Computational QCD

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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
  - 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

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

- \( M^{-1} = (I + \kappa U)^{-1} \) connects \( \Psi \)'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
  - \( \rightarrow \) Sum over all gluons
- \( 32^3 \times 64 \) lattices \( \rightarrow 10^8 \) gluon variables
Computational Issues

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

\[
\frac{1}{m_\pi} \leq \frac{L}{4}
\]

<table>
<thead>
<tr>
<th>L (fm)</th>
<th>(m_\pi) (Mev)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.6</td>
<td>500</td>
</tr>
<tr>
<td>4.0</td>
<td>200</td>
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<tr>
<td>5.7</td>
<td>140</td>
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- Cost \(\sim (m_\pi)^{-7} - (m_\pi)^{-9}\)
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 $\sim 3\%$
Lattice QCD Predictions

$D \rightarrow Kl\nu$

$f_+(q^2)$ vs. $q^2/m_{D_s^*}^2$

- Experiment [Belle, hep-ex/0510003]
- Lattice QCD [Fermilab/MILC, hep-ph/0408306]
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 $T = (192 \pm 11) \text{ MeV}$

**RBC-Bielefeld, preliminary**

pressure increased slightly with smaller quark mass

F. Karsch – p.7/21
Transition temperature in QCD


extrapolation to chiral and continuum limit

\[(r_0 T_c)_{N_f} = (r_0 T_c)_{cont.} + b (m_{PS} r_0)^d + c/N_f^2\]

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

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

\[\Rightarrow T_c = 192(7)(4)\ MeV\]

(1st error: stat. error on $\beta_c$ and $r_0$; 2nd error: $N_f^{-2}$ extrapolation)

F. Karsch – p.9/21
Phase diagram at non-zero chemical potential

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

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

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

$T_c(\mu) = 1 - 0.0056(4)(\mu_B/T)^2$

deForcrand, Philipsen (imag. $\mu$)

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

Bielefeld-Swansea

(O($\mu^2$) reweighting)

search for critical point

RHIC, LHC

low energy RHIC

F. Karsch – p.13/21
Fluctuations in baryon number density

baryon number density fluctuations:
(Bielefeld-Swansea, PRD68 (2003) 014507)

\[ \mu \geq 0, \ n_f = 2 \]

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

\[ = \frac{9}{V} \left( \langle N_B^2 \rangle - \langle N_B \rangle^2 \right) \]

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
Thermal meson correlation functions

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

\[ G^\beta_H(\tau, \vec{r}) = \int_0^\infty d\omega \int \frac{d^3\vec{p}}{(2\pi)^3} \sigma_H(\omega, \vec{p}, T) e^{i\vec{p}\cdot\vec{r}} \frac{\cosh(\omega(\tau - 1/2T))}{\sinh(\omega/2T)} \]

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

spectral representation of the thermal photon rate: \( \omega = |\vec{p}| \)

spectral representation of the thermal dilepton rate:

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

spectral representation of the correlator \( \Rightarrow \) dilepton and photon rates
Charmonium spectral functions

reconstructed correlation functions above $T_c$ from data below $T_c$

\begin{align*}
\langle \chi_{c0} \rangle & \quad (\chi_{c0})^{1.8} \\
\langle J/\psi \rangle & \quad (J/\psi)
\end{align*}

reconstructed spectral functions using the Maximum Entropy Method

\begin{align*}
\frac{G(t) \times G_{\text{recon}}(t)}{G_{\text{recon}}(t)} & \quad \text{for } \omega a \\
\frac{G(t) \times G_{\text{recon}}(t)}{G_{\text{recon}}(t)} & \quad \text{for } \omega a
\end{align*}

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

Note that states with $J \geq 5/2$ lie in representations with lower spins.

Spins identified from degeneracies in continuum limit

<table>
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<tr>
<th>$J$</th>
<th>$n_{G_1}^J$</th>
<th>$n_{G_2}^J$</th>
<th>$n_{H}^J$</th>
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<tr>
<td>$\frac{1}{2}$</td>
<td>1</td>
<td>0</td>
<td>0</td>
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<tr>
<td>$\frac{3}{2}$</td>
<td>0</td>
<td>0</td>
<td>1</td>
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<td>$\frac{5}{2}$</td>
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<td>$\frac{3}{2}$</td>
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<td>$\frac{11}{2}$</td>
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<td>$\frac{15}{2}$</td>
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<td>3</td>
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<tr>
<td>$\frac{17}{2}$</td>
<td>2</td>
<td>1</td>
<td>3</td>
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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

\[ \Gamma(\chi_{c0} \rightarrow J/\psi \gamma) = \frac{1}{8\pi} \frac{|q|}{m_S^2} 2 (2e_c)^2 |E_1(0)|^2 \]

Dudek et al, PRD73, 074507
Moments of parton distributions

Expansion of

\[ O(x) = \int \frac{d\lambda}{4\pi} e^{i\lambda x} \bar{\psi}(-\frac{\lambda}{2 n}) \mathcal{P} e^{-ig \int_{-\lambda/2}^{\lambda/2} d\alpha_n \cdot A(\alpha_n)} \psi(\frac{\lambda}{2 n}) \]

Generates tower of twist-2 operators

\[ O_{q}^{\{\mu_1 \mu_2 \ldots \mu_n\}} = \bar{\psi}_q \gamma^{\{\mu_1} i D^{\mu_2} \ldots i D^{\mu_n\}} \psi_q \]

Diagonal matrix element

\[ \langle P|O_{q}^{\{\mu_1 \mu_2 \ldots \mu_n\}} |P\rangle \sim \int dx \; x^{n-1} q(x) \]

Off-diagonal matrix element

\[ \langle P'|O_{q}^{\{\mu_1 \mu_2 \ldots \mu_n\}} |P\rangle \rightarrow A_{n_1}(t), B_{n_1}(t), C_{n_0}(t) \]

\[ \int dx \; x^{n-1} H(x, \xi, t) \sim \sum \xi^i A_{n_1}(t) + \xi^n C_{n_0}(t) \]

\[ \int dx \; x^{n-1} E(x, \xi, t) \sim \sum \xi^i B_{n_1}(t) - \xi^n C_{n_0}(t) \]

\[ [\gamma \rightarrow \gamma_5 : \; \tilde{A}_{n_1}(t), \tilde{B}_{n_1}(t)] \]
Nucleon axial charge $g_A$ \[ \langle 1 \rangle_{\Delta q}^{u-d} \]

Example of application of chiral perturbation theory
6 low energy parameters describe $m_\pi$ and L dependence
Measure 3 from other lattice observables
Fit 3 to this data
Extrapolate to physical $m_\pi$ and L

LHPC hep-lat/0510062
Nucleon axial charge $g_A$ 

$$\langle 1 \rangle^{u-d}_{\Delta q}$$

[Graph with data points and error bars, labeled with LHPC/hep-lat/0510062]
Moments of structure functions

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

\[ \langle x \rangle_{\Delta u-\Delta d} = a' \left[ 1 - \frac{2g_A^2}{8\pi^2} \right] \left( \frac{m^2}{f^2} \right) \ln \left( \frac{m^2}{f^2} \right) + c' \frac{m^2}{f^2} \]
Chiral Extrapolation of Moments

\[ \langle 1 \rangle_{\Delta u - \Delta d} \quad \langle 1 \rangle_{\delta u - \delta d} \quad \langle x \rangle_{u-d} \quad \langle x \rangle_{\Delta u - \Delta d} \quad \langle x \rangle_{\delta u - \delta d} \quad \langle x' \rangle_{\Delta u - \Delta d} \]
$F_1$ 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: $F_2 / F_1$

\[ \frac{F_2(I=1)}{F_1(I=1)} \]

\[ F_2^0 = 775 \, \text{MeV} \]
\[ F_2^1 = 498 \, \text{MeV} \]
\[ F_2^2 = 359 \, \text{MeV} \]

Expt: $\kappa_p - \kappa_n$
Nucleon spin decomposition

Connected contribution of quark spin and orbital angular momentum

\[ \Delta \Sigma^{u+d}/2 \]

\[ L^{u+d} \]

Contributions to nucleon spin vs. \[ m_\pi^2 \text{ [GeV}^2 \text{]} \]
Nucleon spin decomposition

Connected contribution of quark spin and orbital angular momentum
Transverse size of light-cone wave function

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

\(q(x, \vec{r}_\perp) \text{ model} \) (Burkardt hep-ph/0207047)
Comparison with Phenomenology

N-Delta transition form factor

\[ R_{SM}(%) \]

\[ R_{EM}(%) \]

\[ Q^2 \text{ GeV}^2 \]

\[ C2/M1 \]

\[ E2/M1 \]
Axial N-Delta transition form factors

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