Advanced Computing in Nuclear and Hadronic Physics: Workshop Summary

John W. Negele

Santorini Workshop on Advanced Computing
in Nuclear and Hadronic physics
October 1, 2001

Lattice QCD

Philippe de Forcrand

Insight into chiral symmetry breaking and confinement

Constantia Alexandrou

Calculation of hadron wave functions

Paul Rakow

Calculation of moments of structure functions

Thomas Lippert

Study of sea quark physics

Colin Morningstar

Study of exotic hadrons

Thomas Lippert and J.N.

The technological frontier in lattice QCD:
cost-optimized machines

Experimental Hadronic Physics

Ralph Lange

Accelerator and experiment control and monitor systems

Ferdinand Willeke

Commissioning and operating an accelerator from afar

John Apostolakis

Simulation of physics processes and detector response

David Morrison

Data handling in heavy ion collisions

Gaetano Maron

Computing challenges in nuclear physics experiments: the future

EXPERIMENTAL HADRONIC PHYSICS

CAVEATS:

- PARIS SPHICAS IS THE EXPERT
- EXPERIMENTALISTS TOO GOOD WITH POWERPOINT

ACCELERATOR AND EXPERIMENT CONTROL AND MONITOR SYSTEMS RALPH LANGE
BESSY

- EPICS
  - DEFACTO STANDARD
  - 5 CORE INSTITUTIONS - 120 COLLABORATING INSTITUTIONS
  - SYSTEMS
    - ACCELERATORS, BEAM LINES
    - UP TO ~ 300,000 SIGNALS
  - APPEARS UNDER CONTROL

HOW TO COMMISSION, OPERATE & MAINTAIN A LARGE FUTURE ACCELERATOR FROM AFAR FERDINAND WILLEKE

- ICFA STUDY ON GLOBAL ACCELERATOR NETWORKS
  - EX: LINEAR COLLIDER - TOO COSTLY FOR SINGLE NATION
    TOO LARGE FOR SINGLE LAB
  - REMOTE FACILITY MODEL
    - EQUAL PARTNERS - NO HOST
    - EACH COLLABORATOR RESPONSIBLE FOR MAJOR SECTION OF MACHINE
    - MOST ACTIVITIES DONE REMOTELY
    - ROTATE CONTROL CENTER BETWEEN INSTITUTIONS
    - PERMANENT VIDEOCONFERENCING
    - NEED ON-SITE EXPERT 1% OF TIME
  - WORKSHOP: BNL SUMMER 02
  - APPEARS STRAIGHTFORWARD TECHNICALLY
  - ORGANIZATIONAL & SOCIOLOGICAL CHALLENGES
  - MODELS - ASTRONOMY / ASTROPHYSICS
  - LOTS OF POTENTIAL BENEFITS

SIMULATION OF PHYSICS PROCESSES & DETECTOR RESPONSE JOHN APOSTOLAKIS

EXPT. PHYSICISTS NOT ONLY INVENTED WEB – ALSO INVENTED VIRTUAL REALITY

GEANT 4 GEometry ANd Tracking

TRACKING & GEOMETRICAL PROPAGATION

MODELING OF PHYSICAL INTERACTIONS

VISUALIZATION

FORTRAN 77 → C++

REQUIREMENTS OF LHC, H.I., CP-VIOLATION, COSMIC RAYS ...

NOT YET PARALLEL (PROTOTYPE)

INTERNATIONAL TOOLKIT INTERESTING MODEL FOR LATTICE COMMUNITY

DATA HANDLING IN HEAVY ION COLLISIONS

SCOPE: Au + Au $\sqrt{s} = 200$ GeV 5000 CHARGED TRACKS

$\vec{p} + \vec{p}$ $\sqrt{s} = 500$ GeV GLUON S.F.

DETECTORS PHENIX

PHENIX →

STAR 70 MILLION PIXEL TPC, + PHOBOS & BRAHMS

~ 200 TBYTES OF DATA / YR ~ CDF, D0 < LHC

RHIC COMPUTING FACILITY

~ $8M CONSTRUCTION, $2M/YR REFRESH

COMPUTERS →
DISK →

DISTRIBUTED COMPUTING

PRIMARY EVENT RECONSTRUCTION BNL

SECONDARY SITES: JAPAN, FRANCE, LLNL, MIT ...

5-10 Mbits/sec + FEDEX TAPES

MAJOR CHALLENGE – RAW EXPLORATION →

SEE LINK TO DAVID MORRISON'S TALK:

Phenix

BNL computers

BNL Storage

Conclusions

COMPUTING CHALLENGES IN NUCLEAR PHYSICS

GAETANO MARON

γ ARRAYS: EUROBALL, GAMMASPHERE

⇒ 4π ARRAY AGATA Advanced GAmma Tracking Array

33 M Euro ~ 10 LABS IN EUROPE

FRONT END ELECTRONICS
AND PREPROCESSING

100 Gb/s

PULSE SHAPE ANALYSIS 200 pc's

5 Gb/s

EVENT 10 pc farm

5 Gb/s

TRACK 500 pc farm

1 Gb/s

STORAGE

500-700 TB/y

NUCLEAR STRUCTURE COMMUNITY USING LHC TECHNOLOGY

Lattice QCD in Hadronic Physics

John W. Negele

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Outline

- Introduction and motivation
- Overview of lattice QCD
- Physics opportunities
- Calculation of hadronic observables on the lattice
  - Masses
  - Wave functions
  - Matrix elements
  - Instantons, monopoles, and vortices
- The role of multi-Teraflops Computers

Introduction

Lattice QCD has become an essential tool in hadronic physics

- Only way to solve, rather than model, QCD
- Confluence of advances
    - Lattice field theory
        - Lattice chiral symmetry
        - Improved actions
        - Cluster algorithms
    - Computer technology
        - $ 1 / Mflop
        - 10 Teraflop machines
- Crucial to understand physics of major experimental initiatives
    - Fundamental parameters of Standard Model – weak matrix elements
    - QDC thermodynamics – RHIC and beyond
    - Hadron structure and interactions – focus of this workshop

Motivation

- Understand structure and interactions of hadrons from QCD
- 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 → Coulomb potential

  mesons → N-N potential
- ◦ Most of mass from fermion constituents

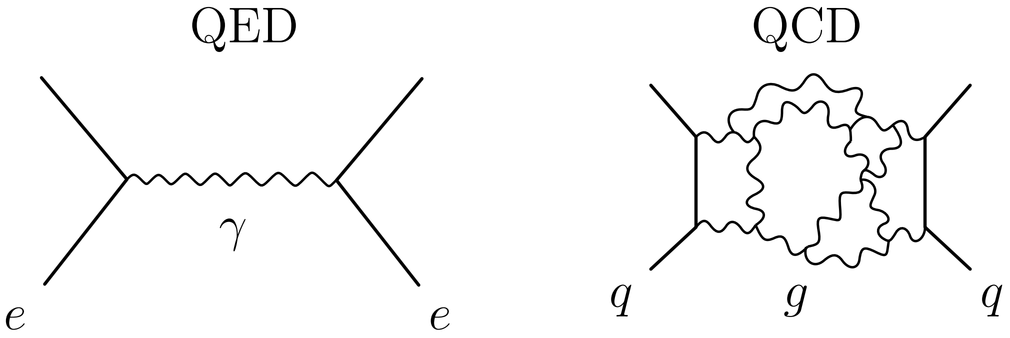
Nucleons

- ◦ Quarks are confined
- ◦ Gluons are essential degrees of freedom

  Carry half of momentum

  Nonpeturbative topological excitations
- ◦ Most of mass generated by interactions

Nonperturbative QCD



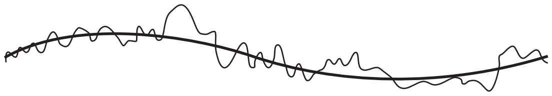
- Fundamental differences relative to QED
  - Self-interacting – highly nonlinear
  - Interaction increases at large distance – confinement
  - Strong coupling $\alpha_s \gg \alpha_{em}$
  - Rich topological structure

- Solution of QCD
  - Present analytical techniques inadequate
  - Numerical evaluation of path integral on space-time lattice

Goals

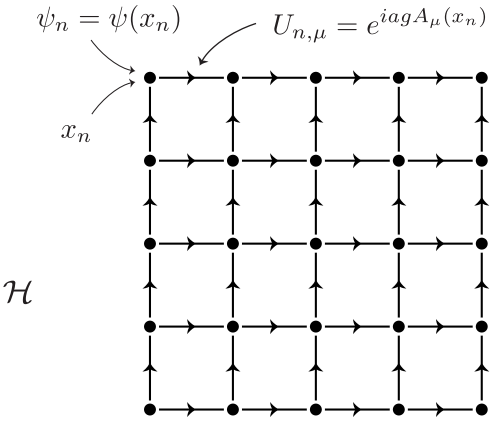
- Use lattice field theory to **solve** QCD with controlled errors
  - Quantitative calculation of properties of nucleon
    - Mass
    - Form factors
    - Light cone distribution of quark and spin densities
  - Understand origin of proton spin
  - Calculate exotics from first principles

- Use lattice field theory for **insight** into how QCD works
  - Identify paths that dominate action



  - Understand mechanism of confinement and chiral symmetry breaking
  - Calculate overlap with trial wave function $\left|\langle \psi_{\text{trial}} \mid \psi_{\text{exact}} \rangle\right|^2$
  - Explore dependence on $m_q \ , \quad N_f \ , \quad N_c$

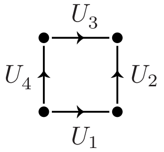
Lattice QCD



Euclidean:

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

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



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

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

INSIGHTS INTO CHIRAL SYMMETRY BREAKING AND CONFINEMENT

INSTANTONS

MINKOWSKI

$$\frac{d^2x}{dt^2} = -\nabla V$$

EUCLIDEAN

$$\frac{d^2x}{d\tau^2} = -\nabla(-V)$$

TUNNELING SOLUTIONS

$it \to \tau$

FIND BY RELAXATION

(COOLING) →

MEASURE DISTRIBUTION →

IN GROUND STATE

OBSERVABLES CALCULATED →

WITH ONLY INSTANTONS CLOSE

TO THOSE CALCULATED WITH ALL GLUONS

$$F^2 \sim \frac{1}{(x^2+\rho^2)^4}$$

SEE QUARK ZERO MODES IN SPECTRUM

$$\psi^2 \sim \frac{1}{(x^2+\rho^2)^3}$$

CONCENTRATED AT INSTANTONS →

DOMINATE PROPAGATOR →

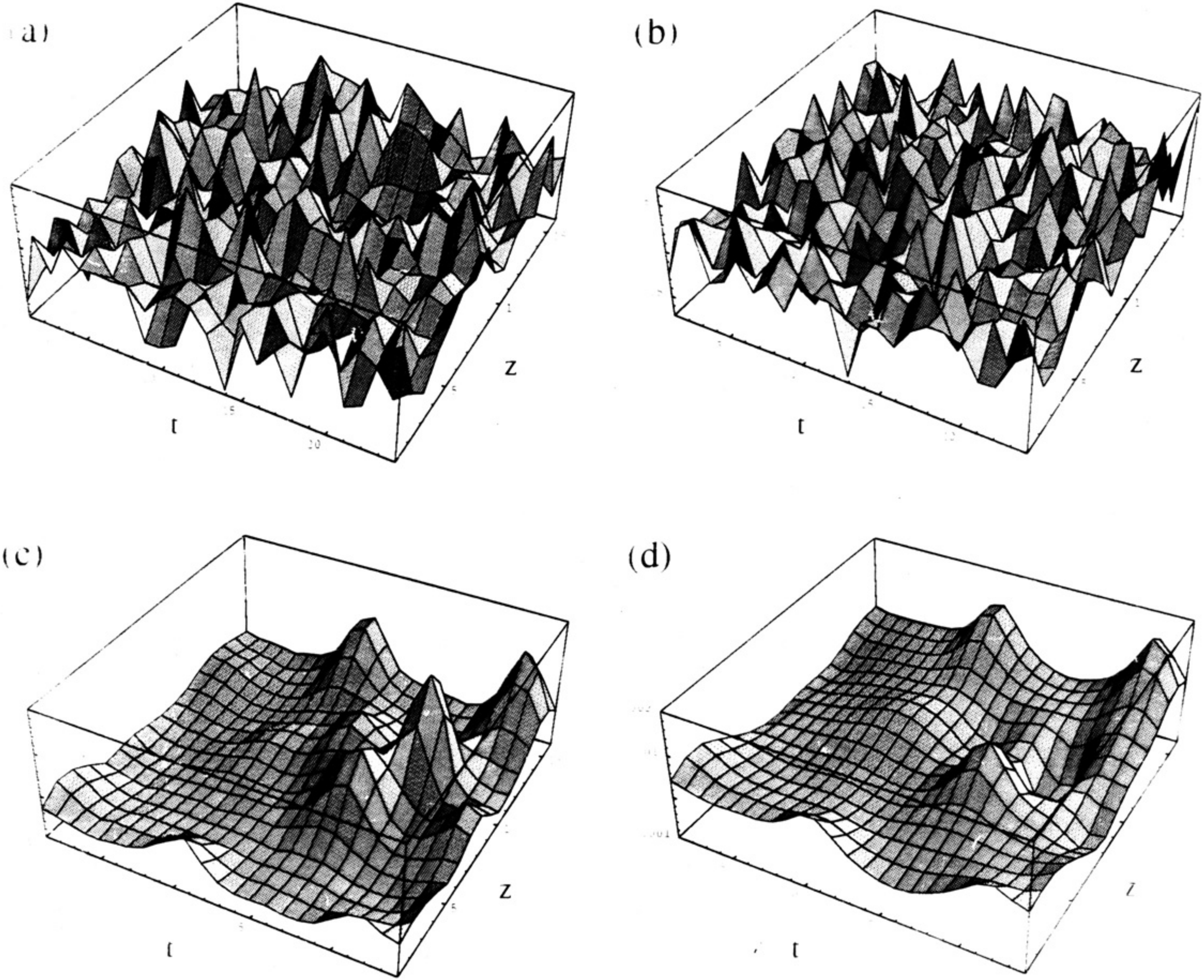
$$\langle \bar{\psi}\psi \rangle = \pi\, \rho(0)$$

MIXING OF ZERO MODES →

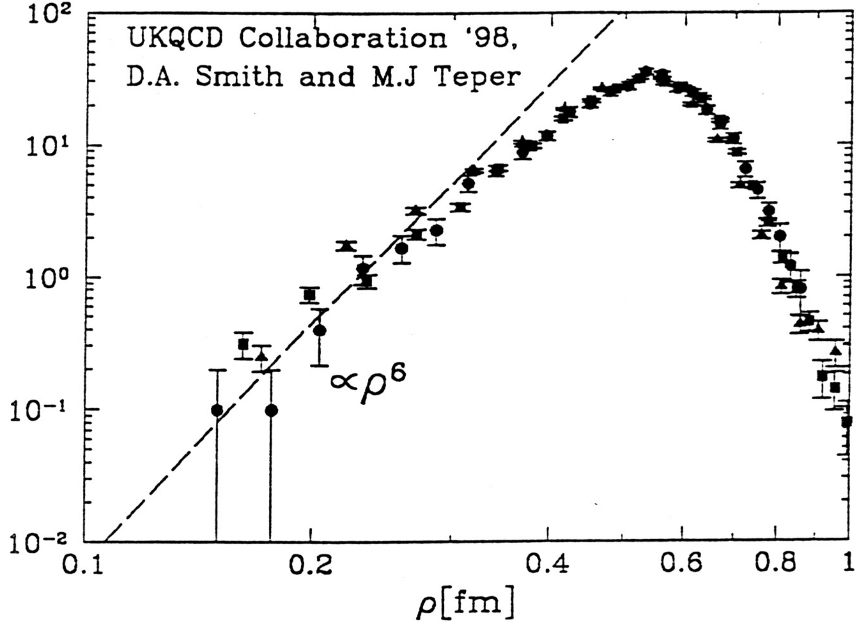
DELOCALIZED $T < T_c$

LOCALIZED $T > T_c$

DO **NOT** PRODUCE CONFINEMENT →

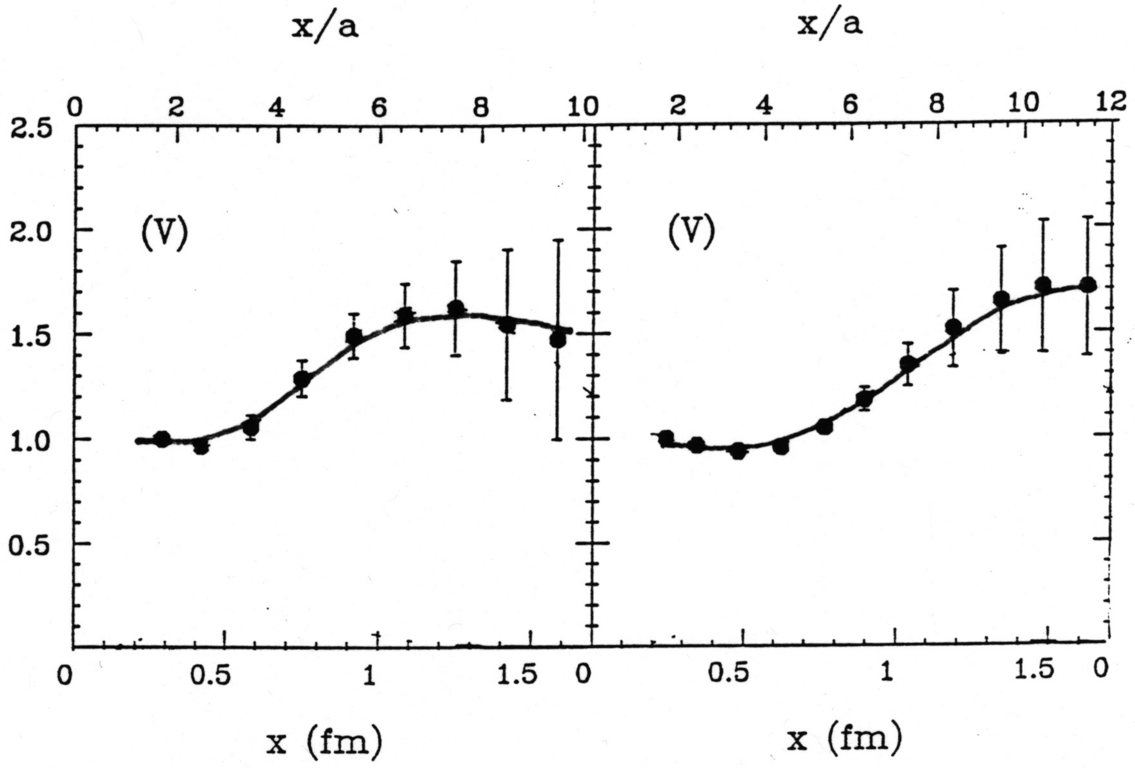

(a)
t
z
(b)
t
z
(c)
t
z
(d)
t
z

UKQCD DATA REPLOTTED BY RINGWALD + SCHREMPP hep-ph 9805492

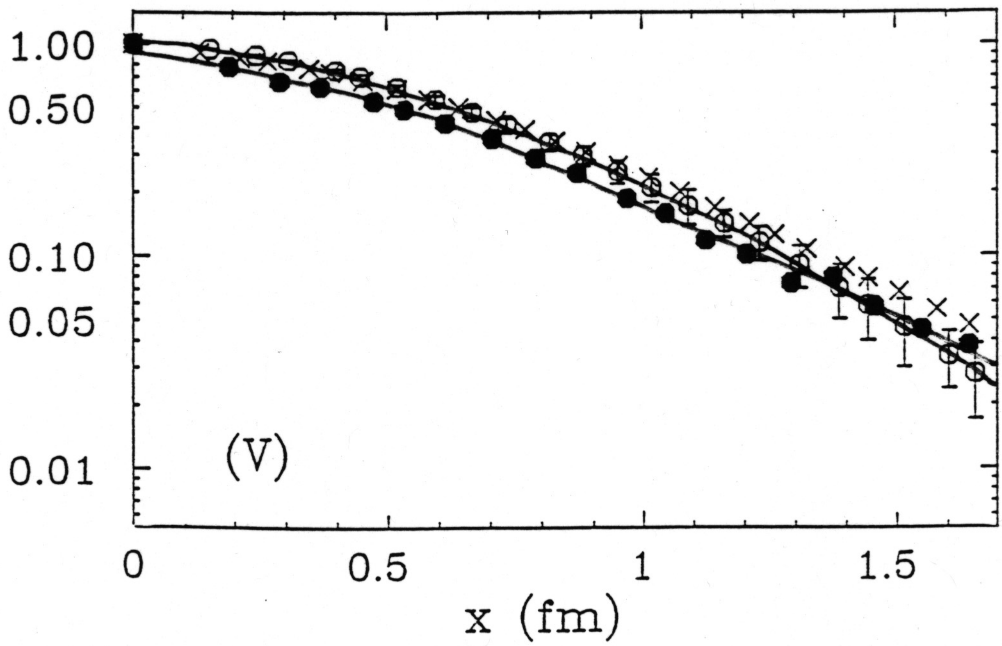


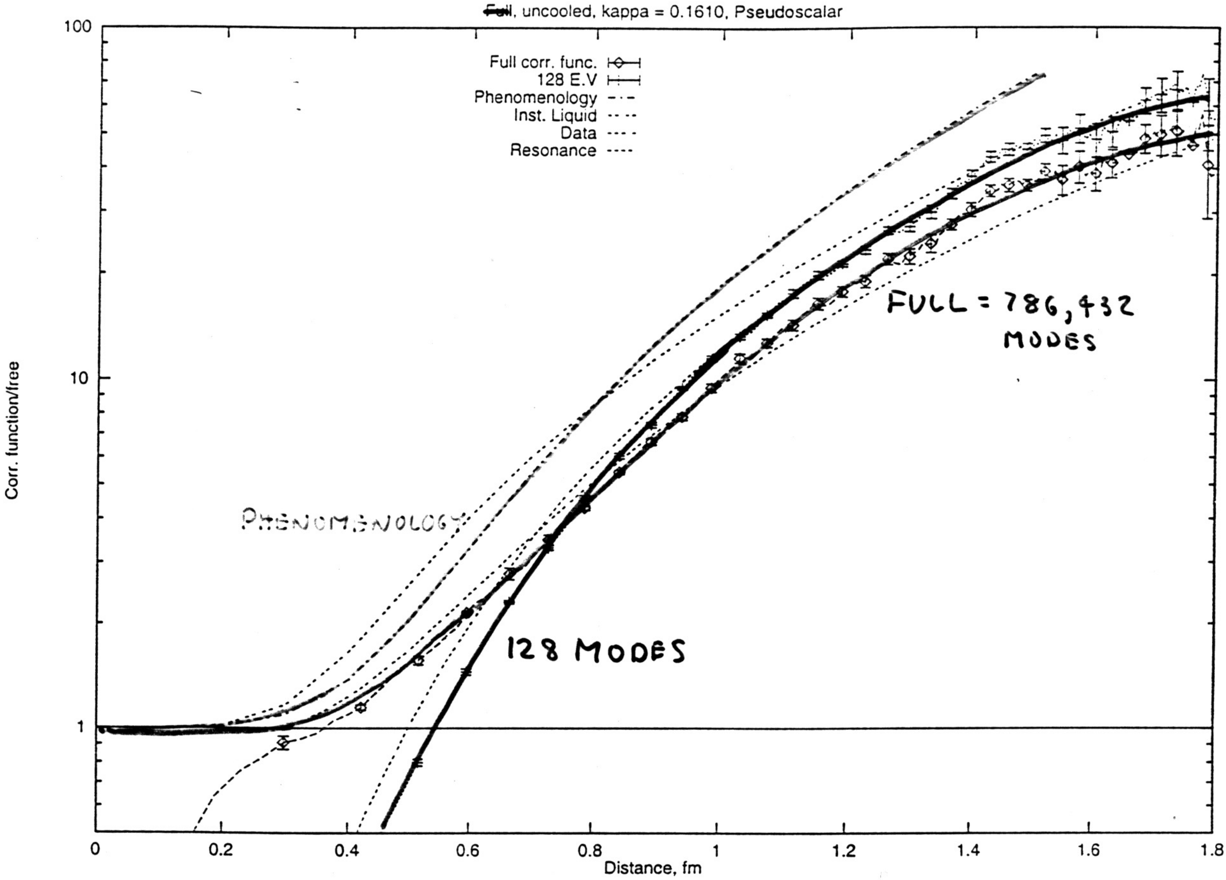
- ALL GLUON CONFIGURATIONS
- INSTANTONS

$$\frac{\langle 0 | J(x)\, J(0) | 0 \rangle_{QCD}}{\langle 0 | J(x)\, J(0) | 0 \rangle_{FREE}} \qquad J = \bar{q}\, \gamma_\mu\, q$$



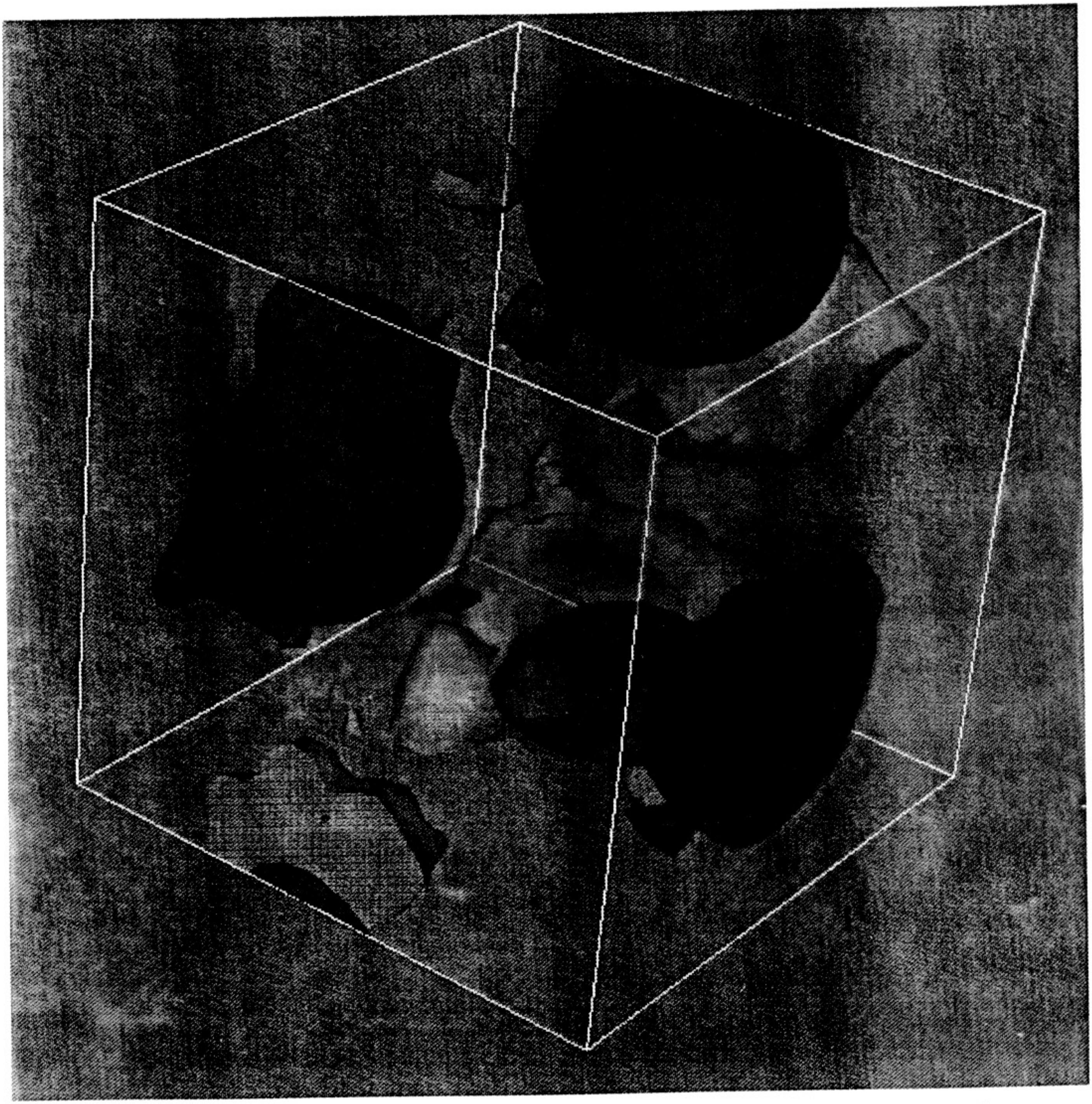
$$\langle \rho | \bar{q}\gamma_0 q(x)\ \bar{q}\gamma_0 q(0) | \rho \rangle$$





QUENCHED $m_a \sim 23$ MeV

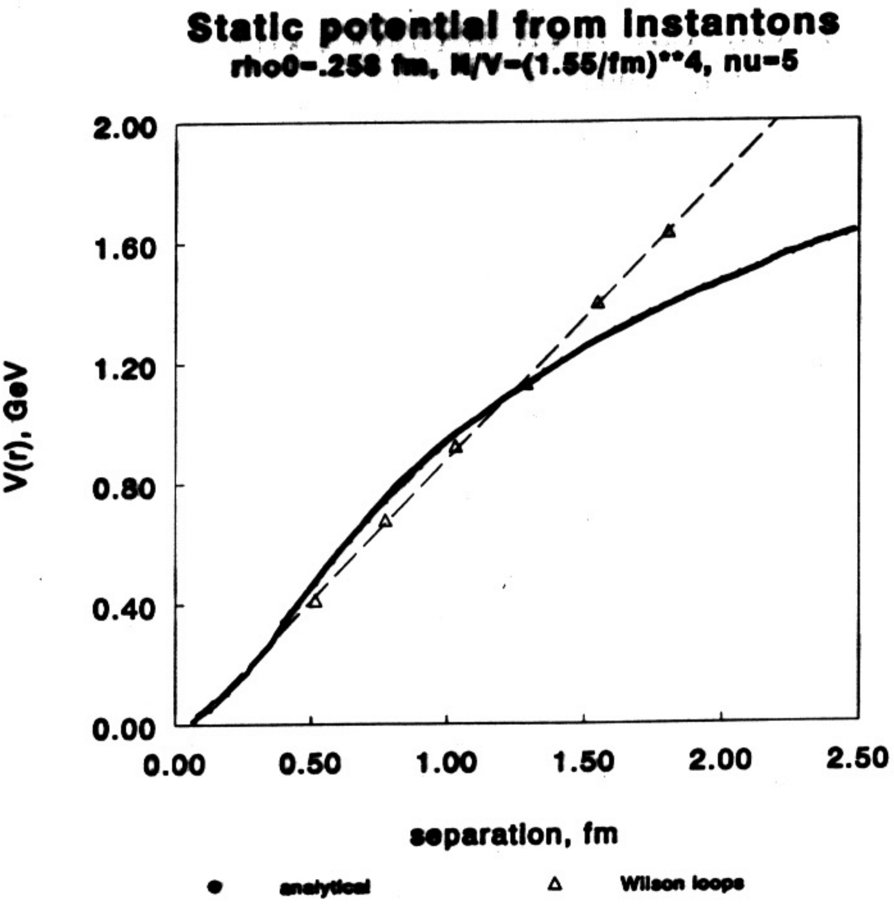
$\bar{\psi} \gamma_5 \psi (x)$ (yellow & blue) **Zero cooling.**



- Dirac eigenmodes see the instantons (no cooling necessary)
- cooling does not distort the instantons very much

Instantons do not confine

Take linear superposition of randomly placed instantons & anti-instantons with random color orientation



2.74 GeV

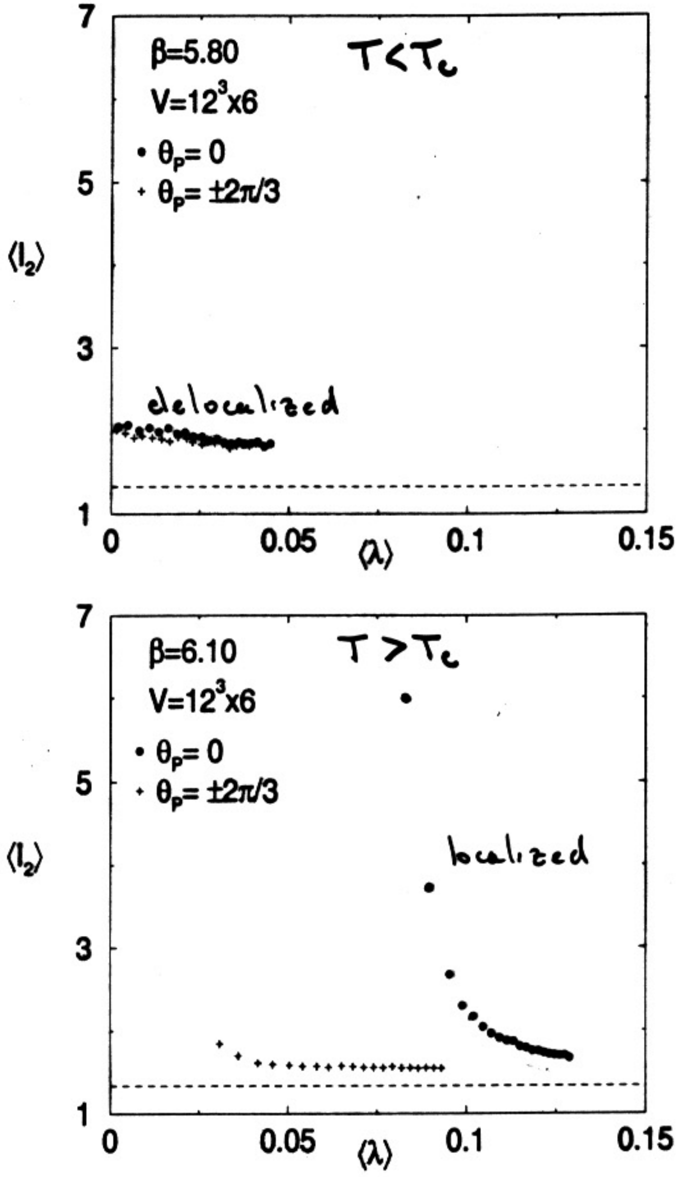
Diakonov & Petrov, hep-lat/9810037

Localization transition

Participation ratio: V $\frac{\sum_x |\psi(x)|^4}{(\sum_x |\psi(x)|^2)^2}$

From 1 (delocalized) to V (localized)

Göckeler et al., hep-lat/0103031



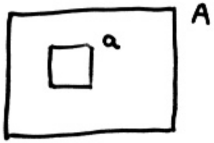
CENTER VORTICES

$\oint e^{i\frac{2\pi}{N}}$

$= -1$ SU(

2-D SHEET IN 4-DIM , LINE IN 3-DIM

WILSON LOOP $\sim (-1)^{\#\text{ ENCLOSED VORTICES}}$



$$W = \sum_{n=0}^{N} \frac{N!}{n!(N-n!)} (-)^n \left(\frac{a}{A}\right)^n \left(1-\frac{a}{A}\right)^{N-n}$$

$$= \left[-\frac{a}{A} + 1 - \frac{a}{A}\right]^N = \left[1 - 2a\underbrace{\frac{N}{A}}_{\rho}\frac{1}{N}\right]^N \to e^{-2\rho a}$$

KEEPING ONLY VORTICES PROJECTED FROM GLUONS GIVES CORRECT STRING TENSION

→

VORTEX STRUCTURE OF VACUUM

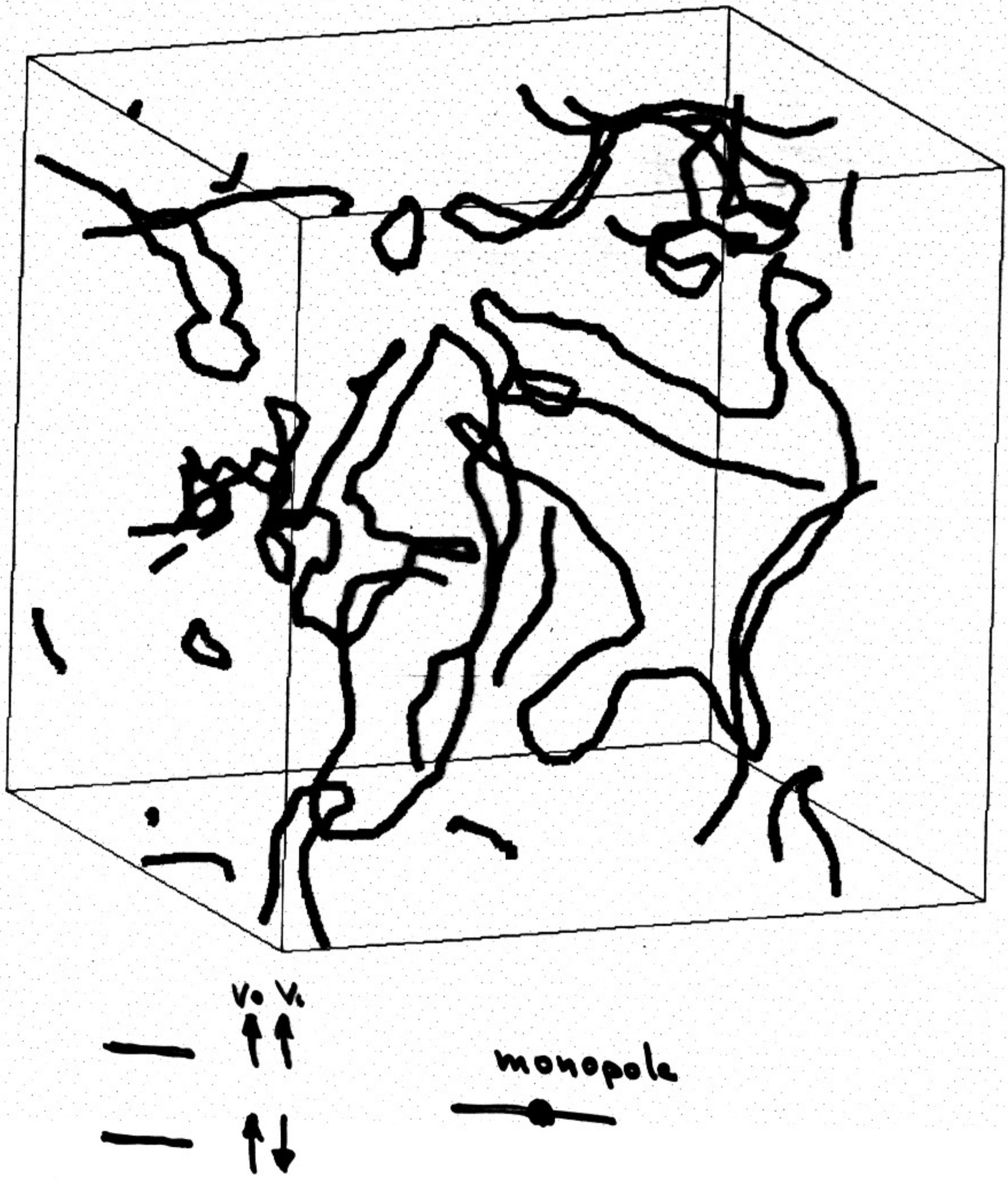
→

PHASE DIAGRAM

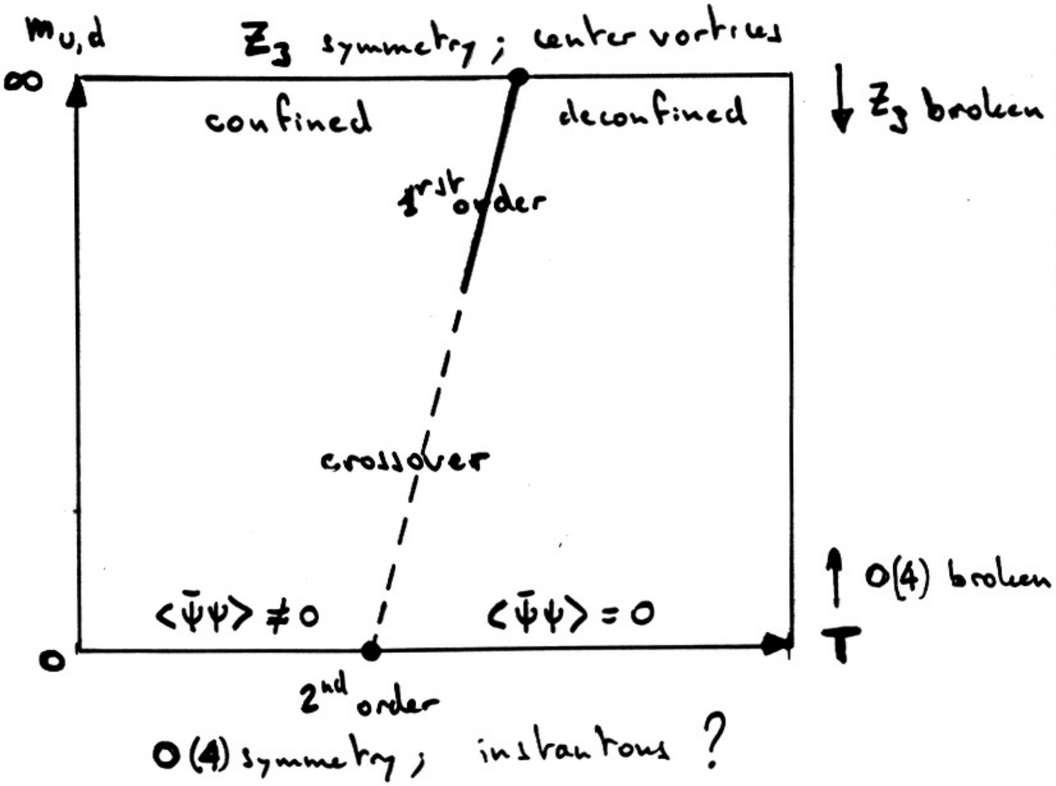
$16^4 \quad \beta = 2.4$

confined

"spaghetti vacuum"



Phase diagram $N_f = 2$



CALCULATION OF HADRON WAVE FUNCTIONS

EVOLUTION IN EUCLIDEAN TIME PRODUCES GROUND STATE

EXPLORE HADRON GROUND STATE WAVE FUNCTION BY:

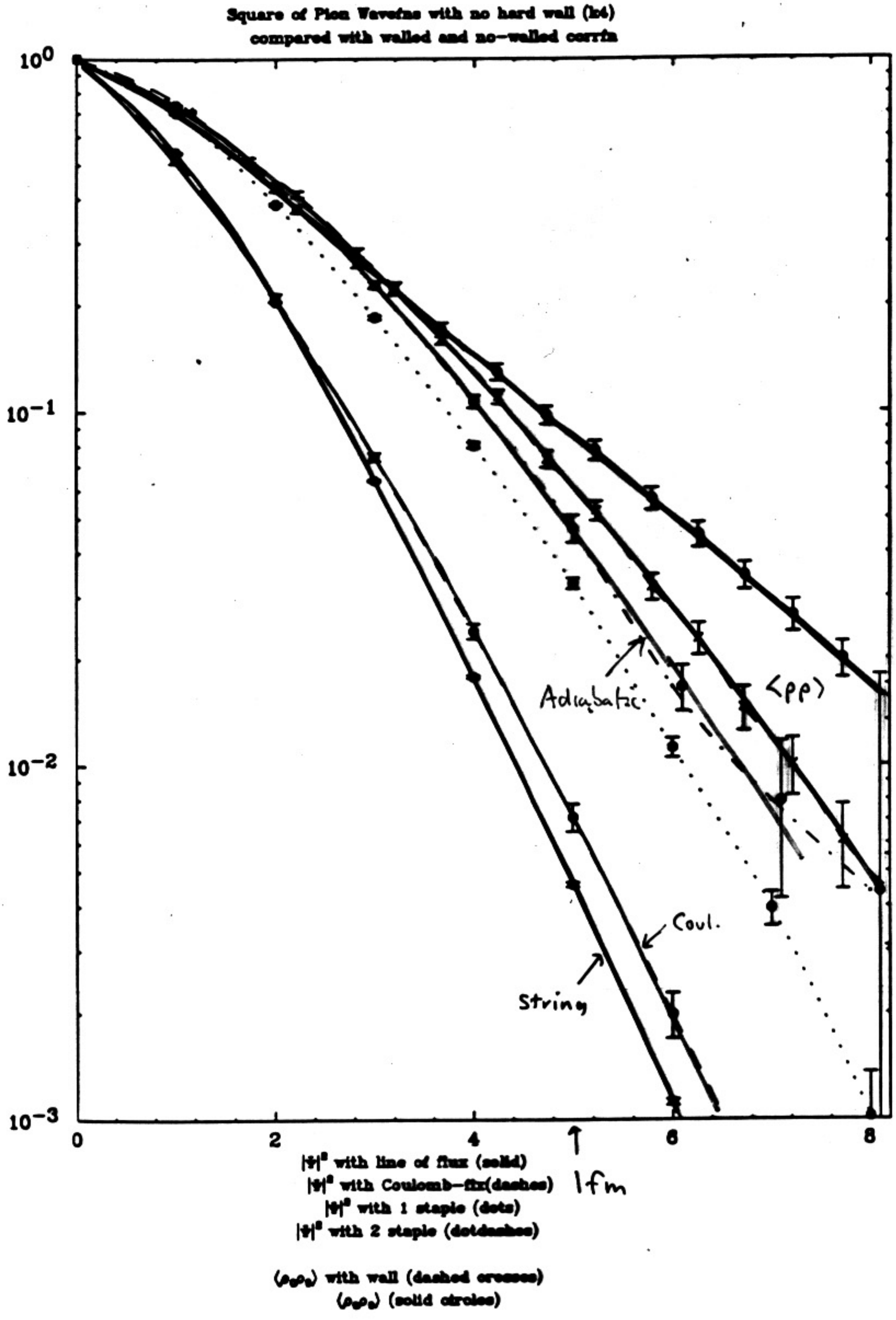
- OVERLAP WITH TRIAL FUNCTION $\langle \Psi_{TRIAL} | \Psi_0 \rangle$
- DENSITY – DENSITY CORRELATION FN $\langle \Psi_0 | \rho(x_1) \rho(x_2) | \Psi_0 \rangle$

EXAMPLE IN PION →

C. ALEXANDROU & Ph. de FORCRAND

- DEFORMATION OF ρ →
- DEFORMATION OF Δ →

$\pi \qquad m_q = 95$



Square of Pion Wavefns with no hard wall (k4) compared with walled and no-walled corrfn

QUARK DISTRIBUTIONS IN MESONS (K.B. TEO)

DEFINITIONS OF WAVEFUNCTIONS

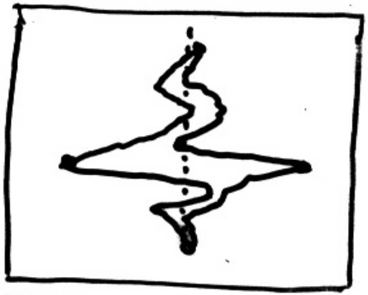
GAUGE FIXED $\langle 0|\psi^\dagger(x)\psi(0)|h\rangle\Big|_{\substack{\text{coul.}\\ \text{or Axial}}}$

STRING $\langle 0|\psi^\dagger(x)e^{i\int A}\psi(0)|h\rangle$

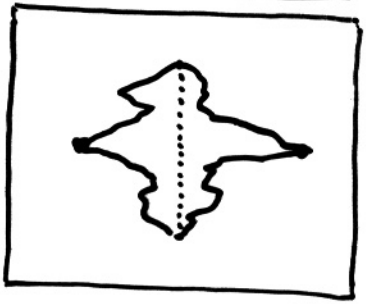
ADIABATIC $\langle\Omega(x)|\psi^\dagger(x)\psi(0)|h\rangle$

CORRELATION FUNCTIONS

$\langle h|\hat{\rho}(x)\,\rho(0)|h\rangle$



$\langle h|\hat{\rho}(x)\,\rho(0)|h\rangle\Big|_{q\bar{q}}$



SEE LINK TO CONSTANTIA ALEXANDROU

Deformation of Pion

Deformation of Delta

CALCULATION OF MOMENTS OF STRUCTURE FUNCTIONS

MOMENTS OF STRUCTURE FUNCTIONS

LINEAR VS CHIRAL EXTRAPOLATIONS

NEED FOR MULTI-TERAFLOPS COMPUTERS

REARRANGED PERTURBATION EXPANSION

Moments of quark and gluon distributions

Moments of quark distributions in the proton

$$\langle x^n\rangle_q = \int_0^1 \mathrm{d}x\, x^n\big(q(x) + (-1)^{n+1}\bar{q}(x)\big)$$
$$\langle x^n\rangle_{\Delta q} = \int_0^1 \mathrm{d}x\, x^n\big(\Delta q(x) + (-1)^{n}\Delta\bar{q}(x)\big)$$
$$\langle x^n\rangle_{\delta q} = \int_0^1 \mathrm{d}x\, x^n\big(\delta q(x) + (-1)^{n+1}\delta\bar{q}(x)\big)$$

where $q = q_\uparrow + q_\downarrow \qquad \Delta q = q_\uparrow - q_\downarrow \qquad \delta q = q_\top + q_\perp$

are related to matrix elements of twist-2 operators

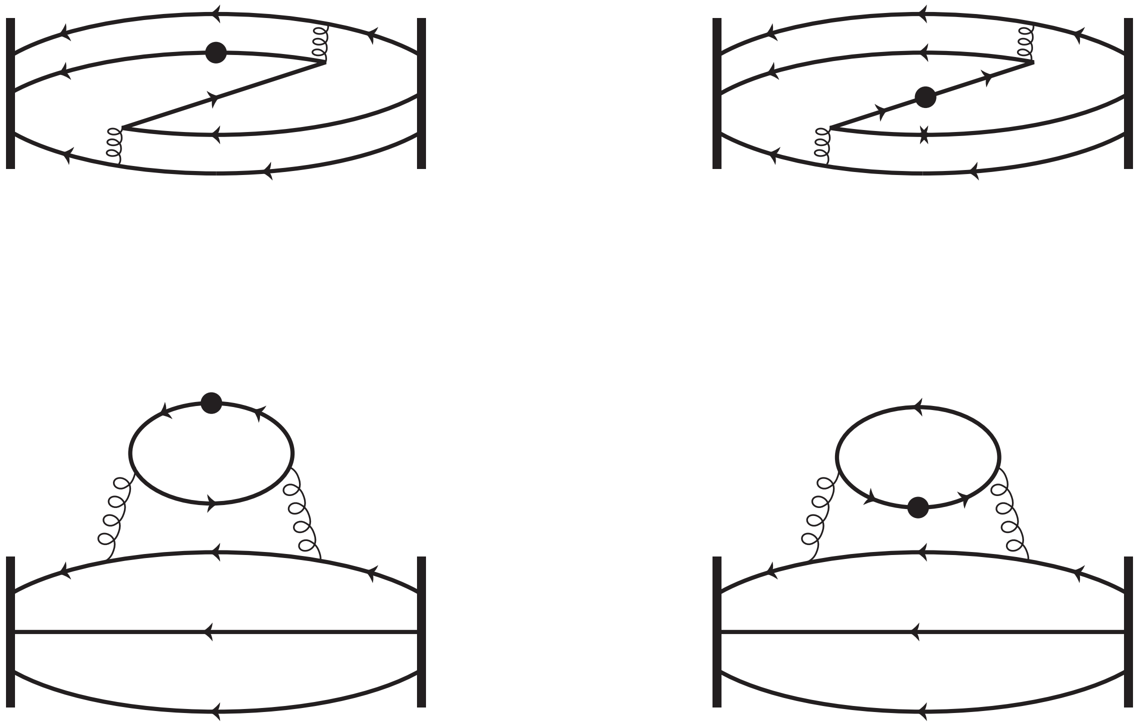
$$\big\langle PS\big|\bar{\psi}\gamma^{\{\mu_1}iD^{\mu_2}\cdots iD^{\mu_n\}}\psi\big|PS\big\rangle = 2\langle x^{n-1}\rangle_q\, P^{\{\mu_1}\cdots P^{\mu_n\}}$$

$$\big\langle PS\big|\bar{\psi}\gamma^{\{\mu_1}\gamma_5 iD^{\mu_2}\cdots iD^{\mu_n\}}\psi\big|PS\big\rangle = 2\langle x^{n-1}\rangle_{\Delta q}\, MS^{\{\mu_1}P^{\mu_2}\cdots P^{\mu_n\}}$$

$$\big\langle PS\big|\bar{\psi}\sigma^{[\alpha\{\mu_1]}\gamma_5 iD^{\mu_2}\cdots iD^{\mu_n\}}\psi\big|PS\big\rangle = 2\langle x^{n-1}\rangle_{\delta q}\, MS^{[\alpha}P^{\{\mu_1]}P^{\mu_2}\cdots P^{\mu_n\}}$$

where $\{\,\}$ ⇒ symmetrization and $[\,]$ ⇒ antisymmetrization

Hadron Matrix Elements on Lattice



- Calculate plateau: measure $\langle \mathcal{O} \rangle$, for m_q, a, L
- Connected diagrams

  $p = 0$

  $p \neq 0$
- Disconnected diagrams
- Extrapolate

  $m_q : m_\pi \to 140\,\text{MeV}$

  $a \to \sim 0.05\,\text{fm}$

  $L \to \sim 5.0\,\text{fm}$
- Note: For $\langle \mathcal{O} \rangle_u - \langle \mathcal{O} \rangle_d$, disconnected diagrams cancel

Chiral Extrapolation of proton matrix elements

- Long-standing puzzle: Linear extrapolation in m_q yields serious discrepancies

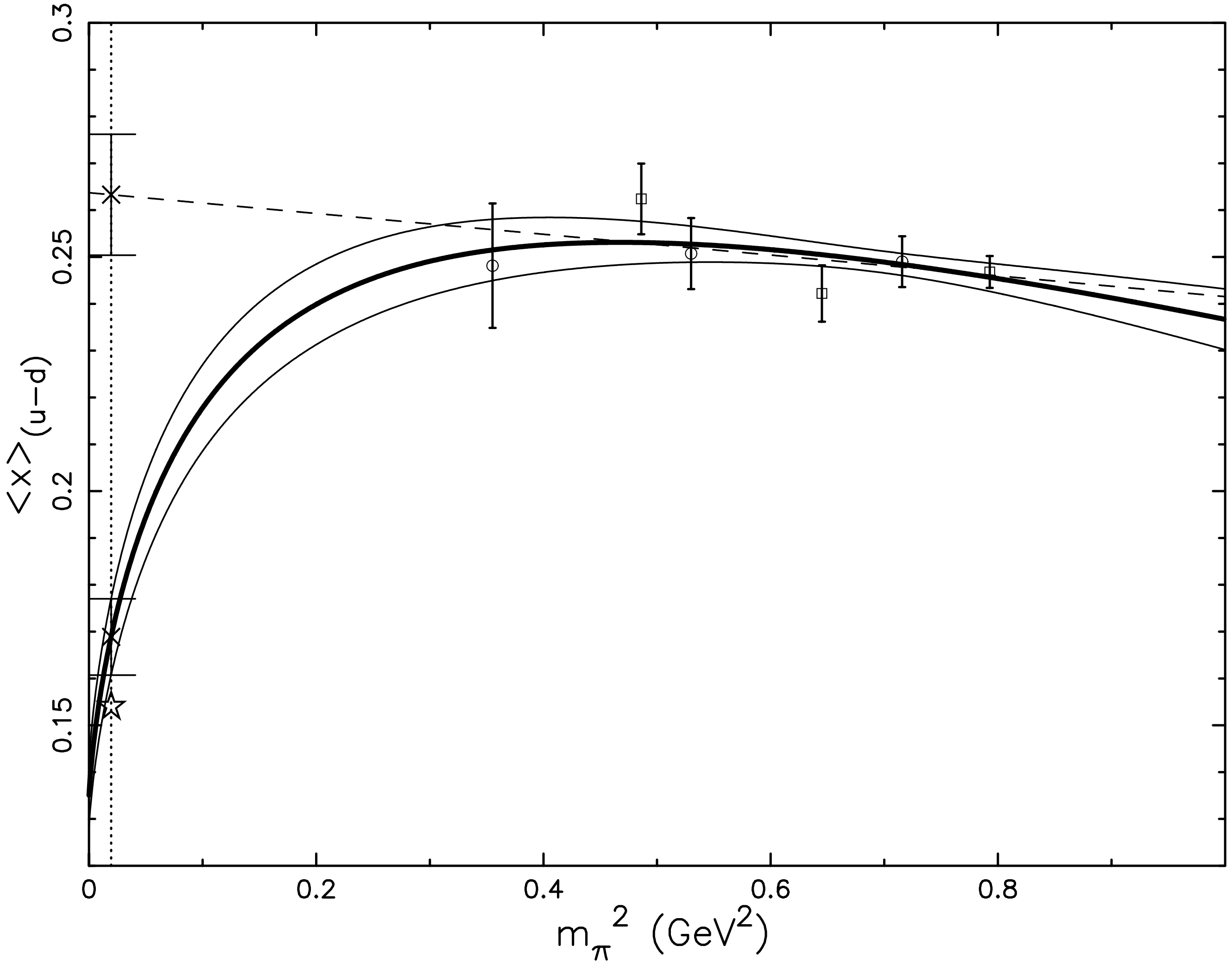
$$\langle x\rangle_u - \langle x\rangle_d \;\sim\; 0.24 - 0.28 \qquad (0.16)$$

$$g_A = \langle 1\rangle_{\Delta u} - \langle 1\rangle_{\Delta d} \sim 1.0 - 1.1 \qquad\qquad (1.26)$$

- Resolution: Chiral extrapolation hep-lat/0103006

Pion cloud is essential

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



SEE LINK TO PAUL RAKOW

CHIRAL EXTRAPOLATION

PERTURBATION EXPANSION
FOR PLAQUETTE

TADPOLE SUMMATION

The Role of Multi-Teraflops Computers

Extrapolate to continuum, infinite volume, and chiral limits:

- $L \to \infty$
- $\frac{1}{g^2} \to 0$
- $m_q : m_\pi^2 \to 0.02$ GeV^2

5% measurement at $m_\pi^2 =$0.05 GeV^2 and lattice spacing $a = 0.1$ fm:

$$N_{\mathrm{OPS}} \sim 0.38 \left[\frac{L}{4}\right]^{4.55} \left[\frac{0.8}{a}\right]^{7.25} \left[\frac{0.3}{m_\pi/m_\rho}\right]^{2.7}$$

~ 8 Tflops-years

STUDY OF SEA QUARK PHYSICS

Thomas Lippert

$$\int d[u] \; \det{}^2 M(u)\, e^{-S_g[u]} = \int d[u] \int d\phi^* d\phi \; e^{-\phi^* M M^\dagger \phi - S_g[u]}$$

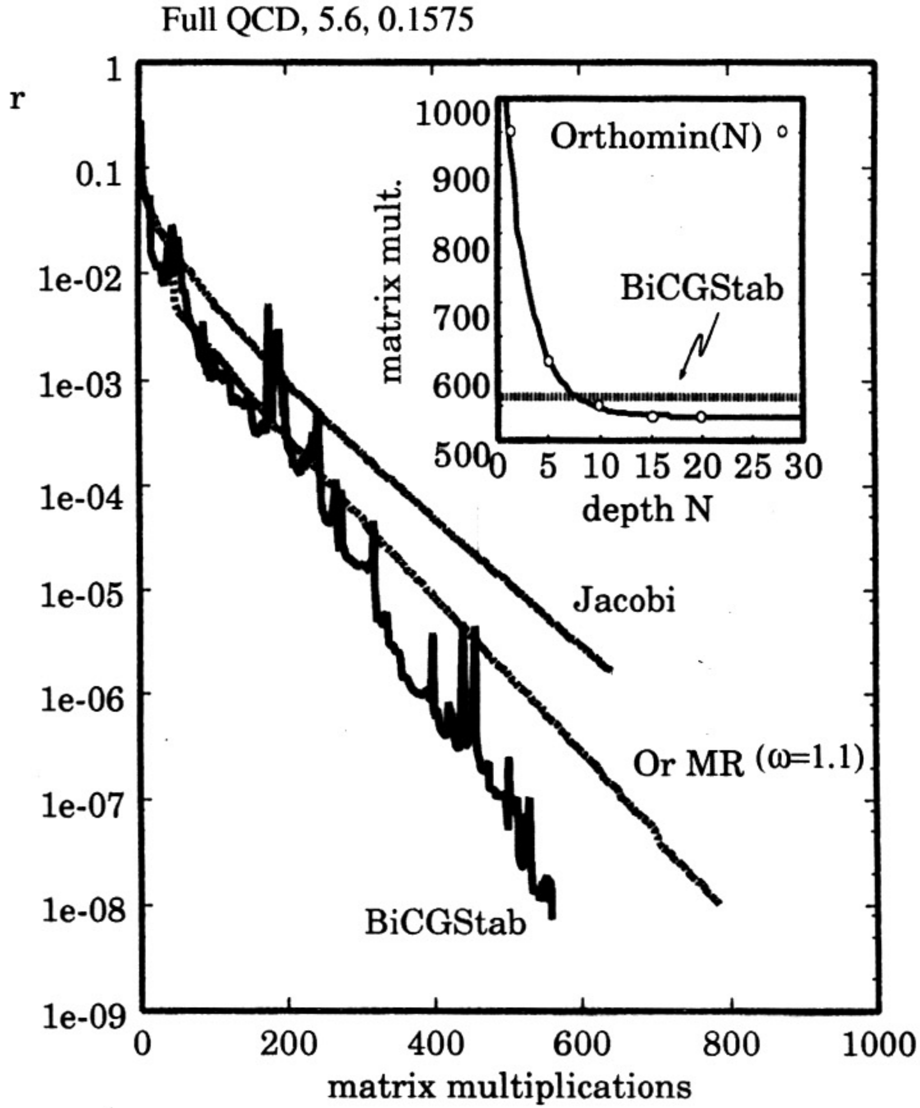
HYBRID M.C.

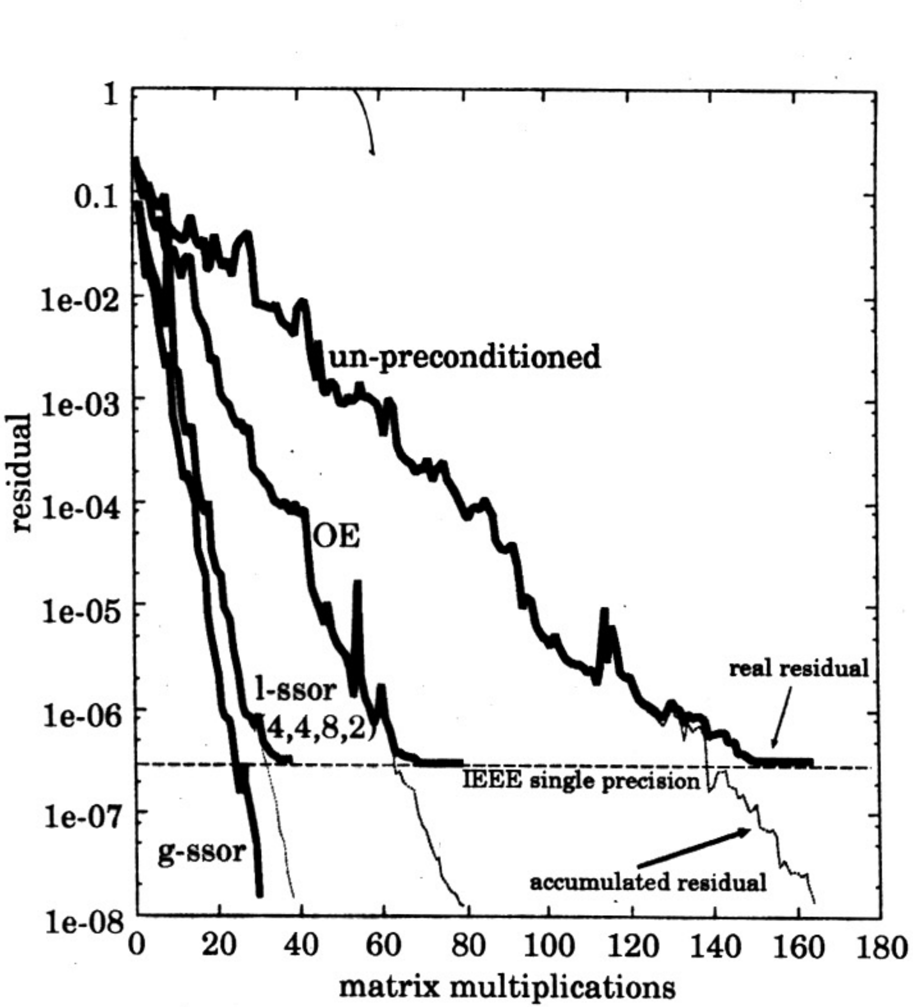
REQUIRES VERY EFFICIENT INVERTER →

RUNNING COUPLING CONSTANT $33 - 2N_f$

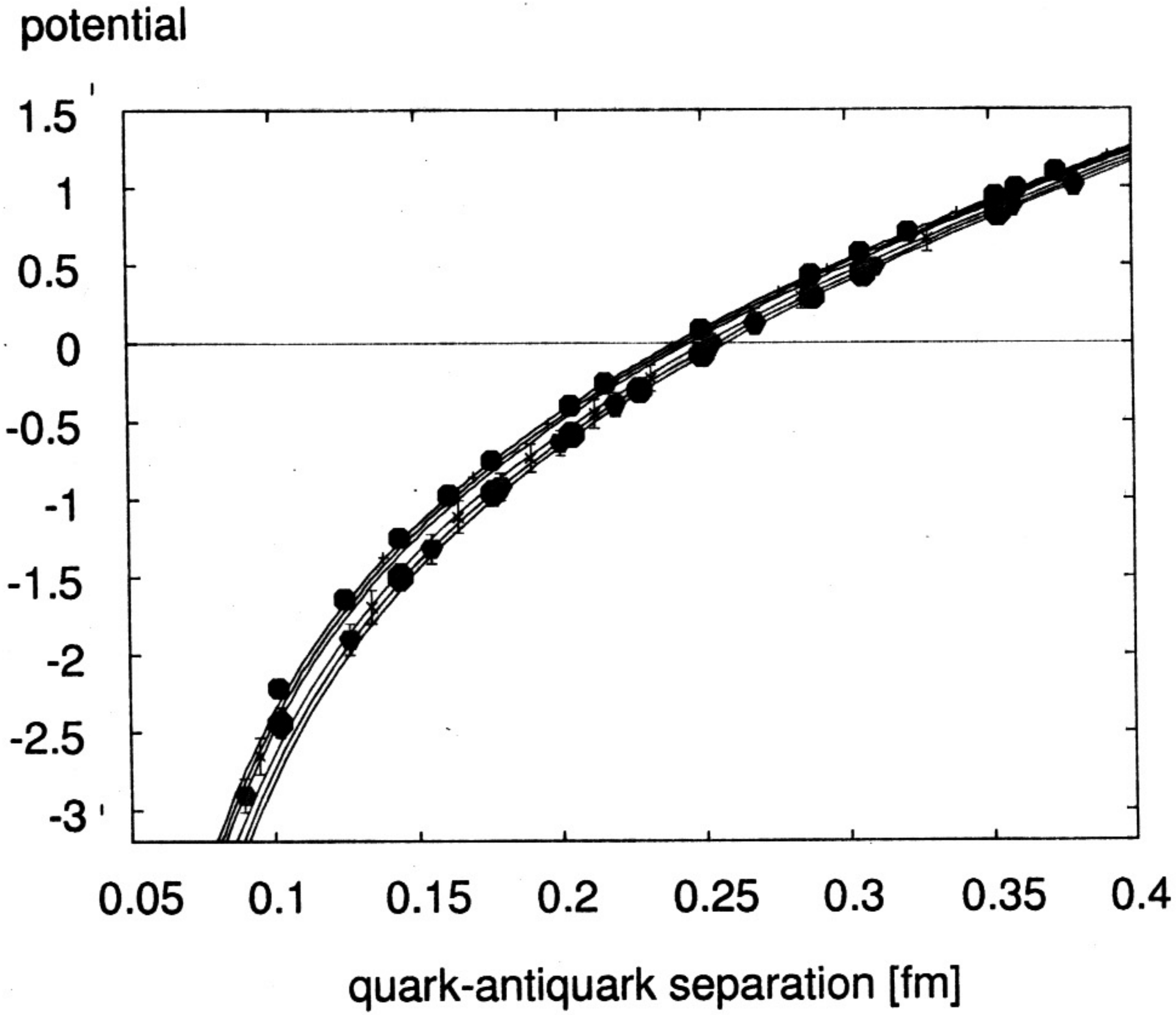
RUNS SLOWER → MORE ATTRACTIVE POTENTIAL →

ELIMINATES DISCREPANCIES IN STRANGE SECTOR


Full QCD, 5.6, 0.1575
r
1
0.1
1e-02
1e-03
1e-04
1e-05
1e-06
1e-07
1e-08
1e-09
0
200
400
600
800
1000
matrix multiplications
1000
900
800
700
600
500
matrix mult.
Orthomin(N)
BiCGStab
0
5
10
15
20
25
30
depth N
Jacobi
Or MR (ω=1.1)
BiCGStab


1
0.1
1e-02
1e-03
1e-04
1e-05
1e-06
1e-07
1e-08
residual
0
20
40
60
80
100
120
140
160
180
matrix multiplications
un-preconditioned
OE
l-ssor
(4,4,8,2)
g-ssor
real residual
IEEE single precision
accumulated residual

N_f dependence



STUDY OF EXOTIC HADRONS

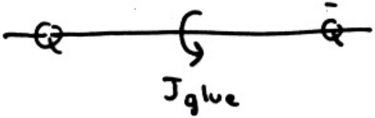
COLIN MORNINGSTAR

QUARK CONFINEMENT PRODUCED BY COLOR FLUX TUBE

(SEE IT ON LATTICE)

N.REL. QUARK MODEL TREATS AS STATIC POTENTIAL

EXCITATION OF FLUX TUBE CAN PRODUCE EXOTIC QUANT. #'s



Λ = PROJECTION OF J_{glue} ALONG AXIS

$$\begin{array}{cccc} = & 0 & 1 & 2 \\ & \Sigma & \Pi & \Delta \end{array}$$

g, u even, odd under CP

$+ \; -$ reflection in plane containing axis

CALCULATE:

ADIABATIC POTENTIALS

BORN OPPENHEIMER W.F.

LATTICE W.F.

SEE LINK TO COLIN MORNINGSTAR

ADIABATIC POTENTIALS

WAVE FUNCTIONS IN ADIABATIC POTENTIALS

LATTICE MASSES IN NRQCD

LATTICE QCD WORKSHOP SUMMARY

LATTICE QCD HAS BECOME AN ESSENTIAL TOOL IN HADRONIC PHYSICS

PROVIDES INSIGHT INTO FUNDAMENTAL ASPECTS OF QCD

ENABLES US TO EXPLORE HADRON WAVE FUNCTIONS

WILL ENABLE CALCULATION OF MOMENTS OF STRUCTURE FNS.

IS REVEALING SEA QUARK PHYSICS

PROVIDES FIRST-PRINCIPLES STUDY OF EXOTIC HADRONS

Cost-Optimized Custom Machines for Lattice QCD

- Highly parallel custom machines much cheaper than general purpose supercomputers

  regular grid structure

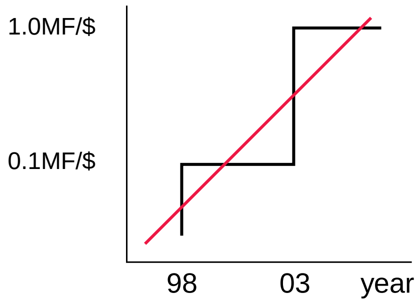
  local communications

  overlapping computation and communications

- Dual approach

  optimization of commodity clusters

  fully custom parallel machine



- Robust strategy to pursue both

4 Compute Engines for Lattice-QCD

- APE100: INFN, 25.6 Gflops (QH4 largest unit) (1994)
- CP-PACS: Tsukuba Center for Computational Physics and HITACHI, 600 Gflops (1996)
- Columbia-QCDSP: Columbia University, 100 Gflops (largest unit?) (1997)
- Cluster Computers: e.g. ALiCE, 160 Gflops (2000)
- APEmille: INFN/DESY, 64 Gflops (largest unit) (2001)

- Columbia-~~QCDSP~~ QCDOC: Columbia University/UKQCD, 10 Tflops (2003)
- apeNEXT: INFN/DESY, 5 Tflops (2004)
- Clusters: Jefferson Lab/MIT, FNAL, 10 Tflops (2004/5)

SUMMARY AND CONCLUSIONS

TWO VIABLE COST-OPTIMIZED TECHNOLOGIES:

CLUSTERS AND CUSTOM MACHINES

$O(1\$/\text{MFLOP})$

SOFTWARE CHALLENGE: PLATFORM INDEPENDENT HIGH LEVEL PHYSICS CODE THAT RUNS EFFICIENTLY ON CLUSTERS AND CUSTOM MACHINES

RESOURCES REQUIRED FOR FUNDAMENTAL IMPACT MODEST ON SCALE OF CONTEMPORARY EXPERIMENTS

\$10 M ↔ 10 TERAFLOPS SUSTAINED

COMMUNITY MUST WEIGH COST/BENEFIT OF THIS INVESTMENT AS PART OF OVERALL INVESTMENT IN FACILITIES FOR HADRONIC PHYSICS