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Lattice QCD from the Nuclear Physics Perspective

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SciDAC March 23 2004

GOAL: Understand the structure and interactions of hadrons and the properties of hadronic matter from first principles

- **Quantitative calculation of experimental observables**
- **Insight into how QCD works**

White Paper: Nuclear Physics with Lattice QCD
http://www-ctp.mit.edu/~negele/WhitePaper.pdf

Introduction

How do hadrons arise from QCD?

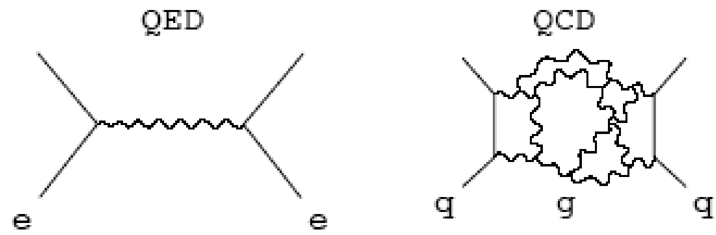
- **Lagrangian constrained by Lorentz invariance, gauge invariance and renormalizability:**

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4}F_{\mu\nu}^2$$

$$D_\mu = \partial_\mu - igA_\mu \qquad\qquad F_{\mu\nu} = \frac{i}{g}[D_\mu, D_\nu]$$

- **Deceptively simple Lagrangian produces amazingly rich and complex structure of strongly interacting matter in our universe**

Nonperturbative QCD



- Fundamental differences relative to QED

  Self-interacting – highly nonlinear

  Interaction increases at large distance – Confinement

  Interaction decreases at short distance – Asymptotic freedom

  Strong coupling $\alpha_s \gg \alpha_{em}$

  Rich topological structure

- Solution of QCD

  Present analytical techniques inadequate

  Numerical evaluation of path integral on space-time lattice

Profound differences between hadrons and other many-body systems

- Atoms, molecules, solids, nuclei, . . .
  - Constituents can be removed
  - Exchanged boson generating interaction may be subsumed into static potential

    Photons $\longrightarrow$ Coulomb potential

    Mesons $\longrightarrow$ N-N potential
  - Most of mass from fermion constituents
- Nucleons
  - Quarks are confined
  - Gluons are essential degrees of freedom

    Carry half of momentum

    Nonpeturbative topological excitations
  - Most of mass generated by interactions

Basic Ideas in Lattice QCD

- **Evolution in Euclidean time**

$$|\psi\rangle \equiv e^{-\beta H}|\phi\rangle = \sum_n e^{-\beta E_n} c_n |\psi_n\rangle \to c_0 e^{-\beta E_0}|\psi_0\rangle$$

- **Lattice Regularization**

$$\phi(x) \to \phi(x_n) \quad , \qquad x_n = na$$

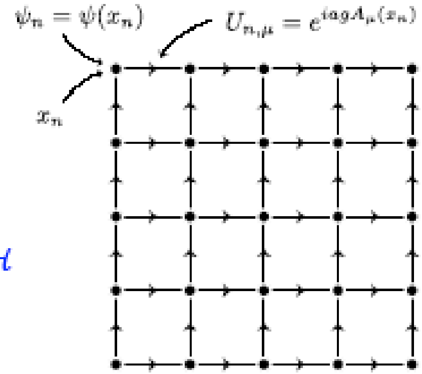
- **Path Integral**

$$e^{-\beta \hat{H}} \to \int \mathcal{D}\left(x(\tau)\right) \, e^{-\int_0^\beta d\tau \, S(x(\tau))}$$

- **Stochastic solution**

$$\int dx \, f(x) P(x) = \frac{1}{N} \sum_{x_i \in P} f(x_i) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

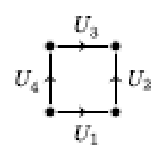
Lattice QCD



Euclidean:

$$e^{i\int dt\, d^3x\, \mathcal{L}} \to e^{-\int d\tau\, d^3x\, \mathcal{H}}$$

$$\begin{aligned}
&\langle T\, e^{-\beta H} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \rangle \\
&= \frac{1}{Z} \int \mathcal{D}[\psi]\mathcal{D}[\bar{\psi}]\mathcal{D}[A] e^{-\int d^4x \left[\bar{\psi}(\partial\!\!\!/ + m + igA\!\!\!/)\psi + \frac{1}{4}F_{\mu\nu}^2\right]} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \\
&\to \prod_n \frac{1}{Z} \int d\psi_n\, d\bar{\psi}_n\, dU_n e^{-\sum\limits_n \left[\bar{\psi} M(U)\psi + S(U)\right]} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \\
&= \prod_n \int dU_n \underbrace{\frac{1}{Z} \det M(U) e^{-S(U)}}_{\text{Sample with M.C.}} \sum M^{-1}(U) M^{-1}(U) \cdots M^{-1}(U) \\
&\to \frac{1}{N} \sum_{\substack{i=1 \\ U_i \in \frac{\det M(U)}{Z} e^{-S(U)}}}^{N} M^{-1}(U_i) M^{-1}(U_i) M^{-1}(U_i)
\end{aligned}$$



$$S(U) = \sum_{\square} \frac{2N}{g^2}\left(1 - N^{-1}\mathrm{ReTr} U_\square\right) \to \tfrac{1}{4}F_{\mu\nu}^2 \qquad U_\square \equiv U_1 U_2 U_3^\dagger U_4^\dagger$$

$$\bar{\psi} M(U)\psi = \sum_n \left[\bar{\psi}_n \psi_n + \kappa(\bar{\psi}_n (1-\gamma_\mu) U_{n,\mu} \psi_{n+\mu} + \bar{\psi}_{n+\mu}(1+\gamma_\mu) U_{n,\mu}^\dagger \psi_n\right]$$

Observables

$$\left\langle T\, e^{-\beta H} \hat{\bar{\psi}}\hat{\bar{\psi}}\hat{\bar{\psi}} \ldots \hat{\psi}\hat{\psi}\hat{\psi} \right\rangle$$

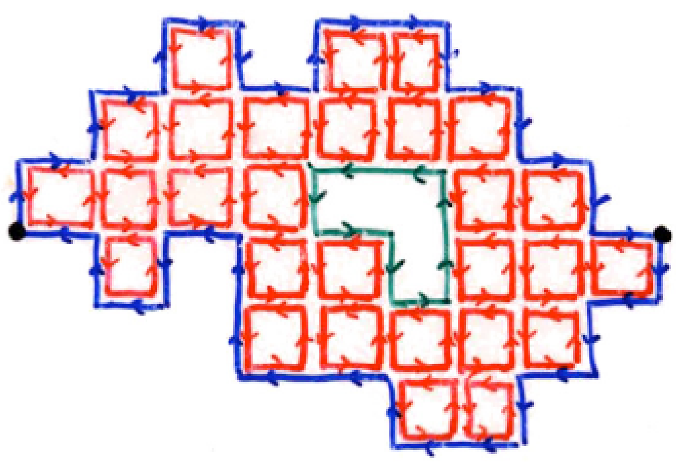
$$= Z^{-1} \int \mathcal{D}(U)\mathcal{D}(\bar{\psi}\psi) e^{-\bar{\psi}M(U)\psi - S(U)} \bar{\psi}\bar{\psi}\bar{\psi}\ldots\psi\psi\psi$$

$$= Z^{-1} \int \mathcal{D}(U) e^{\underbrace{\ln \det M(U)}_{2} - \underbrace{S(U)}_{3}} \sum \underbrace{M^{-1}(U) M^{-1}(U) \ldots M^{-1}(U)}_{1}$$

1. $M^{-1} = (1 + \kappa U)^{-1}$ connects $\bar{\psi}$ and ψ with line of U's
   → Sum over all valence quark paths.

2. $\ln \det M$ generates closed loops of U's
   → Sum over all $\bar{q}q$ excitations from sea
   omit in quenched approximation

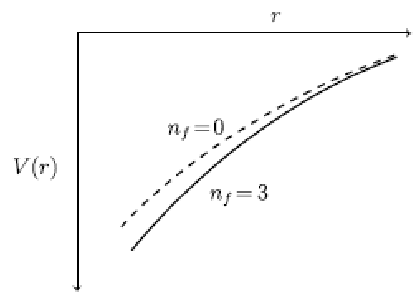
3. $S(U)$ tiles with plaquettes
   → sum all gluons



$32^3 \times 64$ lattice $\Longrightarrow$ 10^8 gluon variables

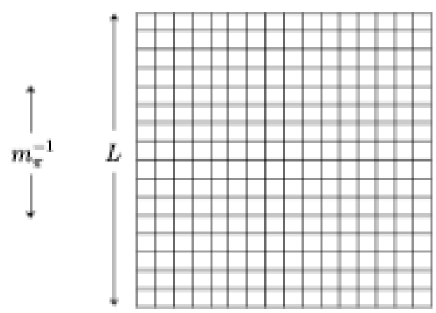
Computational Issues

- Fermion determinant - Full QCD
- Lattice spacing small
- Quark mass small
- Lattice volume large



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

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



Cost ≈ $(m_q)^{-4.5}$ ≈ $(m_\pi)^{-9}$

Current Status

- Include Fermion determinant - Full QCD
- $(m_\pi)^{-9}$ limits calculations to "heavy pion world"
  - Develop physics methodology
  - Understand dependence on quark mass
- Terascale resources required for physical regime

Three Areas of QCD Physics

Lattice calculations essential to understanding physics in each case

- **Heavy Quark Systems**

  Confirm standard model or elucidate physics beyond it

- **QCD Thermodynamics**

  Properties of hadronic matter under extreme conditions

  Foundation for RHIC physics → LHC

- **Hadron Structure**

  Quark and gluon structure of hadrons

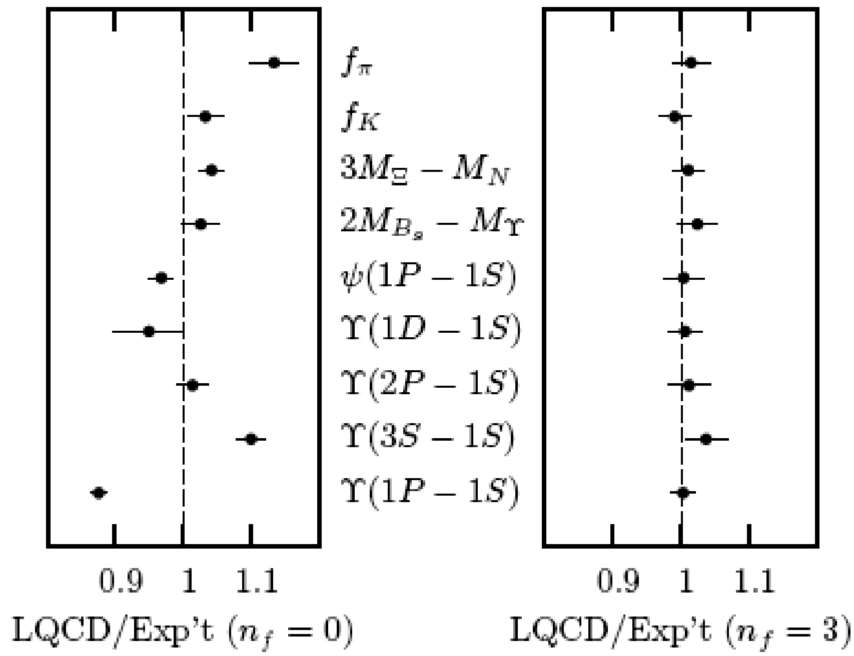
  Spectroscopy

  Hadron-hadron interactions

  Crucial to understand physics from Bates, Jlab, SLAC, Fermilab and RHIC-spin

Precision Agreement in Full QCD

- **Gold-Plated Observables** Davies et al, hep-lat/0304004



Staggered quarks

Asqtad improved action

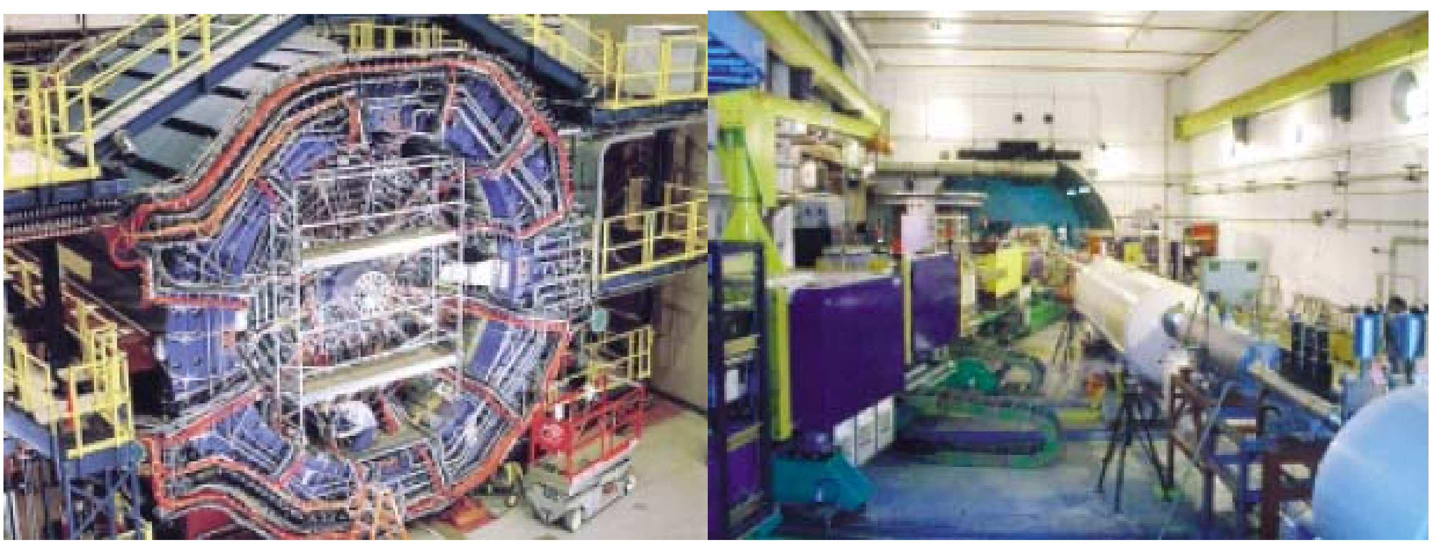
a = 0.13, 0.09 fm

Errors $\sim$ 3%

Gold-plated processes for 8/9 CKM elements

Impact on DOE Nuclear Physics Program

RHIC at BNL



STAR and PHENIX detectors

Impact on DOE Nuclear Physics Program

CEBAF
at
JLab

SOS and HMS spectrometers

Hadron Structure

- Form factors

  G_E , G_M Jlab

  Strangeness FF   Sample, Happex

- Transition form factors

  $N \rightarrow \Delta$ - deformation   Bates, JLab

- Parton Distributions   RHIC spin, Hermes …

  Quark distributions $\langle x \rangle_q$

  Spin distribution - spin crisis $\Delta\Sigma \sim \langle 1 \rangle_{\Delta q}$

  Transversity distribution $\langle 1 \rangle_{\delta q}$

- Generalized Parton Distributions   Jlab

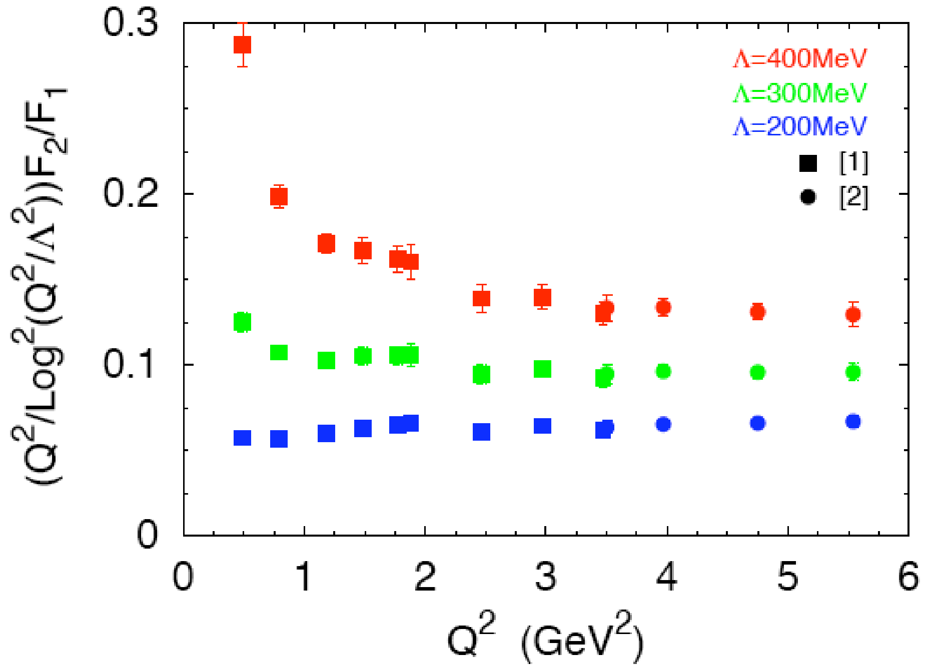
  Total quark angular momentum   J

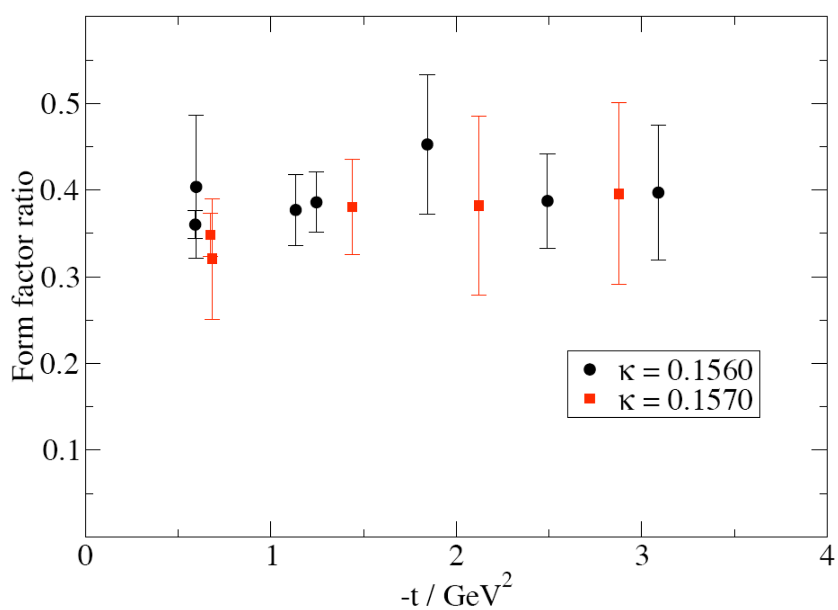
  Transverse structure of nucleon

  Transverse size $\rightarrow 0$ as $x \rightarrow 1$

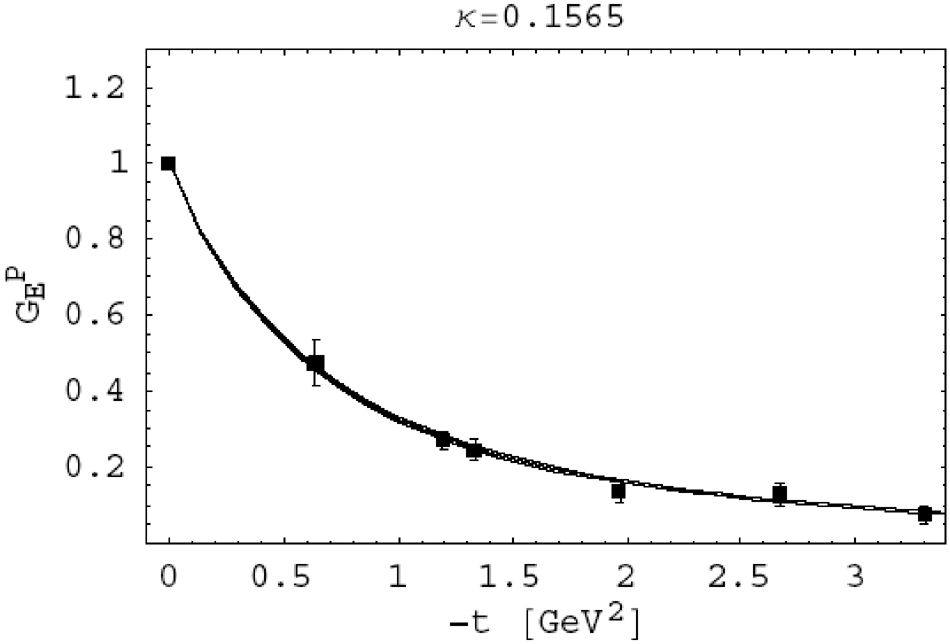
Electromagnetic Form Factors

$$\frac{Q^2 F_2(Q^2)}{\log^2(Q^2/\Lambda^2) F_1(Q^2)} \sim \text{const.}$$

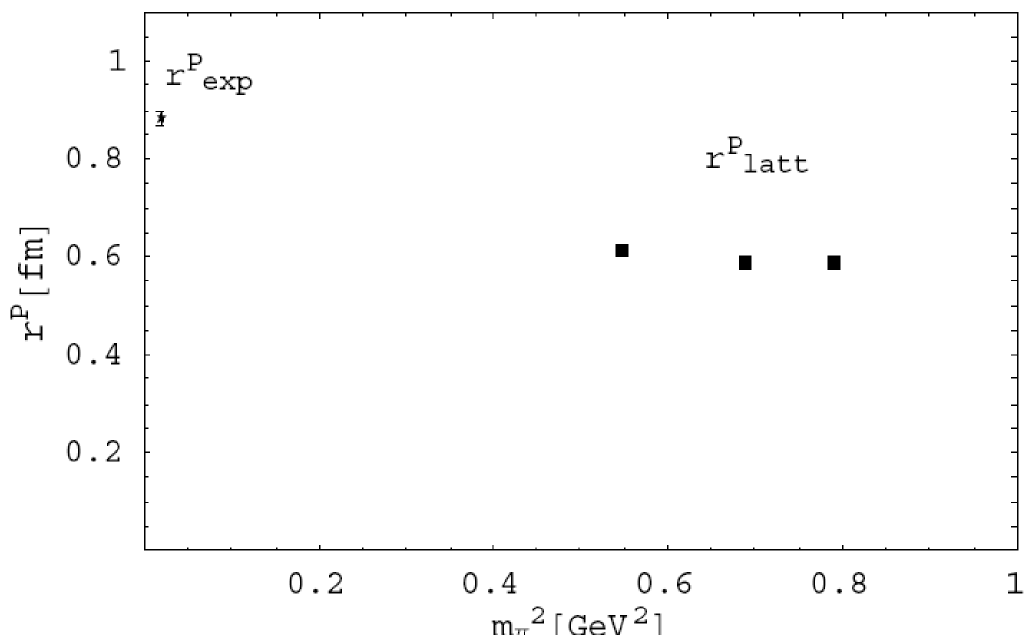




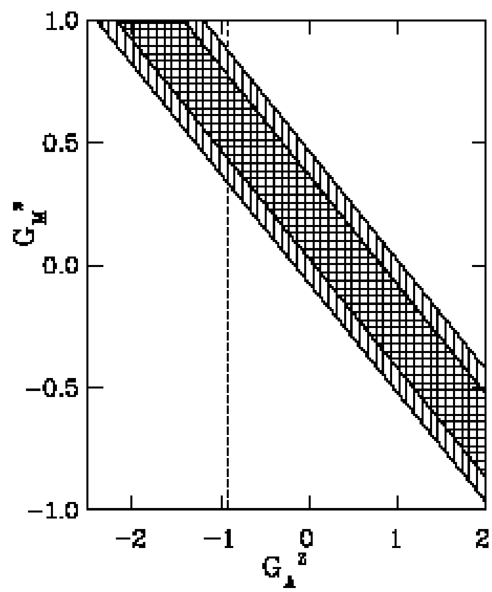
RMS Charge Radius



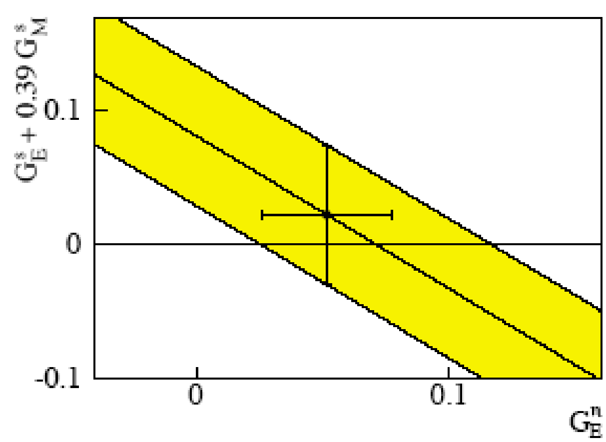
κ	0.1570	0.1565	0.1560
rms[fm]	0.61 ± 0.01	0.59 ± 0.01	0.59 ± 0.01



Strangeness Form Factors from Parity-Violating Electron Scattering



SAMPLE (Bates)



HAPPEX (Jlab)

Nucleon-Delta Transition Form Factor

- **Calculate transition amplitudes**

  M1 dominates

  C2 and E2 vanish if nucleon and delta spherical

- **Lattice calculations**

hep-lat/030007018 Alexandrou, Tsapalis, J.N et. al.

M1/E2 expt

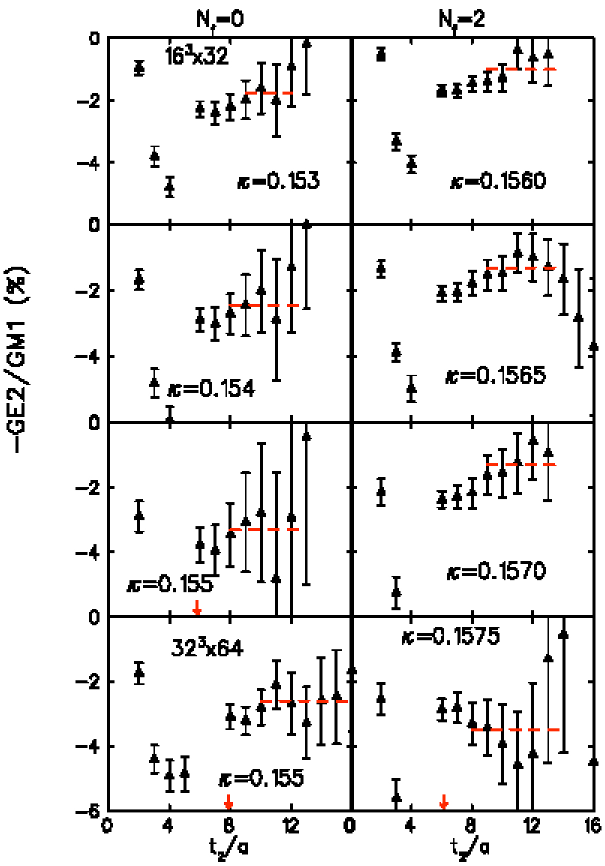
= -1.6 (.4)

Quenched

= -4.8 (1.1)

Full QCD

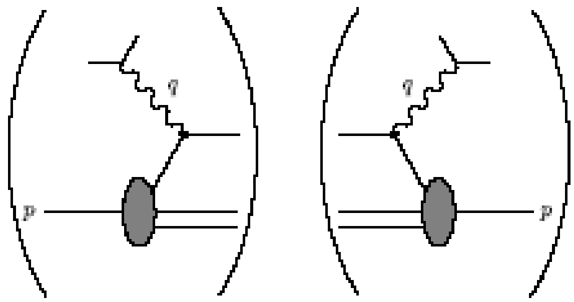
= -3.5 (1.2)



High Energy Scattering Experiments

- Measure matrix elements of quark operators
  $\mathcal{O}^{\mu_1\cdots\mu_n} = \psi\gamma^{\{\mu_1}iD^{\mu_2}\dots iD^{\mu_n\}}\psi$

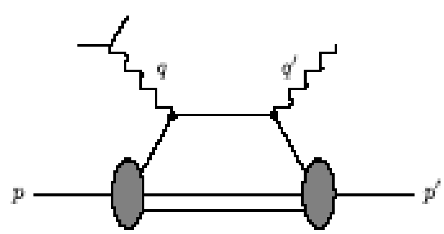
- Deep inelastic scattering



Forward M.E. $\longrightarrow$ moments of quark distribution

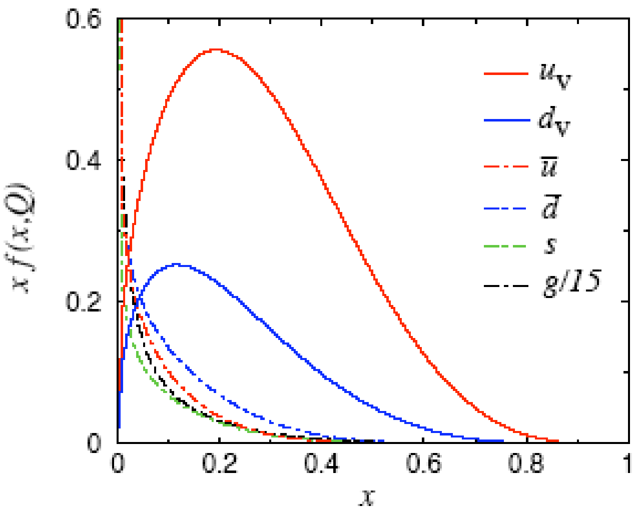
$$\langle p|\mathcal{O}^{\mu_1\cdots\mu_n}|p\rangle \sim \int dx x^{n-1} q(x) p^{\{\mu_1}\dots p^{\mu_n\}}$$

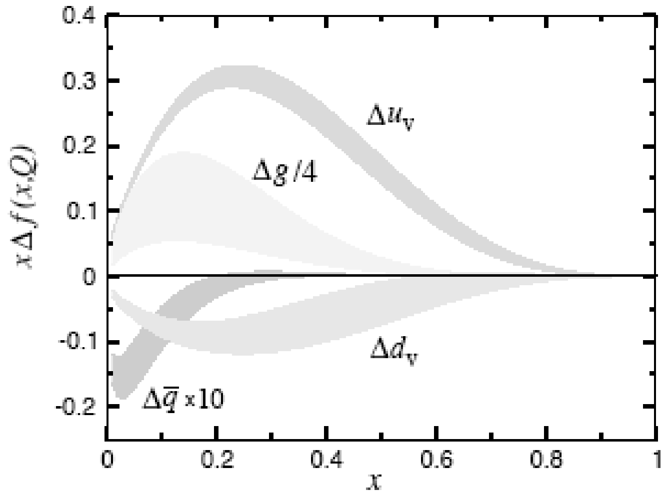
- Deeply virtual Compton scattering



$\langle p|\mathcal{O}^{\mu_1\cdots\mu_n}|p'\rangle$

Forward Matrix Elements





Parton distributions at Q = 5 GeV

Moments of parton distributions

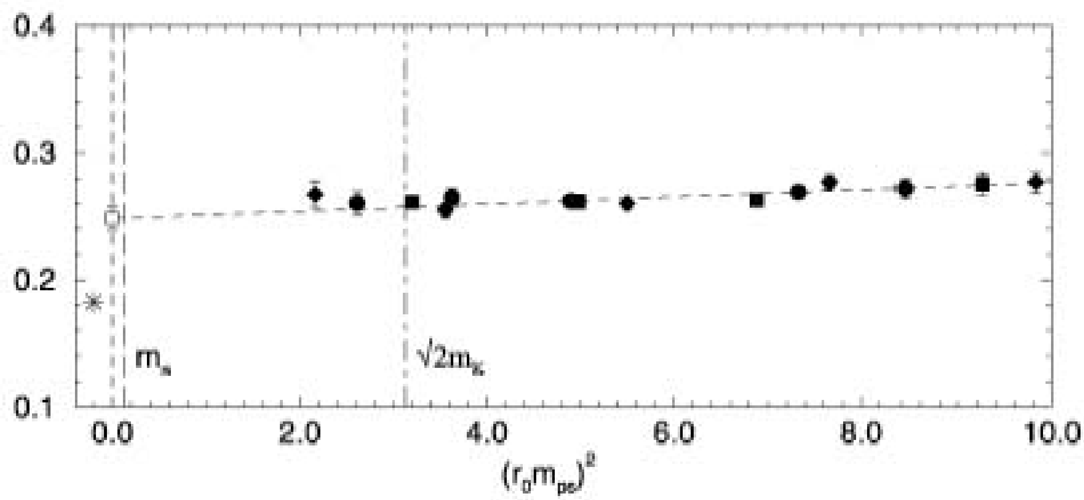
$$\langle p|\bar{\psi}\gamma_\mu D_{\mu_1}\cdots D_{\mu_n}\psi|p\rangle \rightarrow \langle x^n\rangle_q$$

$$\langle p|\bar{\psi}\gamma_5\gamma_\mu D_{\mu_1}\cdots D_{\mu_n}\psi|p\rangle \rightarrow \langle x^n\rangle_{\Delta q}$$

$$\langle p|\bar{\psi}\gamma_5\sigma_{\mu\nu} D_{\mu_1}\cdots D_{\mu_n}\psi|p\rangle \rightarrow \langle x^n\rangle_{\delta q}$$

Momentum Fraction <x>

$\langle x \rangle$ quenched improved Wilson - QCDSF



Chiral Perturbation Theory

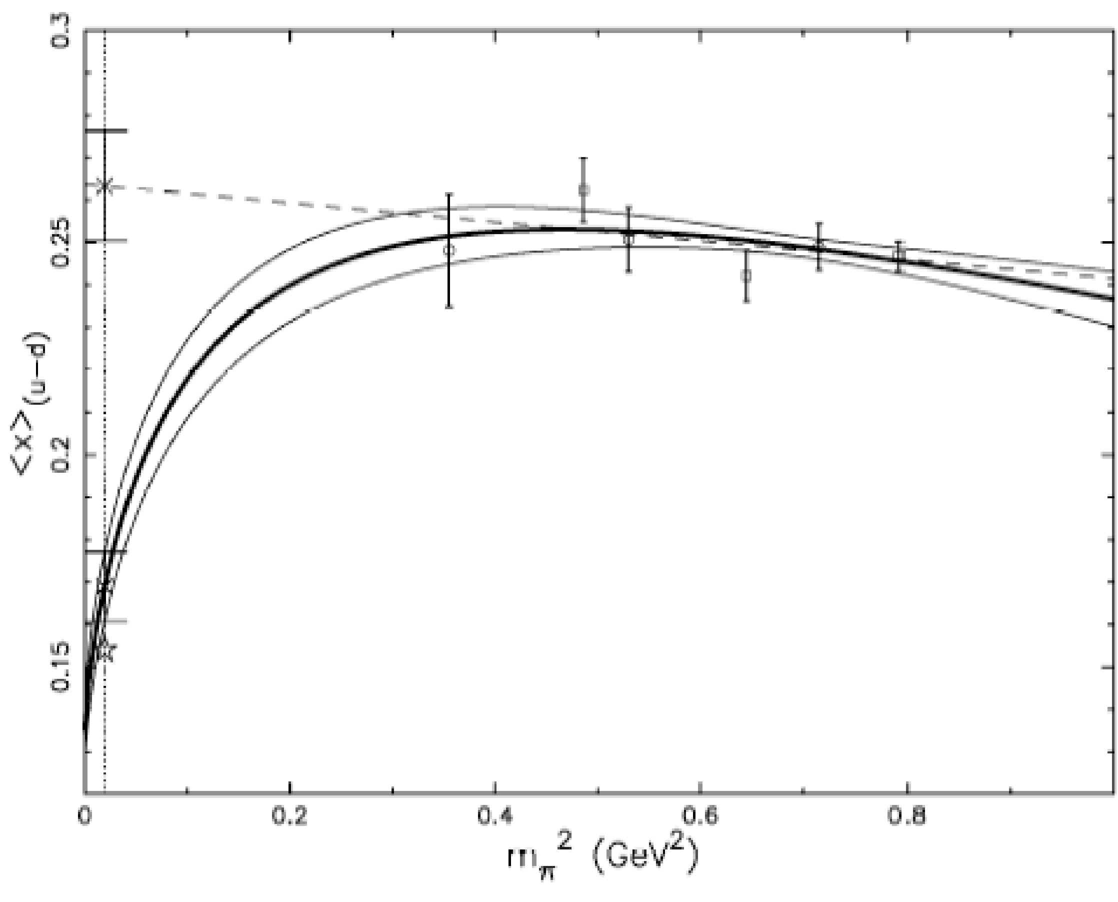
Heavy baryon chiral perturbation theory for nucleon parton distributions

Chen & Ji, Arndt & Savage, Chen & Savage

$$\langle x^n \rangle_u - \langle x^n \rangle_d \sim a_n \left[1 - \frac{(3{g_A}^2+1)m_\pi^2}{(4\pi f_\pi)^2} \ln(m_\pi^2) \right] + \text{analytic terms}$$

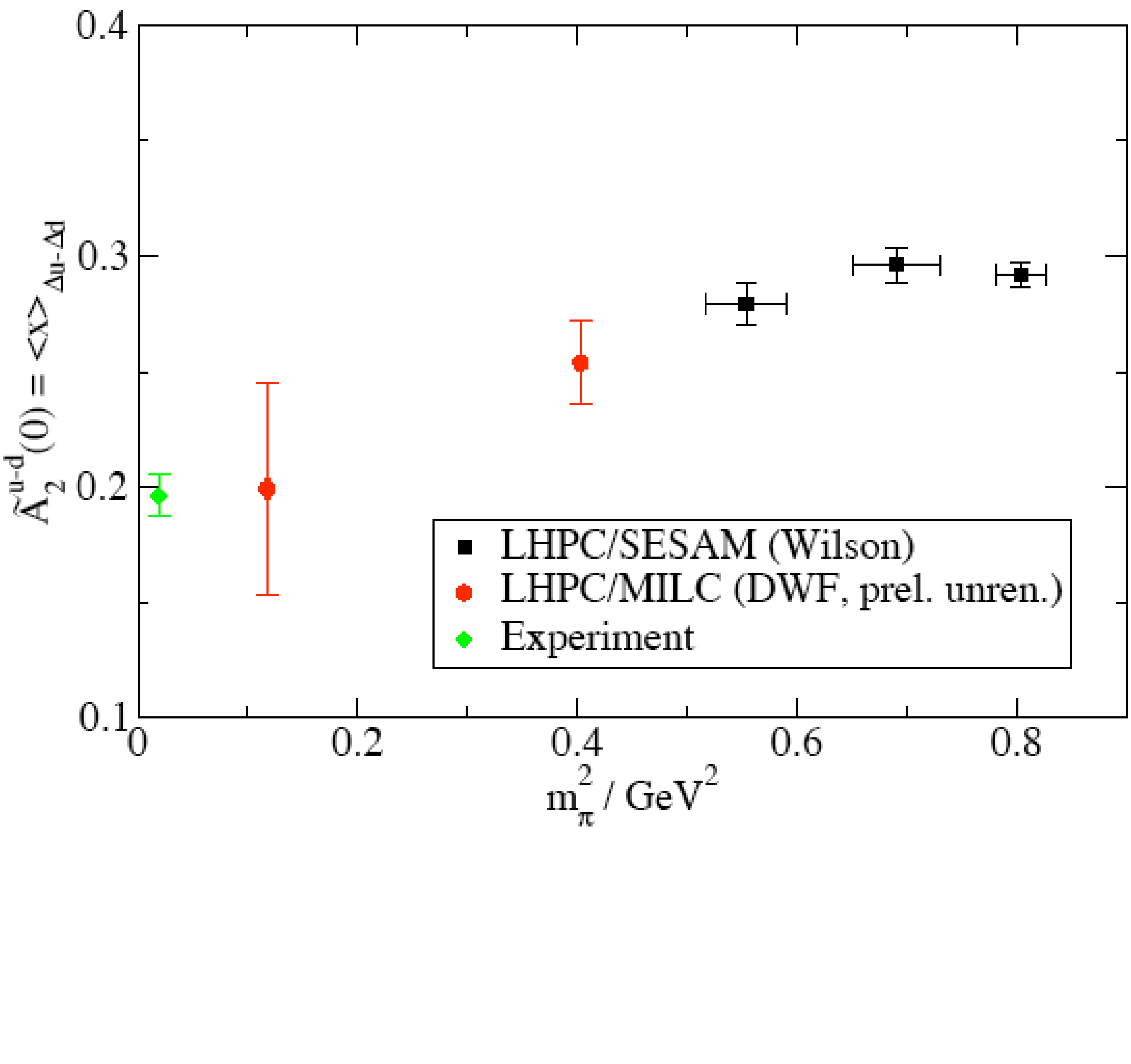
- Physical chiral extrapolation formula hep-lat/0103006

$$\langle x^n \rangle_u - \langle x^n \rangle_d \sim a_n \left[1 - \frac{(3{g_A}^2+1)m_\pi^2}{(4\pi f_\pi)^2} \ln\left(\frac{m_\pi^2}{m_\pi^2+\mu^2} \right) \right] + b_n m_\pi^2$$



Squares full QCD, circles quenched, $\mu = 550 MeV$

$<x>_{\Delta u - \Delta d}$



Off-forward matrix elements

Define generalized form factors

$$\bar{P} = \tfrac{1}{2}(P' + P), \quad \Delta = P' - P, \quad t = \Delta^2$$

$$\langle P'|O^{\mu_1}|P\rangle \sim \langle\gamma^{\mu_1}\rangle A_{10}(t) + \langle\sigma^{\mu_1\alpha}\rangle\Delta_\alpha B_{10}(t)$$

$$\langle P'|O^{\mu_1\mu_2}|P\rangle \sim \langle\gamma^{\{\mu_1}\rangle\bar{P}^{\mu_2\}}A_{20}(t) + \langle\sigma^{\{\mu_1\alpha}\rangle\Delta_\alpha\bar{P}^{\mu_2\}}B_{20}(t) + \langle 1\rangle\Delta^{\{\mu_1}\Delta^{\mu_2\}}C_{20}(t)$$

$$\langle P'|O^{\mu_1\mu_2\mu_3}|P\rangle \sim \langle\gamma^{\{\mu_1}\rangle\bar{P}^{\mu_2}\bar{P}^{\mu_3\}}A_{30}(t) + \langle\sigma^{\{\mu_1\alpha}\rangle\Delta_\alpha\bar{P}^{\mu_2}\bar{P}^{\mu_3\}}B_{30}(t) + \langle\gamma^{\{\mu_1}\rangle\Delta^{\mu_2}\Delta^{\mu_3\}}A_{31}(t) + \langle\sigma^{\{\mu_1\alpha}\rangle\Delta_\alpha\Delta^{\mu_2}\Delta^{\mu_3\}}B_{31}(t)$$

Off-forward matrix elements

- Limits
  - Moments of parton distributions $t \rightarrow 0$

$$A_{n0}(0) = \int dx x^{n-1} q(x)$$

  - Form factors

$$A_{10}(t) = F_1(t) \quad B_{10}(t) = F_2(t)$$

  - Total quark angular momentum

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

- *t*-Dependence

  q(x,t): Transverse Fourier transform of light cone parton distribution at given *x*

  $x \rightarrow 1$: Single Fock space component — slope $\rightarrow 0$

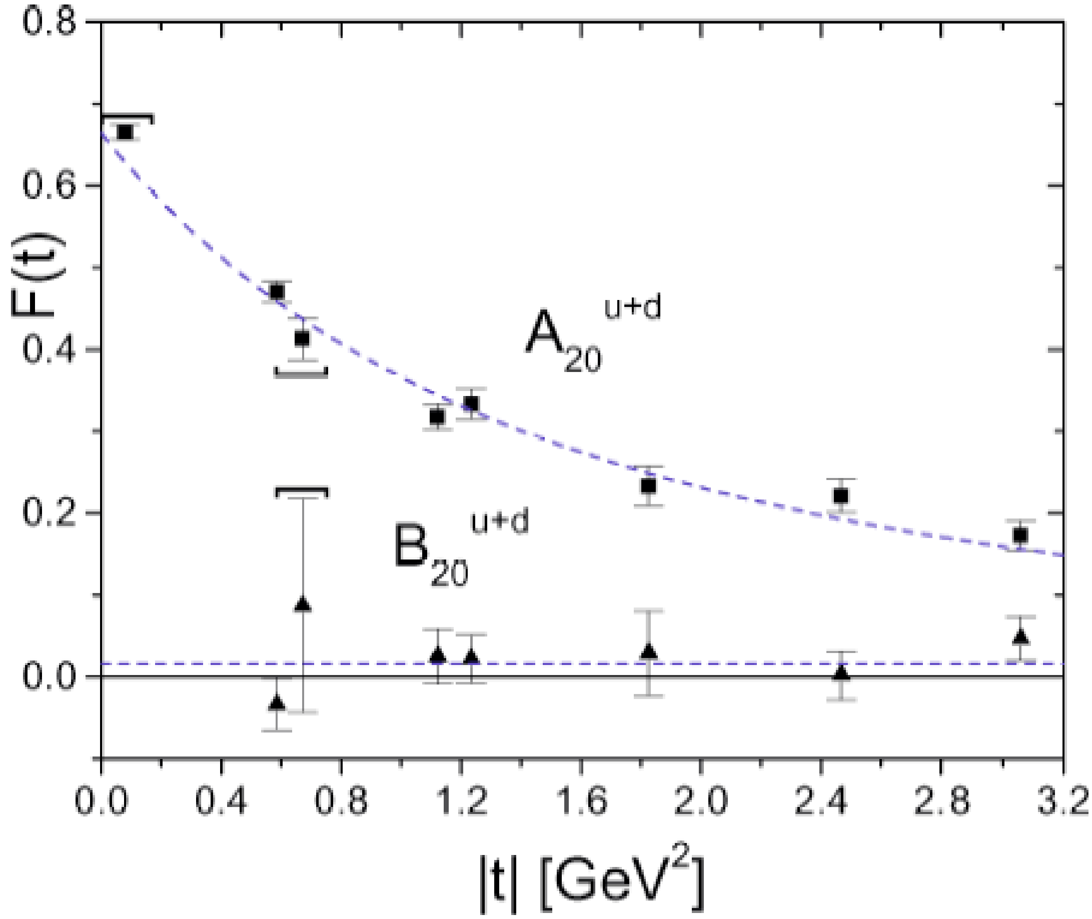
  $x < 1$: Transverse structure — slope steeper

n=2: Quark Angular Momentum

Connected diagrams, $m_\pi = 900$ MeV

$$\frac{1}{2}\Delta\Sigma = \frac{1}{2}[\langle 1\rangle_{\Delta u} + \langle 1\rangle_{\Delta d}]$$
$$\sim \frac{1}{2}\,0.682(18)$$

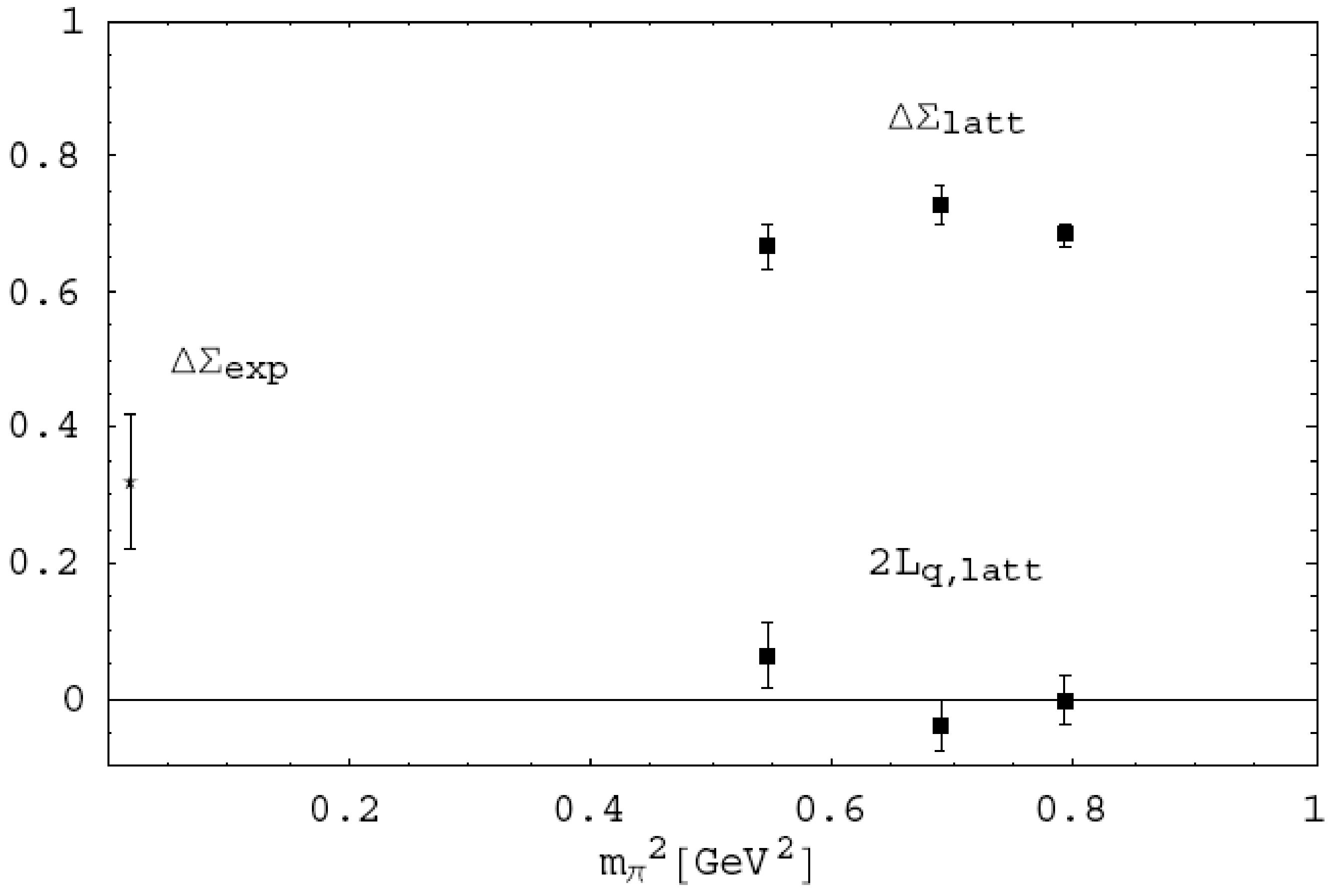
$$J_q = \frac{1}{2}[A_{20}^{u+d}(0) + B_{20}^{u+d}(0)]$$
$$\sim \frac{1}{2}[\langle x\rangle_u + \langle x\rangle_d + 0]$$
$$\sim \frac{1}{2}0.675(7)$$



Quark Angular Momentum

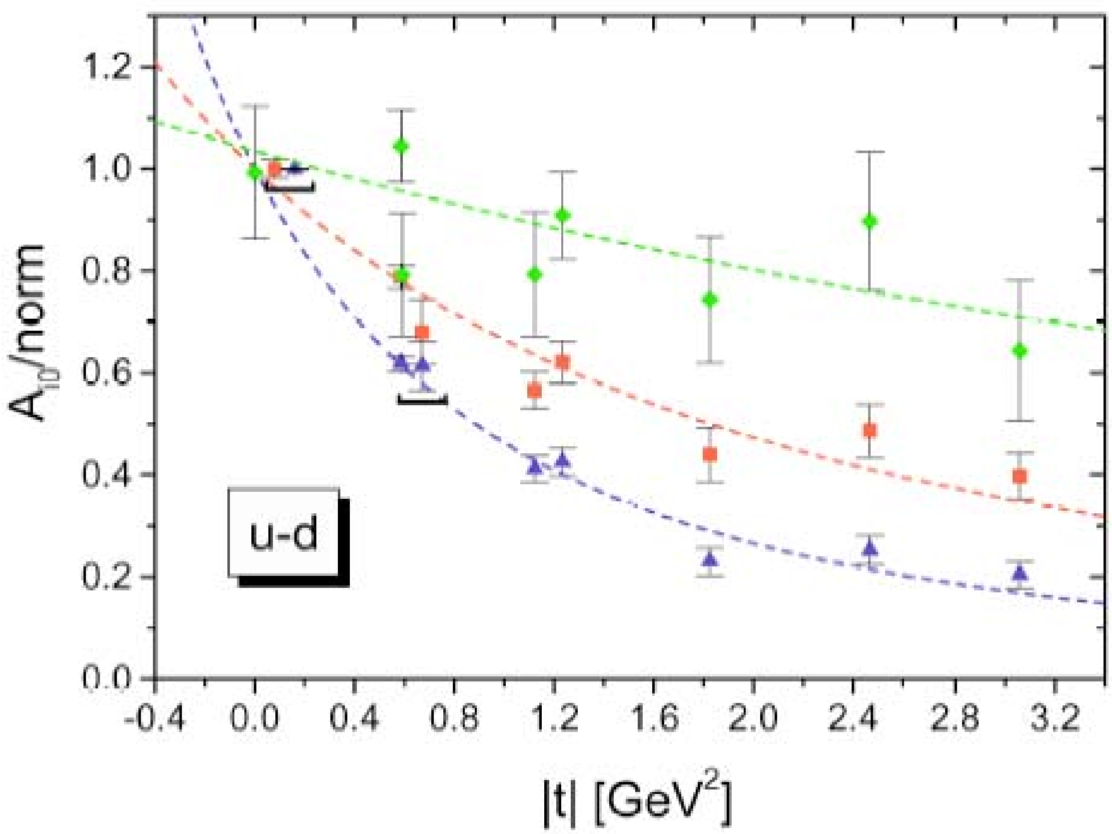
Connected diagram contributions

κ	0.1570	0.1565	0.1560
$\Delta\Sigma$	0.666 ± 0.033	0.727 ± 0.028	0.684 ± 0.018
$2J_q$	0.730 ± 0.035	0.688 ± 0.024	0.682 ± 0.029
$2L_q$	0.064 ± 0.048	-0.039 ± 0.037	-0.002 ± 0.034

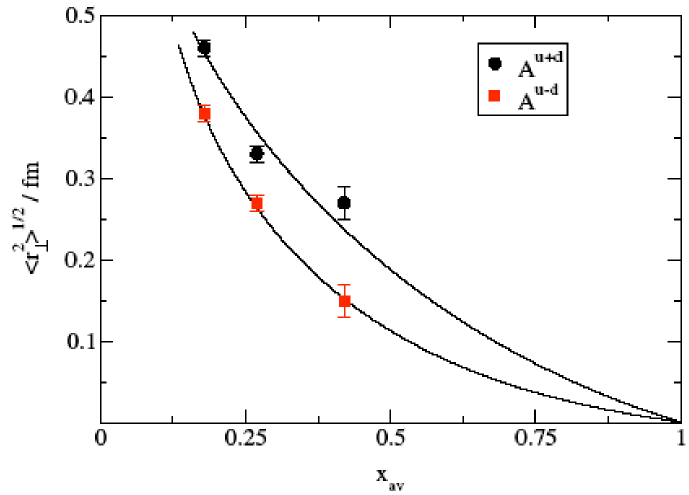


Transverse Structure of Parton Distribution

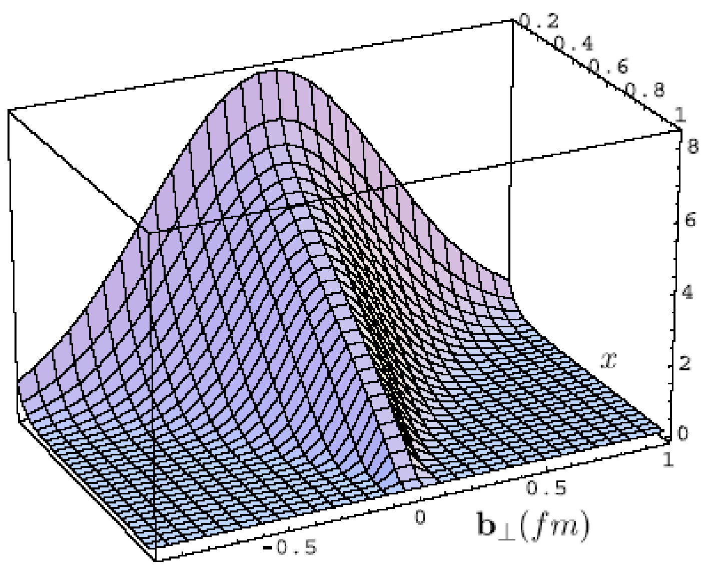
- Transverse Fourier transform of light cone parton distribution
- Expect slope $\to 0$ as $x \to 1$
- Expect higher moments have smaller slope
- Lattice results for n = 1, 2, 3 ($m_\pi = 900$MeV)
- Factorization Ansatz invalid



Smeared transverse structure



$$x_{\rm av}^{(n)} = \frac{\int d^2b_\perp \int_{-1}^{1} dx\, x \cdot x^{n-1} q(x,\vec{b}_\perp)}{\int d^2b_\perp \int_{-1}^{1} dx\, x^{n-1} q(x,\vec{b}_\perp)}$$



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

Spectroscopy

- N* Spectroscopy JLab

    Number and structure of states

- Exotics JLab

    Glueballs

    Exotic mesons - gluonic excitations

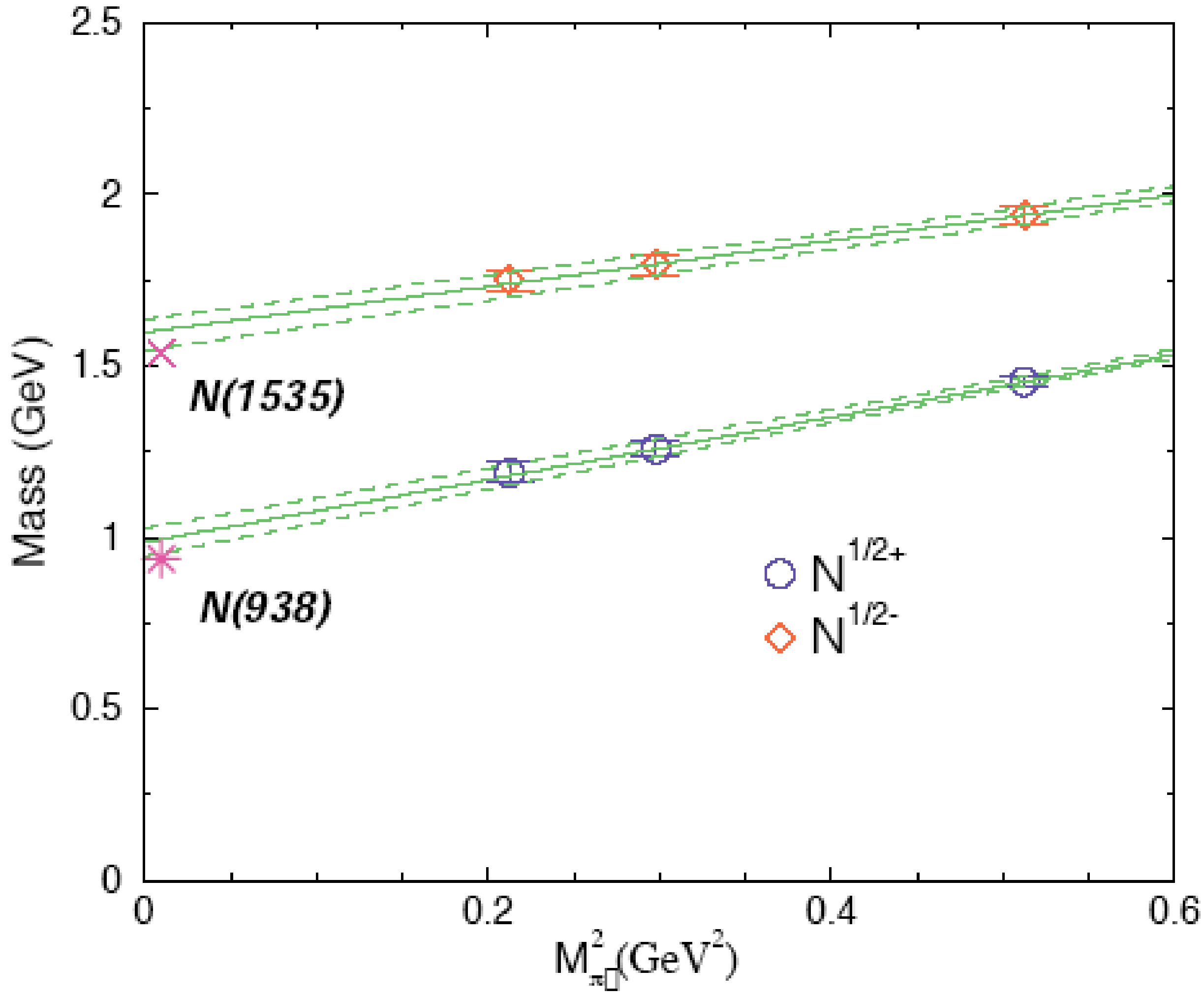
    Pentaquark

- Hadronic Interactions

    Heavy-light meson and baryon interactions

    - Light quark exchange
    - Gluon contributions

Nucleon Parity Partner



Quark mass extrapolation of nucleon and its parity partner

D. Richards *et.al.* hep-lat/0011025

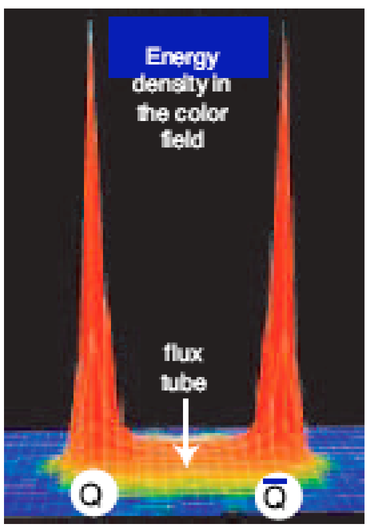
Exotic Mesons

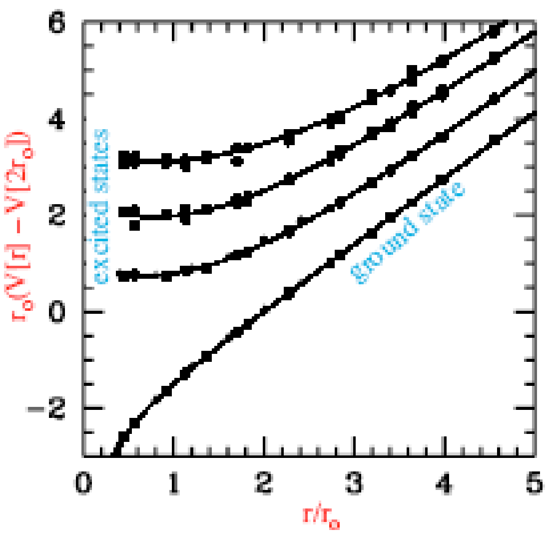
Exotics - mesonic states not accessible to quark model

Window on gluonic excitations of flux tube

Exploration of mechanisms of *confinement*.

Ideal spectrum between heavy quarks





Bali Juge, Kuti, Morningstar

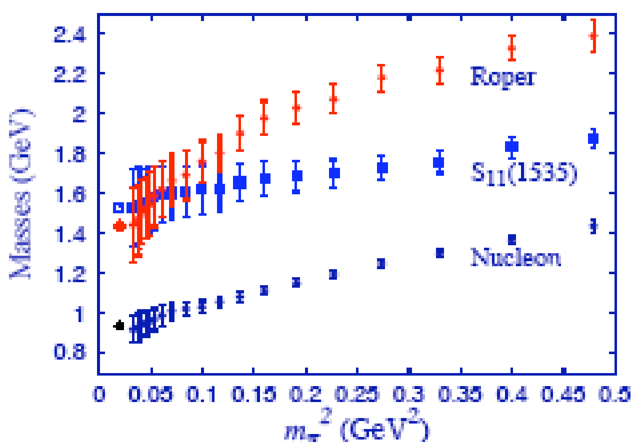
Roper Resonance

Lightest radial excitation of nucleon

Quark model predicts equal-spacing ordering of states

$$m_N < m_{N^{1/2-}} < m_{\text{Roper}}$$

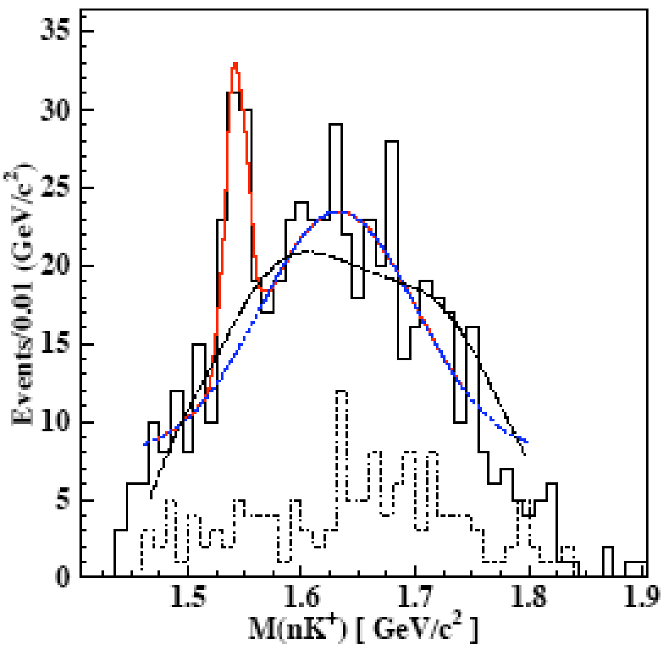
Resolution of observed Roper(1440) with QCD



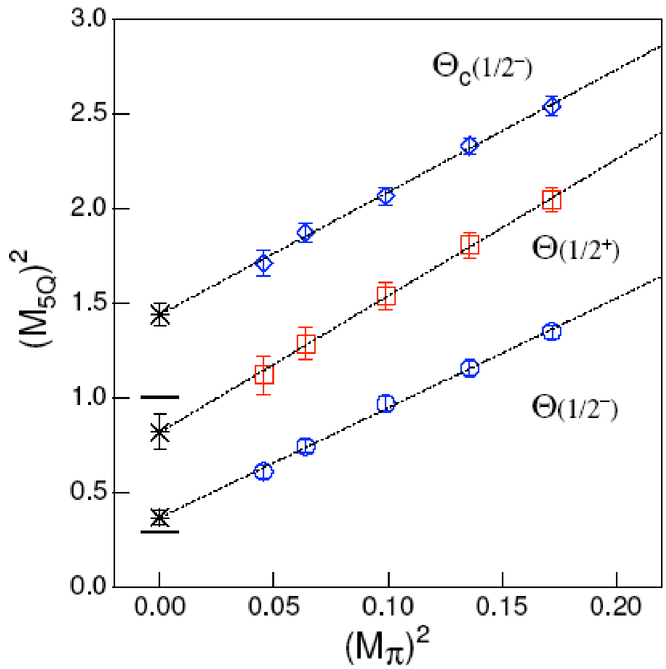
S.J. Dong *et al.*, hep-lat/0306199

Pentaquarks

Θ (1540} observed at SPRing8, Jlab,…



Stepanyan et.al. hep-ex/0307018



Sasaki hep-lat/0310014

S = +1 five quark state $uudd\bar{s}$

Diquark model - positive parity $(ud)(ud)\bar{s}$

Quark model - negative parity

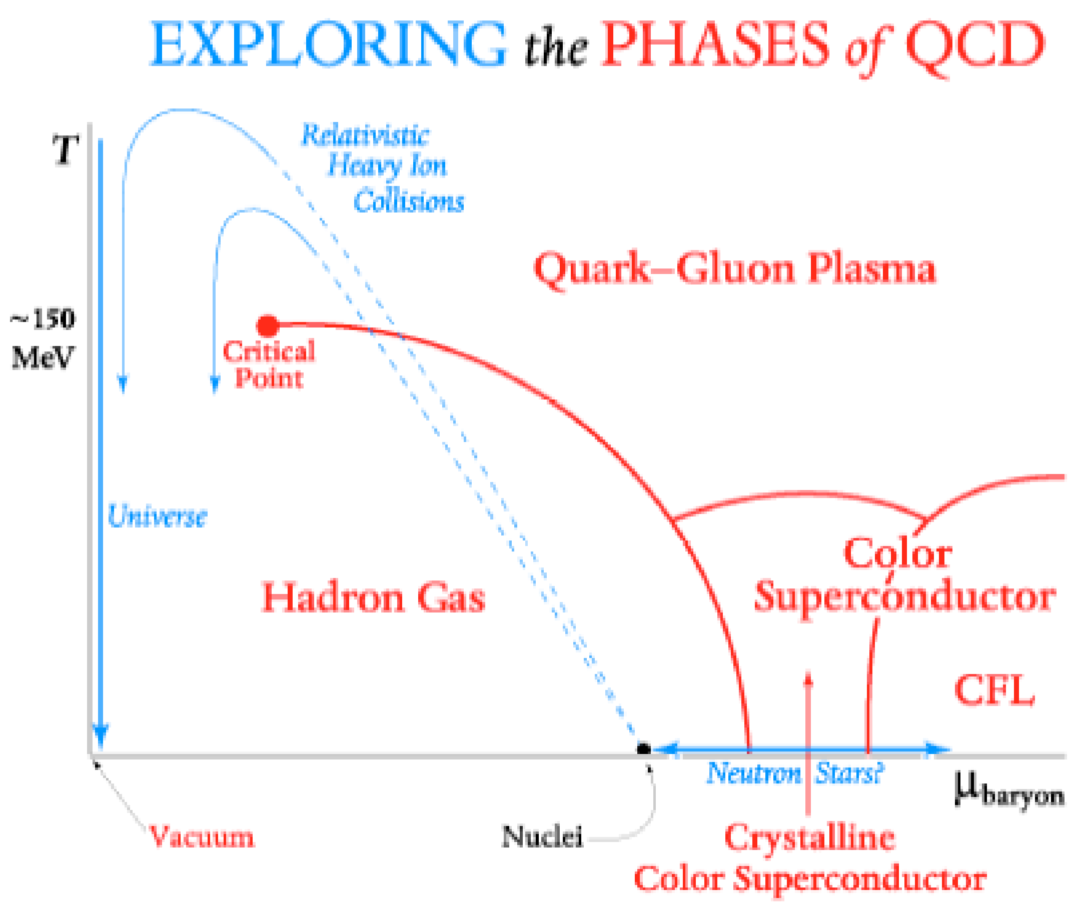
Preliminary lattice calculations in heavy pion world

QCD Thermodynamics

- Phase diagram of QCD
- Zero baryon density ($\mu = 0$)
  - Transition to Quark Gluon Plasma
  - E(T), P(T)
- Non-zero baryon density ($\mu \neq 0$)
  - Critical point - RHIC signatures
  - Equation of state - neutron stars
  - Superconducting phases
- Quark number susceptibility
  - Event by event fluctuations
- Quark-antiquark potential
  - J/Ψ production
- Current correlation functions - spectral function
  - Dilepton and photon emission
  - Transport coefficients

QCD Thermodynamics

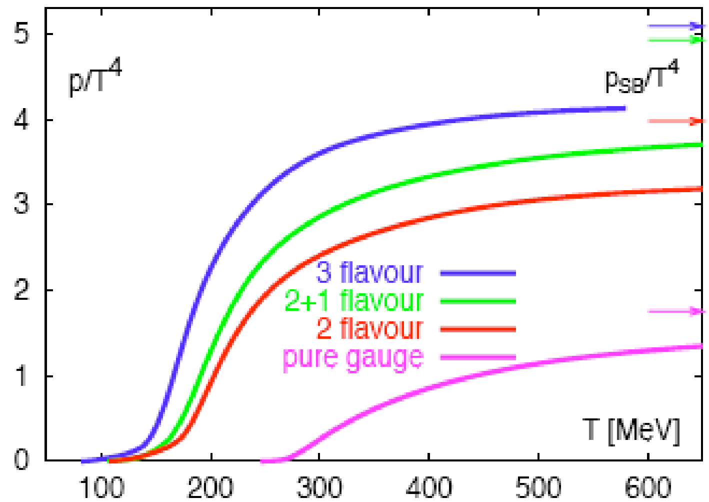
- QCD phase diagram



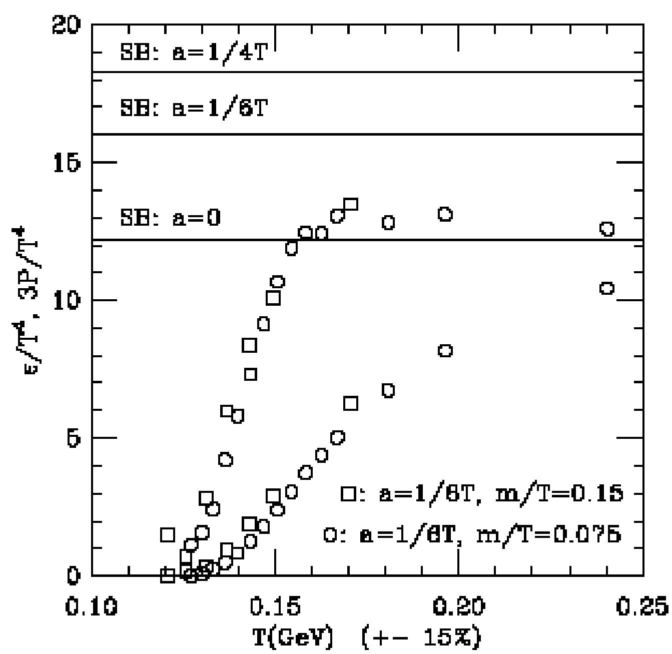
- Currently restricted to $\mu \sim 0$

Equation of State at $\mu = 0$

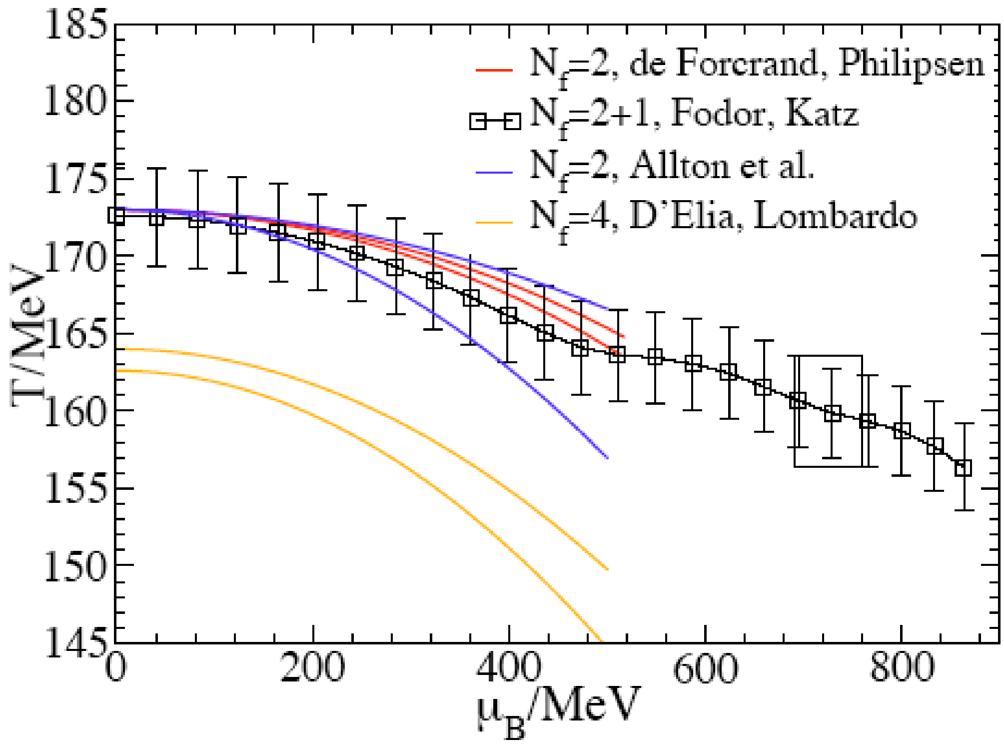
- **Equation of state** (F. Karsch hep-lat/0106019)



- **Pressure and energy density for 2 flavors** (MILC)



Finite Baryon Density



- Three methods for calculation

  Reweighting

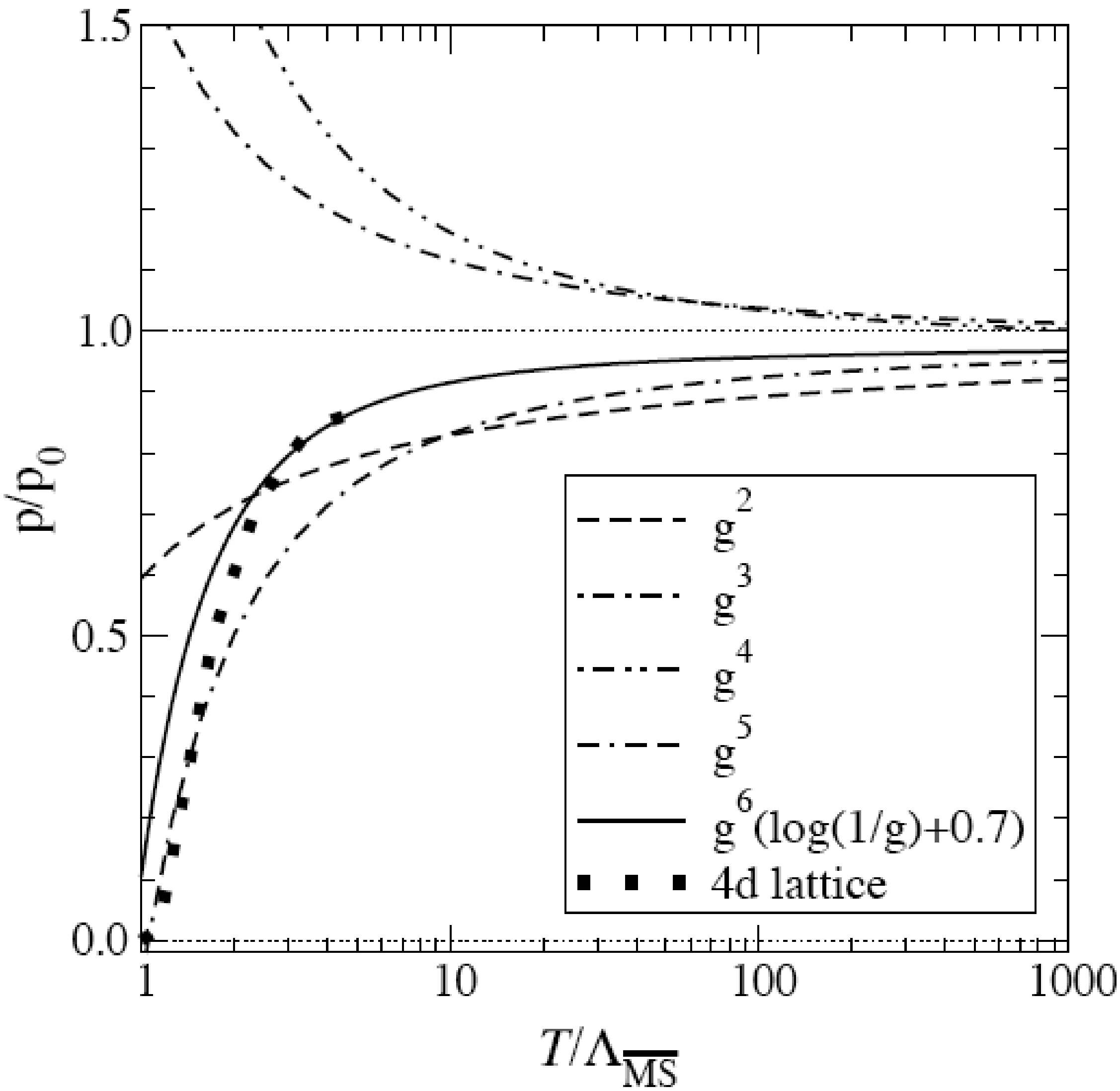
  Expansion around $\mu = 0$

  Analytic continuation with complex μ

- Open question - large μ

  Cluster algorithms ?

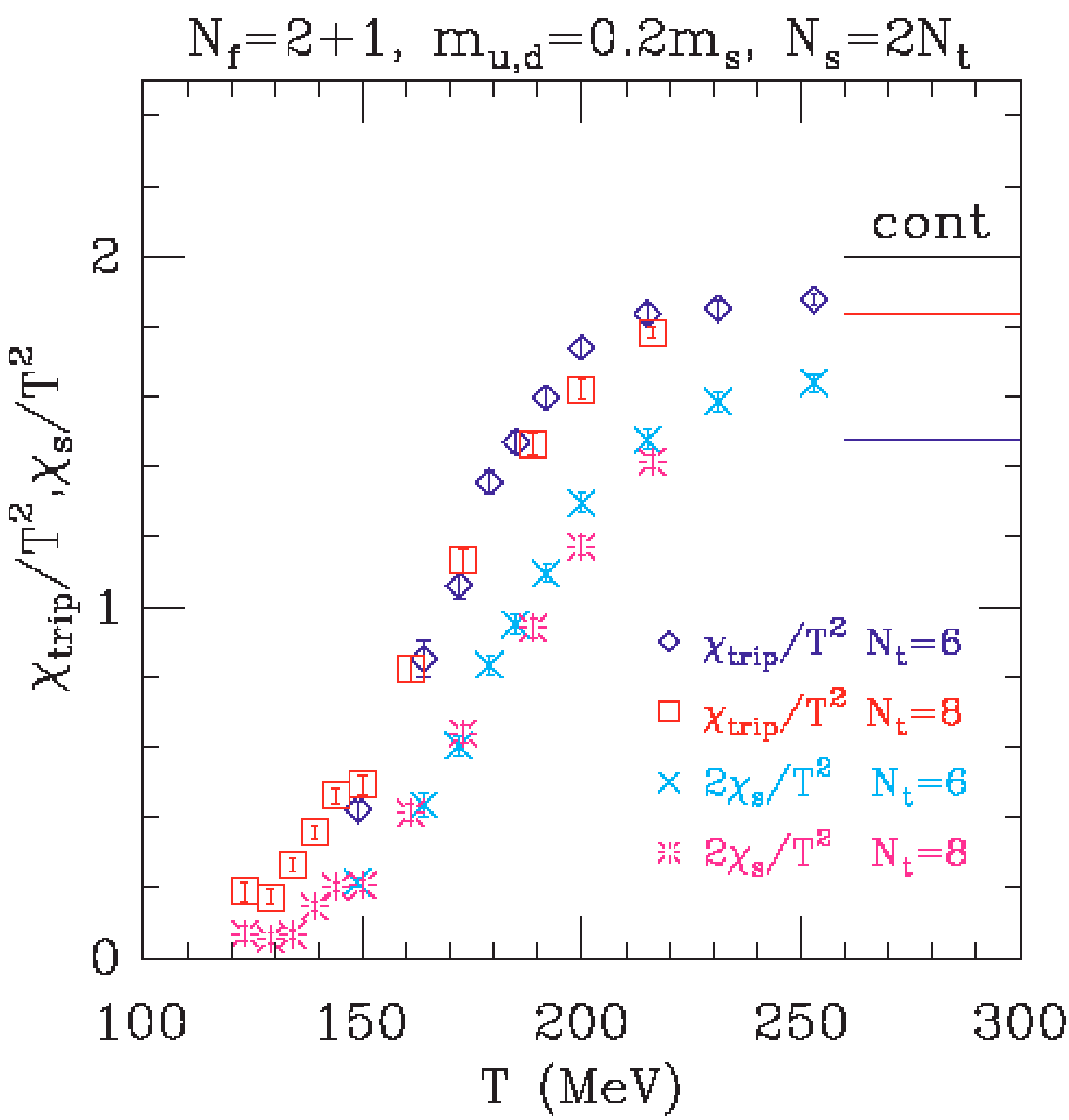
Matching to Perturbative QCD



(Kajantie, Laine, Rummukainen, Schroder hep-ph/0211321)

- Dimensionally reduced effective theory
  Integrate out 'hard' modes $\sim \pi T$
  Integrate out 'soft' modes $\sim gT$
  Calculate p_G in 3-D
  $p = 1 + g^2 + g^3 + g^4 + g^5 + g^6 \ln g + \#g^6$

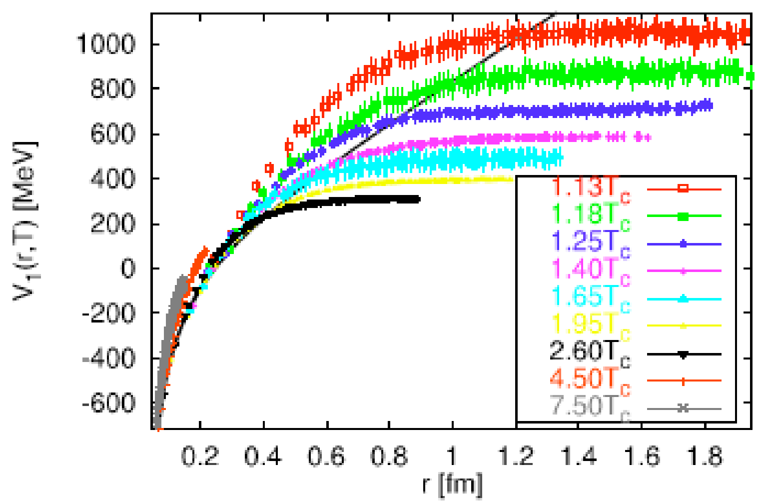
Quark Susceptibility

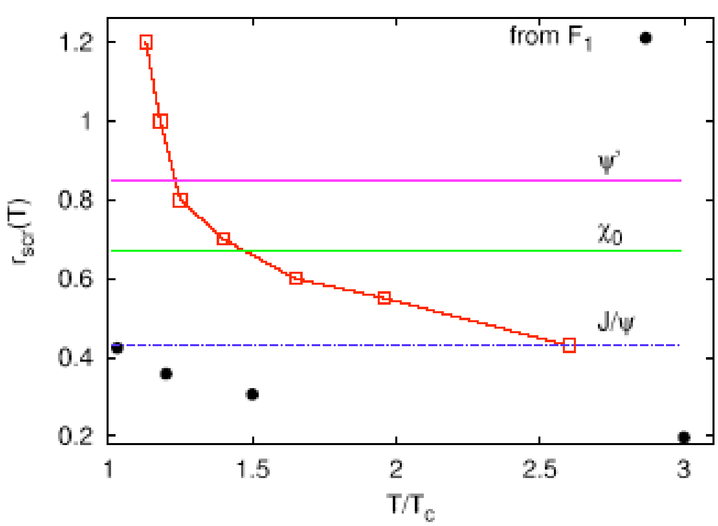


Triplet quark susceptibility, related to fluctuations in isospin density, and strange quark susceptibility, related to fluctuations in strangeness density (C. Benard *et.al.* hep-lat/0209079)

Screening of Heavy Quark Potential

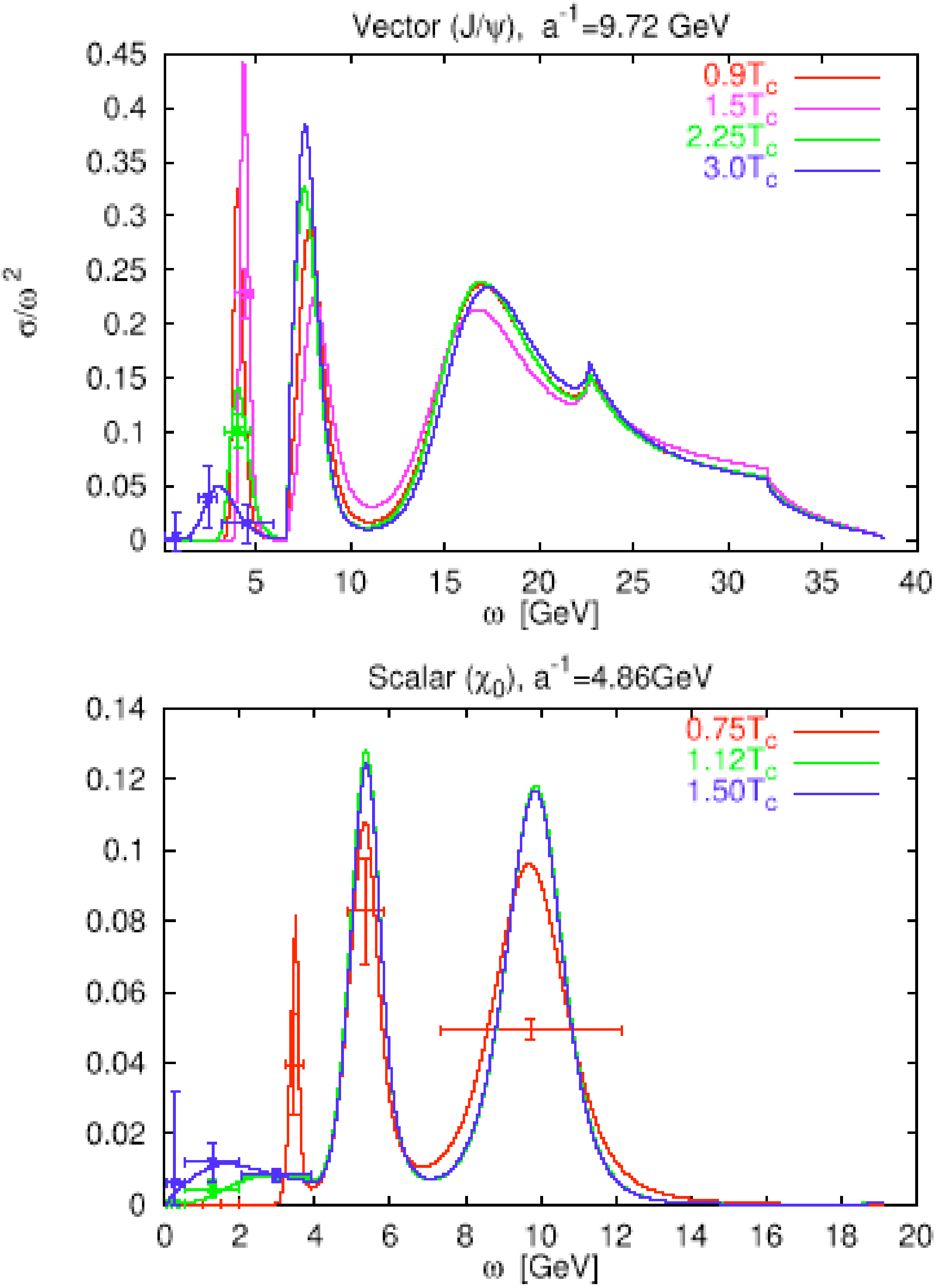
- Why, how can J/ψ exist in the plasma ?
- The free energy $F_1(r,T)$ and the internal energy $V_1(r,T)$ of a static singlet $Q\bar{Q}$ pair, $F_1(r,T) = V_1(r,T) - TS_1(r,T)$





Kaczmarek et al hep-lat/0309121

Spectral Functions



J/Ψ survives up to 2.25 T_C

Petreczky et al hep-lat/0309012

Fundamental aspects of QCD

Insight into how QCD works

- Confinement

  Mechanism, flux tubes

- Chiral symmetry breaking

  Instantons, zero modes

- Low energy effective theory

  Parameters of chiral perturbation theory

- Structure of wave functions

  Variational wave functions

  Density-density correlation functions

- Configurations that dominate path integral

  Instantons

- Dependence on parameters of QCD

  N_c , N_f , gauge group, m_q

Long Term Effort

- Quantities for which we already have theoretical and computational tools

  Need 10's of Teraflops - Petaflops for precision calculations at level of few percent

- Challenges with the potential for opening still more vistas

  Example: Finite chemical potential

  Cluster algorithms

- Need sustained effort at leading edge of technology curve

Lattice QCD Initiative

Coherent National Plan

Cost optimized hardware: QCDOC and Clusters

SciDAC Computational Infrastructure

- **Software development**

  Uniform optimized software for all platforms

- **Cluster development**

Hardware Plan

- **10 Tflops QCDOC at BNL in 04**

  Plan $1 per sustained Mflops in 04

  General purpose machines $20-50

- **10 Tflops clusters at Jlab, FNAL in 05 and 06**
- **Joint high energy and nuclear physics funding**

  $4M committed in HEP

  Seek Nuclear and ASCR support

SciDAC Software

Uniform QCD physics software environment

Highly optimized for each platform

QCD–API Level Structure

Level 3
Dirac Operators, CG Routines, etc.

QDP lib Level 2	
Data Parallel QCD Lattice Operations (overlapping Algebra and Messaging) e.g. A = SHIFT(B, mu) * C ; Global sums, etc	
Lattice Wide Linear Algebra (No Communication) e.g. A = B * C	Lattice Wide Data Movement (Pure Communication) e.g. Atemp = SHIFT(A, mu-dir)

QLA lib Level 1	QMP lib
Single Site & Vector Lin Alg API e.g. SU(3), Dirac algebra, etc.	Message Passing API (Maps Lattice into Network)

Current and Planned Clusters

- Prototype Clusters

  99 64 Gflops Alpha cluster @ MIT

  99 48 Gflops Alpha cluster @ JLab

  01 80 node P3 cluster @ FNAL

- SciDAC Clusters ($\sim$ \$2M + Lab matching)

  Myrinet

  8/02 48 node dual P4 cluster @ FNAL

  9/02 128 node single P4 cluster @ JLab

  2/03 128 node dual P4 cluster @ FNAL

  Gigabit Ethernet

  6/03 256 node dual P4 cluster @ JLab

  Next Generation Technology

  9-12/03 Clusters @ FNAL and JLab

- Propose 10^{+} Tflops clusters at FNAL and JLab in FY05 and FY06

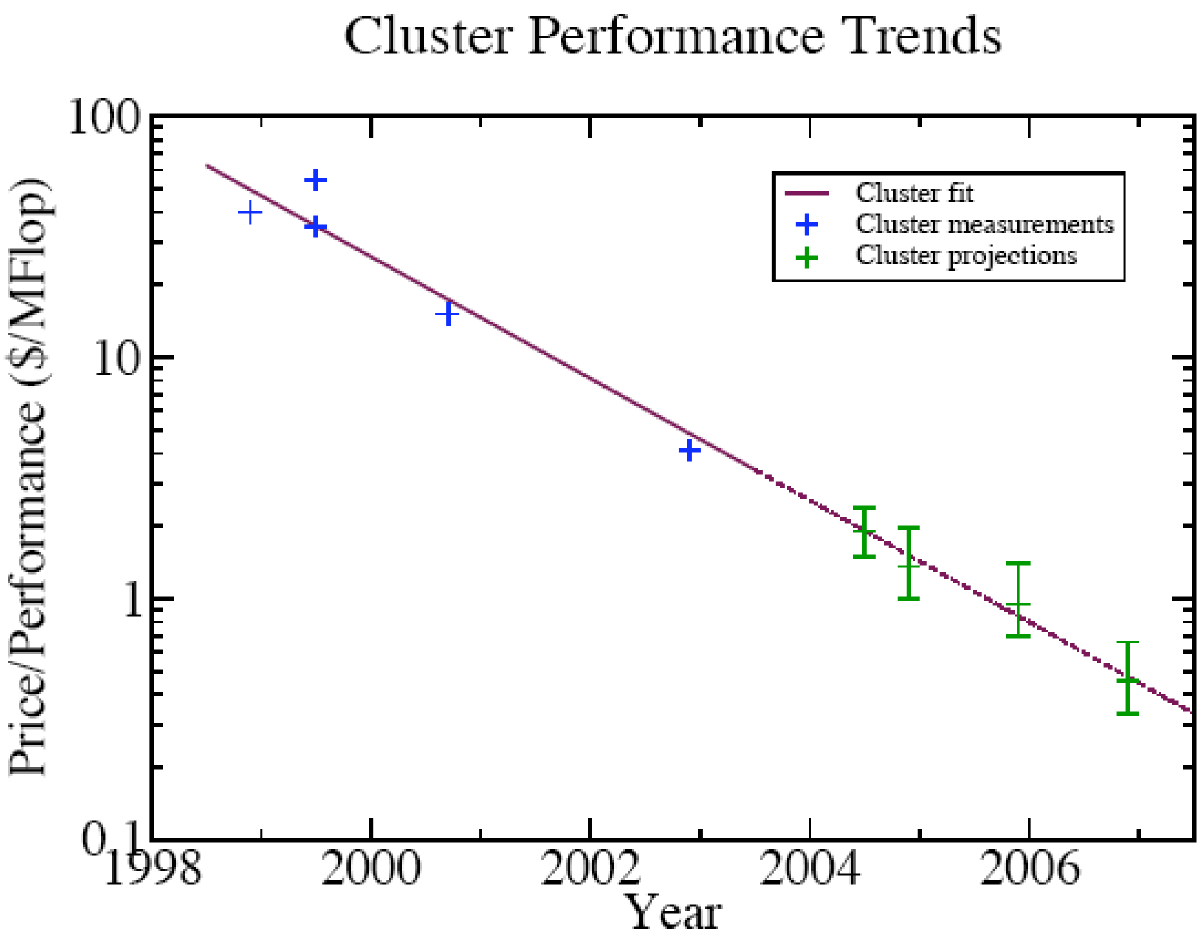
FNAL Myrinet Cluster

- 128 Node dual Xeon
- 2.4 GHz P4
- Commissioned 1/03

Jlab GigE Cluster

- 256 Node single Xeon
- 2.66 GHz P4
- 3 dual GigE cards
- $ 1950/node
- Commissioned 9/03

Projected Cluster Performance



Staggered fermion inverter at FNAL

Summary

- Lattice QCD poised to provide fundamental understanding of hadrons and hadronic matter
- Essential tool for understanding contemporary experiments
- Demonstrated methodology in “heavy pion world”
- Computer technology ready for 10’s of Teraflops at $1/sustained Mflops.
- Sustained effort at leading edge of technology curve provides outstanding opportunity for fundamental advances in Nuclear Physics