Lattice QCD in Hadronic Physics

John W. Negele

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

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
    - $1 / \text{Mflop}$
    - 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 $\rightarrow$ Coulomb potential
    - mesons $\rightarrow$ N-N potential
  - Most of mass from fermion constituents

Nucleons
  - Quarks are confined
  - Gluons are essential degrees of freedom
    - Carry half of momentum
    - Nonperturbative 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
    \[ |\langle \psi_{\text{trial}} | \psi_{\text{exact}} \rangle|^2 \]
  ○ Explore dependence on
    \[ m_q, \quad N_f, \quad N_c \]
Lattice QCD

Euclidean:

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

\[
\langle T e^{-\beta H} \psi \psi \cdot \cdot \cdot \bar{\psi} \bar{\psi} \bar{\psi} \rangle
\]

\[
= \frac{1}{Z} \int \mathcal{D}[\psi] \mathcal{D}[\bar{\psi}] \mathcal{D}[A] e^{-\int d^4x [\bar{\psi}(\partial + m + igA) \psi + \frac{1}{4} F_{\mu\nu}^2]} \bar{\psi} \psi \psi \cdot \cdot \cdot \bar{\psi} \bar{\psi} \bar{\psi}
\]

\[
\to \prod_n \frac{1}{Z} \int d\psi_n d\bar{\psi}_n dU_n e^{-\sum_n [\bar{\psi} M(U) \psi + S(U)]} \bar{\psi} \psi \psi \cdot \cdot \cdot \bar{\psi} \bar{\psi} \bar{\psi}
\]

\[
= \prod_n \int dU_n \frac{1}{Z \det M(U)} e^{-S(U)} \sum M^{-1}(U)M^{-1}(U) \cdots M^{-1}(U)
\]

Sample with M.C.

\[
\to \frac{1}{N} \sum_{U_i \in \frac{\det M(U)}{Z} e^{-S(U)}} M^{-1}(U_i)M^{-1}(U_i)M^{-1}(U_i)
\]

\[
S(U) = \sum_{\Box} \frac{2N}{g^2} (1 - N^{-1} \text{ReTr} U_{\Box}) \to \frac{1}{4} F_{\mu\nu}^2 U_{\Box} \equiv U_1 U_2 U_3 U_4^t \u^t
\]

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

\[ \langle T e^{-\beta H} \hat{\psi} \hat{\psi} \hat{\psi} \cdots \hat{\psi} \hat{\psi} \rangle \]
\[ = Z^{-1} \int D(U) e^{\ln \det M(U) - S(U)} M^{-1}(U) e^{-\bar{\psi} M(U) \psi} \]
\[ = Z^{-1} \int D(U) e^{\ln \det M(U) - S(U)} \sum M^{-1}(U) M^{-1}(U) \cdots M^{-1}(U) \]

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

2. \( \ln \det M \) generates closed loops of \( U \)'s
   \[ \rightarrow \text{Sum over all } \bar{q}q \text{ excitations from sea} \]
   \[ \text{omit in quenched approximation} \]

3. \( S(U) \) tiles with plaquettes
   \[ \rightarrow \text{sum all gluons} \]

32^3 \times 64 \text{ lattice} \rightarrow 10^8 \text{ gluon variables}
Physics Opportunities

Nucleon structure

- Form factors

  Electromagnetic \( G_E(q^2) \) \( G_M(q^2) \)

  Pion cloud essential – demanding lattice calculation
  
  large volume \( L^3 \)
  
  small \( m_q \)

  Axial \( G_A \)

Strange form factor

  Parity-violating electron scattering measures
  strange quark content of nucleon
  
  \( \langle r^2 \rangle^{1/2}_{\text{strange}}, \langle \mu \rangle_{\text{strange}} \)

  Sea quark physics – disconnected diagrams
Nucleon structure (cont.)

\[ x f(x, Q) \]

Parton distributions at \( Q = 5 \) GeV

- Moments of quark and gluon distributions

Leading twist

\[
\langle p | \bar{\psi} \gamma_\mu D \cdots D \psi | p \rangle \rightarrow \int dx \, x^n (q_\uparrow(x) + q_\downarrow(x))
\]

\[
\langle p | \bar{\psi} \gamma_5 \gamma_\mu D \cdots D \psi | p \rangle \rightarrow \int dx \, x^n (q_\uparrow(x) - q_\downarrow(x))
\]

\[
\langle p | \bar{\psi} \gamma_5 \sigma_{\mu\nu} D \cdots D \psi | p \rangle \rightarrow \int dx \, x^n (q_\uparrow(x) - q_\downarrow(x))
\]

Higher twist

\[ \langle p | \bar{\psi} \tilde{F}^{\mu\nu} \gamma_5 \gamma_\mu \psi | p \rangle, \ldots \]

Generalized parton distributions

\[ \langle p' | \bar{\psi} O D \cdots D | p \rangle \]
Physics Opportunities *(cont.)*

**Spectroscopy**

- $N^*$ spectrum
  - Number and structure of states
  - Flux tube confinement
  - Fine and hyperfine structure
  - Transition form factors

- Glueballs
- Exotics, $H$
Physics Opportunities (cont.)

Hadron-hadron interactions

- Heavy-light mesons and baryon interactions
  - Light quark exchange
  - Gluon contributions

Fundamental aspects of QCD

- Chiral symmetry breaking
  - Role of instantons, zero modes
- Confinement
  - Role of center vortices, monopoles
- Dense hadronic matter
  - Phases and equation of state

Adiabatic potential for $I = S = 0$ heavy-light mesons
Overlap between $|\psi_J\rangle$ and $|0\rangle$

\[
\langle J(t_3) J(t_1) \rangle = \sum_n |\langle \psi_J | n \rangle|^2 e^{-E_n (t_3 - t_1)}
\]

\[
A = \sum_n |\langle \psi_J | n \rangle|^2
\]

\[
B = |\langle \psi_J | 0 \rangle|^2
\]

\[
\frac{B}{A} = \frac{|\langle \psi_J | 0 \rangle|^2}{\sum_n |\langle \psi_J | n \rangle|^2} = \frac{|\langle \Psi_J | 0 \rangle|^2}{\langle J J \rangle} = P(0)
\]

\[
\frac{A - B}{B} = \frac{\sum_{n \neq 0} |\langle \psi_J | n \rangle|^2}{|\langle \psi_J | 0 \rangle|^2} = \frac{P(n > 0)}{P(0)}
\]

Optimize

- Vary parameters in trial function to maximize $P(0)$
- Tool to study physics of wave functions
CALCULATION OF MASSES AND WAVE FUNCTIONS:

2-POINT FUNCTIONS

\[ -\frac{\partial}{\partial H} \]
\[ \langle T e^{\int_{t_1}^{t_2} J(t) J^+(t') dt'} \rangle \]
\[ = \langle 0 | J \sum_n e^{-E_n(t_1-t_2)} \langle n | J^+ | \Omega \rangle \]]
\[ \rightarrow_{t_1 \to t_2} |\langle 0 | J | \Omega \rangle|^2 e^{-E_0(t_1-t_2)} \]

\( E_0 = \text{mass of lowest hadron} \)
\( \text{with quantum numbers of } J^+(|\Omega\rangle) \)

\[ \langle 0 | J | \Omega \rangle = \langle \Psi_0 | \Psi_J \rangle \]
\( \text{overlap of ground state } \Psi_0 \)
\( \text{with trial function } \Psi_J \)
Lattice Measurement of Overlap

- Graph 1: Graph showing $D(t)$ versus $t$ with two curves labeled A and B. The number of data points is $N = 65$.

- Graph 2: Graph showing $P(0)$ versus $\langle r \rangle^{1/2}$ with several data points.
Definition of Wave Functional of Quarks & Gluons

Explicitly or implicitly specify W.F. for Gluons \( \Psi[n(\vec{r}), \vec{A}(\vec{r})] \)

We consider 3 definitions

1) Axial Gauge \( \equiv \) String W.F. for Glue

\[
\left. \langle \Omega \left| \bar{q}(x) q(0) \right| \hbar \rangle \right|_{\text{AXIAL}} = \langle \Omega \left| e^{i \int_0^x A \cdot dx'} \bar{q}(x) q(0) \right| \hbar \rangle
\]

\[
\Psi[A]
\]

2) Coulomb Gauge Analogous (Write for QED)

\[
\left. \langle \Omega \left| \bar{q}(x) q(0) \right| \hbar \rangle \right|_{\text{COULOMB}} = \langle \Omega \left| e^{i \int d^3x \vec{E}_{\text{COUL}}(x) \cdot \vec{A}(x)} \bar{q}(x) q(0) \right| \hbar \rangle
\]

\[
\Psi[A]
\]

\[
\int \vec{A} \cdot \vec{E}_{\text{COUL}} = \int \vec{A} \cdot \vec{\nabla} \phi = -\int (\vec{\nabla} \cdot \vec{A}) \phi \rightarrow 0
\]

3) Adiabatic

\[
\left. \langle \hat{\Omega} \left| \bar{q}(x) q(0) \right| \hbar \rangle \right|
\]

\[
| \hat{\Omega}(x) \rangle = \text{QCD Ground State with static } q\bar{q}
\]

Compare \( |\psi|^2 \) with density \( \langle h \left| \hat{\rho}(x) \hat{\rho}(0) \right| h \rangle \)
Quark Distributions in Mesons

Definitions of Wave Functions

Gauge Fixed: \[ \langle 0 | \psi(x) \psi(0) | h \rangle \]

String: \[ \langle 0(\psi(x)e^{iS_A} \psi(0)) | h \rangle \]

Adiabatic: \[ \langle s(x) | \psi(x) \psi(0) | h \rangle \]

Correlation Functions

\[ \langle h | \hat{\rho}(x) \rho(0) | h \rangle \]

\[ \langle h | \hat{\rho}(x) \rho(0) | h \rangle \bigg|_{\bar{q}q} \]
Square of Pion Waves with no hard wall (k4)
compared with walled and no-walled correl.

| $|\eta|^2$ with line of flux (solid) |
| $|\eta|^2$ with Coulomb-flux(dashes) |
| $|\eta|^2$ with 1 staple (dots) |
| $|\eta|^2$ with 2 staple (dotdashes) |

(\pi^0) with wall (dashed crosses)
(\pi^0) (solid circles)
Calculation of Matrix Elements on Euclidean Lattice

\( J^\dagger: \) Current with quantum number of proton

\[ |\psi_J\rangle = J^\dagger|\Omega\rangle \quad \text{Trial function} \]

\[
\langle T J(t_3) \mathcal{O}(t_2) J^\dagger(t_1) \rangle = \sum_{m,n} \langle \psi_J|n\rangle \langle n|\mathcal{O}|m\rangle \langle m|\psi_J\rangle e^{-E_n(t_3-t_2)-E_m(t_2-t_1)}
\]

\[
|\langle \psi_J|0\rangle|^2 \langle 0|\mathcal{O}|0\rangle e^{-E_0(t_3-t_1)}
\]

Want \( |\langle \psi_J|n\rangle|^2 \sim \delta_{n0} \) for best plateau

Normalize:

\[
\langle T J(t_3) J^\dagger(t_1) \rangle = \sum_n |\langle \psi_J|n\rangle|^2 e^{-E_n(t_3-t_1)}
\]

\[
|\langle \psi_J|0\rangle|^2 e^{-E_0(t_3-t_1)} \quad \xrightarrow{t_3-t_1 \gg 1} \quad |\langle \psi_J|0\rangle|^2 e^{-E_0(t_3-t_1)}
\]

\[
\langle 0|\mathcal{O}|0\rangle = \frac{\langle J\mathcal{O}J^\dagger \rangle}{\langle JJ^\dagger \rangle} = \frac{\begin{array}{c}
\bullet
\
\end{array}}{\begin{array}{c}
\otimes
\end{array}}
\]
• Calculate plateau: measure $\langle O \rangle$, for $m_q$, $a$, $L$

• Connected diagrams
  
  \[ p = 0 \]
  
  \[ p \neq 0 \]

• Disconnected diagrams

• Extrapolate

  \[ m_q : m_\pi \rightarrow 140 \text{ MeV} \]
  
  \[ a \rightarrow \sim 0.05 \text{ fm} \]
  
  \[ L \rightarrow \sim 5.0 \text{ fm} \]

• Note: For $\langle O \rangle_u - \langle O \rangle_d$, disconnected diagrams cancel
Moments of quark and gluon distributions

Moments of quark distributions in the proton

\[ \langle x^n \rangle_q = \int_0^1 dx \, x^n (q(x) + (-1)^{n+1} \bar{q}(x)) \]

\[ \langle x^n \rangle_{\Delta q} = \int_0^1 dx \, x^n (\Delta q(x) + (-1)^n \Delta \bar{q}(x)) \]

\[ \langle x^n \rangle_{\delta q} = \int_0^1 dx \, x^n (\delta q(x) + (-1)^{n+1} \delta \bar{q}(x)) \]

where \( q = q_\uparrow + q_\downarrow \quad \Delta q = q_\uparrow - q_\downarrow \quad \delta q = q_\perp + q_\perp \)

are related to matrix elements of twist-2 operators

\[ \langle PS | \bar{\psi} \gamma^{\mu_1} i D^{\mu_2} \ldots i D^{\mu_n} \psi | PS \rangle = 2 \langle x^{n-1} \rangle_q P^{\mu_1} \ldots P^{\mu_n} \]

\[ \langle PS | \bar{\psi} \gamma^{\mu_1} \gamma_5 i D^{\mu_2} \ldots i D^{\mu_n} \psi | PS \rangle = 2 \langle x^{n-1} \rangle_{\Delta q} MS^{\mu_1} P^{\mu_2} \ldots P^{\mu_n} \]

\[ \langle PS | \bar{\psi} \sigma^{\alpha} \gamma^{\mu_1} \gamma_5 i D^{\mu_2} \ldots i D^{\mu_n} \psi | PS \rangle = 2 \langle x^{n-1} \rangle_{\delta q} MS^{\alpha} P^{\mu_1} P^{\mu_2} \ldots P^{\mu_n} \]

where \{ \} \Rightarrow \text{symmetrization and} \ [ ] \Rightarrow \text{antisymmetrization}
Plateaus in full QCD for operators with $p = 0$
**Rule of Classical Solutions in Quantum Field Theory**

**Instantons (Points)**

**Monopole Lines**

**Vortex Sheets**

**Example: Instantons**

**Tunneling Solution**

\[ i + \alpha \rightarrow \frac{d^2x}{dt^2} = -\nabla (\nu) \]

**Find by Relaxation**

("cooling")

**Measure Distribution**

**In Ground State**

**Find Observables Calculated with Only Instantons Close to Those Including All Gluons**

See Quark Zero Modes in Spectrum

**Localized at Instantons**

**Domiante \( \rho, \pi, q^1 \) Contributions to 2-Point Functions**
UKQCD DATA REPRODUCED BY RINGUARD & SCHREMPF hep-ph 9805492
ALL GLUON CONFIGURATIONS

\[ \frac{\langle 0 | J(x) J(0) | 0 \rangle_{\text{QCD}}}{\langle 0 | J(x) J(0) | 0 \rangle_{\text{FRSB}}} \]

\[ J = \bar{q} \gamma_{\mu} q \]

\begin{align*}
\langle 0 | \bar{q} \gamma_5 \gamma_\mu q(x) \bar{q} \gamma_0 \gamma_\nu q(0) | 0 \rangle
\end{align*}

\begin{align*}
x (\text{fm})
\end{align*}

\begin{align*}
\text{(V)}
\end{align*}
Figure 5-8: The lowest 64 modes of the Dirac operator on one selected lattice after 0 and 100 relaxation steps. $\kappa = 0.1600$ on both graphs and large negative values on the lower graph indicated that $\kappa_c$ for this configuration is much lower ($\approx 0.125$).
QUENCHED $m_a \sim 23$ MeV
The Role of Multi-Teraflops Computers

Extrapolate to continuum, infinite volume, and chiral limits:

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

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

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

$\sim 8 \text{ Tflops-years}$
UKQCD DATA REPRODUCED BY RINGUACO & SCHERER

UKQCD Collaboration '98,
D.A. Smith and M.J. Teper

\[ D(\rho) \left[ \text{1/fm}^6 \right] \]

\[ \rho [\text{fm}] \]

\[ \alpha \rho^6 \]
Chiral Extrapolation of proton matrix elements

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

\[ \langle x \rangle_u - \langle x \rangle_d \sim 0.24 - 0.28 \quad (0.16) \]

\[ g_A = \langle 1 \rangle_{\Delta u} - \langle 1 \rangle_{\Delta d} \sim 1.0 - 1.1 \quad (1.26) \]

- Resolution: Chiral extrapolation

Pion cloud is essential

\[ \langle x^n \rangle_u - \langle x^n \rangle_d \sim a_n \left[ 1 - \frac{(3g_A^2 + 1)m^2_\pi}{(4\pi f_\pi)^2} \ln \left( \frac{m^2_\pi}{m^2_\pi + \mu^2} \right) \right] + b_n m^2_\pi \]
Chiral Extrapolation of proton magnetic moment

D. Leinweber, D. Lu, and A. Thomas  
hep-lat/0103006

![Graph showing the relationship between nucleon magnetic moment ($\mu_N$) and $m_\pi^2$.]
Workshop talks

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*