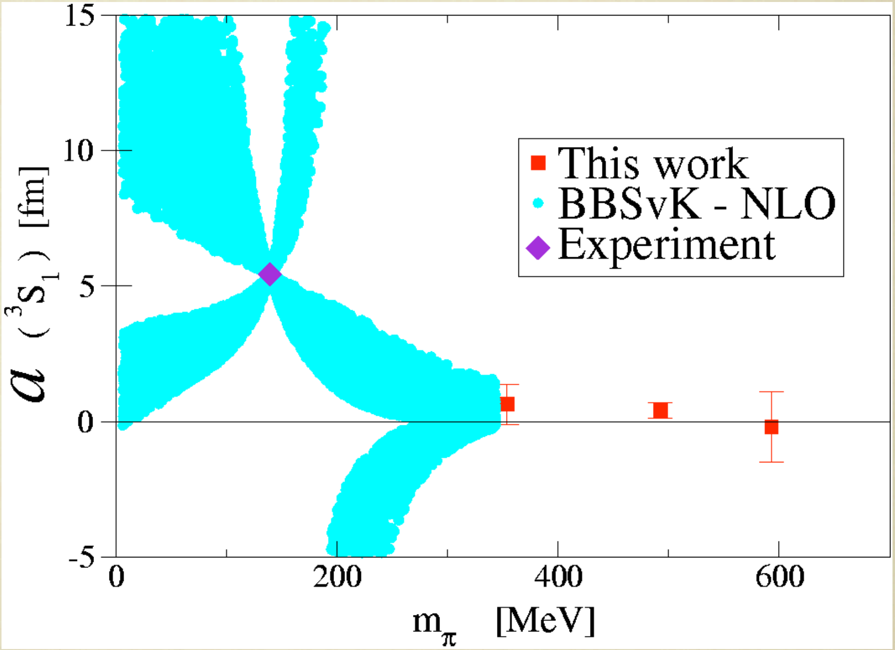
NPLQCD hep-lat/0506013

Nucleon-nucleon scattering length

Large N-N scattering length much more demanding

Requires calculation far closer to chiral limit





NPLQCD hep-lat/0602010

Opportunities and challenges

- Petascale resources will enable precision calculation of present thermodyanmic and structure observables
  - Chiral sea and valence fermions
  - Smaller lattice spacing - continuum limit
  - Larger lattice volume - infinite volume limit
  - Chiral regime: masses down to physical pion mass
  - Renormalization - higher loops and/or nonperturbative
- Nucleon scattering length
- Anisotropic lattices for extensive spectroscopy

New observables and theoretical issues

- Transport coefficients
- Disconnected diagrams
  - Flavor singlet matrix elements, strangeness form factors
- Gluon distributions
- Mixing of gluon and flavor singlet operators
- Operator mixing of higher moments of structure functions and generalized form factors
- Higher twist operators
- Neutron electric dipole moment - strong CP and theta angle
- Polarizabilities
- Changes between free and interacting nucleon
  - Example: difference between moments of structure functions of free n and p and of deuteron
- Observables in unstable states, eg, delta

Resources

- Computational resources
  - Big science: beyond scope of traditional theory resources
  - Sustained Petaflops in next 5 years
  - Partnership between NP, HEP, ASCR, SciDAC, NNSA
- Theorists
  - Innovative ideas crucial
  - Mastery of theoretical physics and computational science
  - As in all nuclear theory, need theory initiatives to attract and mentor the brightest and most creative theorists