Lattice QCD and Hadrons

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- overview
- hadron spectrum and fundamental constants of QCD
- topics in hadron physics
- issues and progress with chiral symmetry
- weak interactions of hadrons
- QCD thermodynamics
- conclusions
Center for computational Physics
University of Tsukuba

- Founded in 1992
- Emphasis on
  - Development of HPC systems suitable for computational physics
  - Close collaboration of physicists and computer scientists

- Computing facility
  - CP-PACS parallel system
    - MPP with 2048PU/0.6Tflops peak
    - Developed at the Center with Hitachi Ltd.
    - #1 of Top500-November 1996
  - GRAPE-6 system
    - Dedicated to gravity calculations
    - Developed at U. Tokyo
    - 8Tflops equivalent
Lattice QCD

- Quantum Chromodynamics (QCD)
  - Fundamental theory of quarks and gluons and their strong interactions
  - Knowing 1 coupling constant $\alpha_s$ and 6 quark masses $m_u, m_d, m_s, m_c, m_b, m_t$ will allow full understanding of strong interactions (Yukawa’s dream)

- Lattice QCD and numerical simulation
  - Provides the mean for first-principles realization of the dream
  - With computers instead of pencils in your hand
Lattice QCD and PaNic2002

PaNic02 Plenary program

- Sep.30
  Quark confinement and deconfinement
- Oct.1
  Nucleon structure and hadron interaction
  Nuclear matter at high density
- Oct.2
  Flavored matter and astrophysics
  Neutrino physics
- Oct.3
  Hadron physics with leptons and hadrons
  Structure functions of nucleon
- Oct.4
  CP violation and rare K-decays
  Precision frontier and beyond standard model

LQCD

Finite-temperature/density behavior

structure functions/form factors

Weak amplitudes of K and B mesons
Organization of this talk

- Hadron spectrum and fundamental constants of QCD
  - Fundamental verification of QCD at low energies
  - Determination of quark mass and strong coupling constant
- Topics in hadron physics
  - Nucleon structure functions
- Issues and progress with chiral symmetry
  - Chiral extrapolation of observables
  - Chirally symmetric fermion formulations
- Weak amplitudes of hadrons
  - $\bar{K}K$ decays and CP violation
  - $K$ and $B$ meson amplitudes and constraints on the CKM matrix
- Finite temperature/density QCD
  - Status at zero density
  - Progress toward non-zero density
Light hadron mass spectrum

- Benchmark calculation to verify QCD
- Indispensable for determination of QCD scale and quark masses
- Essential to control various systematic errors down to a few % level
  - Finite lattice size $L > 3\text{fm}$
  - Finite quark mass $m_q \neq 0$
  - Finite lattice spacing $a \neq 0$

Experimental spectrum
CP-PACS result for the quenched spectrum’98

- Sea quark effects ignored
- General pattern reproduced, but clear systematic deviation beyond 10% precision
- Completes the calculation started in ’81 (Hamber-Parisi/Weingarten)

\[ \text{use } m_\pi, m_\rho \text{ for fixing } a \text{ and } m_{ud} \]
\[ \text{use } m_K \text{ for fixing } m_s \]

Calculated quenched spectrum
Input dependence in quenched QCD

- Details of disagreement depends on input, but overall agreement not possible

\[ \text{use } m_K \text{ for fixing } m_s \]
\[ \text{use } m_\phi \text{ for fixing } m_s \]

- Predictions in quenched QCD suffer from uncertainties depending on input

Calculated quenched spectrum
Strange quark mass in quenched QCD

- 25% discrepancy in the predicted value of strange quark mass

- Clearly illustrates
  - limitation of quenched QCD
  - necessity of full QCD with dynamical quarks

\[
m_s(\overline{MS}, 2\text{GeV}) = \begin{cases} 
142^{+28}_{-6} \text{ MeV} & \phi \text{ meson mass input} \\
114^{+8}_{-6} \text{ MeV} & K \text{ meson mass input}
\end{cases}
\]
QCD simulation with dynamical quarks

- **Spectrum of quarks**
  - 3 *light quarks* ($u,d,s$) \( m < 1\text{GeV} \)
  - Need dynamical simulation
  - 3 *heavy quarks* ($c,b,t$) \( m > 1\text{GeV} \)
  - Quenching sufficient

- **Dynamical quark simulation (full QCD)**
  - Costs 100-1000 times more computing power
  - Algorithm for *odd number of quarks* now available

- **Two-flavor full QCD** \( N_f = 2 \)
  - $u$ and $d$ quark dynamical simulation
  - $s$ quark quenched approximation
  - Number of studies: SESAM/UKQCD/MILC/CP-PACS/JLQCD

- **Two+one-flavor full QCD** \( N_f = 2 + 1 \)
  - $s$ quark also treated dynamically
  - Extensive studies have begun: MILC/CP-PACS-JLQCD
Sea quark effects in the spectrum

- K*-K and Ω-K mass difference (Meson hyperfine splitting)
  - too small in quenched QCD
  - Much closer agreement for two-flavor full QCD
Sea quark effects in quark masses

- Significant decrease by inclusion of sea quark effects
- Input dependence of strange quark mass also reduced

**Graphical Representation:**
- **Up & Down Quark**
  - Quenched value
- **Strange Quark**
  - Two-flavor full QCD
  - K-input
Light quark masses (u, d, s) $m_q^{\overline{MS}}(2\text{GeV})$

- Significant sea quark effects
  - Large uncertainty ($\sim 20\%$) depending on input in quenched theory
  - Sizable decrease ($\sim 25\%$) from quenched to two-flavor full QCD

- Lighter than naïve quark model values

- Nf=3 simulations being pursued to obtain physical values of light quark masses, e.g., Hein et al hep-lat/0209077

Real world; three flavors?

CP-PACS Collab. Hep-lat/0004010
Heavy quark masses (c, b)

- Charm quark mass
  - J. Rolf and S. Sint  Lattice01
  - Fully non-perturbative determination in the continuum in quenched QCD
  - $m_c^{\overline{MS}}(m_c) = 1.314(45)\text{GeV}$

- Bottom quark mass
  - Not straightforward since $m_b > 1/a$
  - Use
    $$M_B = m_b^{\text{pole}} + E_b - \delta m$$
    - $M_B, E_B$ Monte Carlo
    - $\delta m$ pert. theory
  - G. Gimenez et al (’00)
    - $m_b^{\overline{MS}}(m_b) = 4.27(9)\text{GeV}$

compiled by T. Kaneko (Lattice ‘01)
Hep-lat/0111005
Strong coupling constant $\alpha_s(\mu)$

- Another fundamental parameter of QCD
- Large number of high energy determinations from experiments
- Lattice determinations:
  - Method I (Lepage et al '91):
    - Calculate short-distance observables as a function of $\alpha_s(1/a)$ at cutoff scale 1/a
    - The scale 1/a is fixed from hadron mass
  - Method II (Luescher et al '93)
    - Non-perturbative determination of the RG evolution by Schrodinger functional finite-size technique
Scale dependence of $\alpha_s(\mu)$

- Non-perturbative determination by Alpha Collaboration for two-flavor full QCD (Lattice02)
- Indicates perturbative evolution for $p > \text{a few GeV}$
- Similar results for quenched QCD ('94)
- Physical scale yet to be determined

M. Della Morte et al hep-lat/0209023
Determination of $\alpha_s^{\overline{MS}}(M_Z)^{N_f=5}$

□ Comments

- Davies et al '97(hep-lat/9703010):
  Involved extrapolation of $N_f=0$ (quenched) and $N_f=2$ data to $N_f=3$

- QCDSF-UKQCD '01(hep-lat/0103023)
  Continuum estimate with systematic $N_f=2$ simulations

- Davies et al '02(hep-lat/0209121):
  Preliminary result based on MILC $N_f=3$ configurations at $a=0.13\text{fm}$

□ Systematic $N_f=3$ full QCD determination expected in a few years
Topics in hadron physics

- Progress in hadron spectroscopy
  - Eta’ meson mass and U(1) problem
  - Glueballs
  - Multiquark states
  - Excited string states etc

- Hadron structure
  - Moments of nucleon structure functions
  - Form factors

- Hadron scattering amplitudes
  - Scattering length
  - Phase shift
Moments of nucleon structure functions (I)

- A number of calculations
  - QCDSF (quenched)'96
  - Alpha (quenched)'98
  - QCDSF+UKQCD (full)'01-'02
  - LHPC+SESAM (full)'02

- No large sea quark effects observed for non-singlet moments

- No large scaling violation

- Lattice predictions do not agree with experiment

Compiled in M. Goeckeler et al hep-lat/0209160
Moments of nucleon structure functions (II)

- Linear chiral extrapolation misses experiment

- Possible reasons:
  - Quenching? No
  - O(a) error? No
  - Chiral extrapolation itself?

- Chiral perturbation theory:

\[
\langle x^n \rangle = a_n \left( 1 - \frac{3g_A^2 + 1}{(4\pi f)^2}m^2 / \ln \frac{m^2}{\Lambda^2} + cm^2 \cdots \right)
\]

- Pion not light enough to see curvature?
- An effective model can reproduce experiment

\[
\langle x^n \rangle = a_n \left( 1 - \frac{3g_A^2 + 1}{(4\pi f)^2}m^2 / \ln \frac{m^2}{\Lambda^2} + dm^2 \right)
\]

From D. Dolgov et al hep-lat/0201021

W. Detmold et al hep-lat/0103006
Moments of nucleon structure functions (II)

- Linear chiral extrapolation misses experiment
- Possible reasons:
  - Quenching? No
  - O(a) error? No
  - Chiral extrapolation itself?
- Chiral perturbation theory:
  \[ \langle x^n \rangle = a_n \left( 1 - \frac{3g_A^2}{(4\pi f)^2} m^2 + \ln \frac{m^2}{\Lambda^2} + \cdots \right) \]
  - Pion not light enough to see curvature?
  - An effective model can reproduce experiment

From D. Dolgov et al hep-lat/0201021

\[ \langle x \rangle_{u-d} \]

\[ m^2_{\pi} \]

W. Detmold et al hep-lat/0103006
A general issue with chiral extrapolation

- Current lattice data often fails to see logarithmic singularity expected from chiral perturbation theory.
- Often causes sizable (10-20%) uncertainties in the extrapolated result.
- Pion mass in current simulations (~500MeV) too heavy; needs to be reduced.
- Lattice fermion action with exact chiral symmetry much desired (conventional Wilson and KS action breaks chiral symmetry).
Lattice fermion with exact chiral symmetry

- Theoretically based on the Ginsparg-Wilson relation:

\[ D\gamma_5 + \gamma_5 D = 2aDR\gamma_5 D \]

- Domain-wall fermion  Kaplan(‘92)/Furman-Shamir(‘94)
- Overlap formalism  Neuberger-Narayanan(‘92,’97)
- Fixed point action  Hasenfratz-Neidermyer(‘94)

- Avoids the Nielesen-Ninomiya Theorem by using “infinitely” many fields (hence needs more computer power)

- quenched calculations show very promising results: good chiral property, small scaling violation, …
A test in quenched QCD

- Chiral logarithm behavior of pion mass in quenched QCD
  Sharpe/Bernard-Golterman ’91

\[ m_\pi^2 = A m_0 (1 - \delta \ln m_0 + b m_0 + \ldots) \]

- Nice confirmation with the new fermion formalism
  - T. Draper et al : overlap fermion
  - C. Gattringer et al : fixed point fermion

- Reached very light pion mass
  - \( m_\pi \sim 170 \text{MeV} \) (T. Draper et al)
  - Similar results from other chiral formalisms

\( \delta = 0.26(3) \)

T. Draper et al hep-lat/0208045
Weak amplitudes of hadrons

- First principles calculation of strong interaction corrections to weak amplitudes of hadrons
- Understand old and new issues in hadronic weak interactions
  - $I=1/2$ rule and direct CP violation in $K\to\pi\pi$ decay
- Constraints on the CKM mixing matrix
  - Neutral $K$ and $B$ meson mixings
  - $B$ meson decay form factors

\[
\text{Measured weak amplitude} = \text{Known factor including CKM matrix} \times \langle h' | H_{\text{weak}} | h \rangle
\]

QCD matrix element
I=1/2 rule and CP violation in K decays

- **Weak interaction decays of K mesons**
  
  \[ \frac{\text{Re} A_0(K \rightarrow \pi\pi(I = 0))}{\text{Re} A_2(K \rightarrow \pi\pi(I = 2))} \approx 22 \]

  - I=1/2 rule

  - CP violation
    
    \[ \frac{\varepsilon'}{\varepsilon} = \begin{cases} 
    (20.7 \pm 2.8) \times 10^{-3} & \text{KTeV experiment (FNAL)} \\
    (15.3 \pm 2.6) \times 10^{-3} & \text{NA48 experiment (CERN)} 
    \end{cases} \]

- **Crucial numbers to verify the Standard Model understanding of CP violation**

- **Chiral symmetry crucial because of the chiral structure of weak interactions**

- **Two large-scale calculations using domain-wall QCD**
  
  - RIKEN-BNL-Columbia  
    
    T. Blum et al hep-lat/0110124
  
  - CP-PACS  
    
    J. Noaki et al hep-lat/0108013
I=1/2 rule

- Reasonable agreement with experiment for I=2
- About half of experiment for I=0
- RIKEN-BNL-Columbia obtains a somewhat different result (smaller I=2 and larger I=0)
CP violation parameter $\epsilon'/\epsilon$

- Small and negative in disagreement with experiment
- Similar result from RIKEN-BNL-Columbia

Possible reasons:
- Connected with insufficient enhancement of $I=1/2$ rule
- Method of calculation (K reduction) may have serious problems

Still a big problem requiring further work

\[
\frac{\epsilon'}{\epsilon} = \frac{\omega}{\sqrt{2}|\epsilon|} \left[ \frac{\text{Im} A_2}{\text{Re} A_2} - \frac{\text{Im} A_0}{\text{Re} A_0} \right]
\]
Constraints on the CKM matrix

\[
\text{Measured weak amplitude} = \text{Known factor including CKM matrix} \times \left\langle h' | H_{\text{weak}} | h \right\rangle
\]

\[QCD \text{ matrix element}\]

- \( K^0 - \bar{K}^0 \) mixing
  \[\varepsilon_K \propto \bar{\eta} \left[ (1 - \rho) A + B \right]^2 \hat{B}_K \]
  \[\left\langle \bar{K}^0 | \bar{s} \gamma_\mu (1 - \gamma_5) d \bar{s} \gamma_\mu (1 - \gamma_5) d | K^0 \right\rangle = \frac{8}{3} f_K B_K M_K^2 \]

- \( B_{d,s}^0 - \bar{B}_{d,s}^0 \) mixing
  \[\Delta M_{B_q} \propto \left( \rho^2 + \bar{\eta}^2 \right) f_{B_q}^2 B_{B_q} \]
  \[\left\langle B_q^0 | \bar{b} \gamma_\mu (1 - \gamma_5) q \bar{b} \gamma_\mu (1 - \gamma_5) q | B_q^0 \right\rangle = \frac{8}{3} f_{B_q}^2 B_{B_q} M_{B_q}^2 \quad \xi = \frac{f_{B_s}}{f_{B_d}} \sqrt{\frac{B_{B_s}}{B_{B_d}}} \]
Lattice results for $B_K$

- Previous best result obtained with conventional KS fermion action
- Recent Domain-wall results indicates a smaller value
- Full QCD calculation yet to be made with domain-wall fermion
- Current best estimate:

$$B_K = 0.628(42) - 0.532(11)$$

$\hat{B}_K = 0.87^{+0.06}_{-0.13}$  \text{RG-invariant B parameter}$\quad$\text{CP-PACS hep-lat/0105020}

$\quad$\text{RBC hep-lat/0110075}
Full QCD results for $f_B$

- Two-flavor full QCD result begins to accumulate
- $f_{B_d}$: possibly large uncertainty due to chiral extrapolation

- Best estimate from two-flavor full QCD:
  \[
  f_{B_d} = 198(30)^{+0}_{-34} \text{ MeV} \\
  f_{B_d}/f_{B_s} = 1.16(5)^{+24}_{-0}
  \]

N. Yamada at Lattice2002
Results for $B_B$

- Still mostly quenched (only one calculation in full QCD)
- Sea quark effects small
- Uncertainty with chiral extrapolation is small
- Current best estimate:

$$B_{B_d} = 1.33(12)$$

$$B_{B_d} / B_{B_s} = 1.00(3)$$

Compilation by N. Yamada at Lattice02

N. Yamada at Lattice2002
Summary of lattice results for CKM matrix

\[ \hat{B}_K = 0.87^{+0.06}_{-0.13} \]
\[ f_{B_d} \sqrt{B_{B_d}} = 0.227(37)^{+0}_{-34} \text{GeV} \]
\[ \xi = 1.16(5)^{+24}_{-0} \]

Cf. numbers used in the figure left

\[ \hat{B}_K = 0.87^{+0.06}_{-0.13} \]
\[ f_{B_d} \sqrt{B_{B_d}} = 0.227(28) \text{GeV} \]
\[ \xi = 1.16^{+3}_{-5} \]

Better control of chiral extrapolation needed

status 2002  http://www.ckmfitter.in2p3.fr/
Finite temperature/density QCD

- Status for $T>0$ and $\mu=0$
  - Expected phase diagram
  - Recent results

- Progress toward $\mu \neq 0$
  - Reweighting
  - Taylor expansion
  - Analytic continuation

Remarks
- Still mostly (improved) KS fermion action
- Still mostly Temporal size $N_t=4-8$
  - i.e., coarse lattice $a^{-1} \approx 0.6-1.2 GeV$
Phase diagram expected at $\mu=0$

$N_f = 2 + 1 \, QCD$

Tricritical point

$m_{ud} \propto (m_s^* - m_s)^{5/2}$

Second-order

D=3 Z(3) Potts universality

D=3 Ising universality

Where is the physical point?
Nature of the 2\textsuperscript{nd} order endline

- Existence of the endline well established
  - JLQCD/Bielefeld/Columbia

- Binder cumulant test to distinguish universality class

\begin{equation}
B_4 = \frac{\langle (\delta \psi \psi)^4 \rangle}{\langle (\delta \psi \psi)^2 \rangle^2}
\end{equation}

- Clear evidence of Ising universality as predicted by S. Gavin et al
  - S. Gavin et al hep-ph/9311350

Karsch et al hep-lat/0107020
Previous work by
JLQCD/Columbia

Schmidt (Bielefeld-Swansea) @Lattice2002

$m_{ud} = 0.03, m_s = 0.045, 0.06$

$12^3 \times 4$

Binder cumulant

Christ (Columbia) @Lattice2002

$m_{ud} = m_s = 0.015 - 0.045$

$8^3 \times 4, 16^3 \times 4, 32^3 \times 4$

Ch. Schmidt et al hep-lat/0209009

Cross-over at the physical point indicated with the KS fermion simulations

NB first-order with Wilson fermion; old controversy still remains
Progress with finite chemical potential

- Reweighting method to move from $\mu=0$ to $\mu \neq 0$
  - Budapest (Fodor et al)
- Taylor expansion around $\mu=0$
  - Bielefeld-Swansea
- Analytic continuation from $\text{Im}\mu \neq 0$ to $\text{Re}\mu \neq 0$
  - Forcrand et al/Lombardo et al
- Glasgow attempts ('92-'98) failed at $T=0$, but resurrected at $T \neq 0$ by Fodor-Katz

Schematic phase diagram (assuming cross-over at $T=0$)
Reweighting in chemical potential $\mu$

- **Fodor-Katz strategy**
  Z. Fodor et al. hep-lat/0104001
  - Reweight in $\beta$ and $\mu$ such that width of $\omega$ is minimal
  - Turned out to work for small volume;
    $$\mu a \leq \left( N_t \cdot N_s^3 \right)^{-1/4}$$
  - Use Lee-Yang zero analysis to locate the end-point $E$

*From Fodor et al. hep-lat/0208078*
Results

- **End point:**
  \[ T_E = 160 \pm 3.5 \text{ MeV} \]
  \[ \mu_E = 725 \pm 35 \text{ MeV} \]
  \[ NF=2+1 \]
  \[ [m_{ud}=0.025, m_s=0.2] \]
  \[ (4, 6, 8)^3x4 \]

  Z. Fodor et al hep-lat/0106002

- **Equation of state**
  Pressure \( p \)
  Energy density \( e \)
  \[ NF=2+1 \]
  \[ [m_{ud}=0.025, m_s=0.2] \]
  \[ (8, 10, 12)^3x4 \]

  Z. Fodor et al hep-lat/0208078
Taylor expansion in chemical potential $\mu$

- Taylor expansion should converge up to the endpoint
  \[
  \text{Tr} \ln D(\mu) = \text{Tr} \ln D(\mu = 0) + \text{Tr} D(\mu = 0)^{-1} \frac{\partial D}{\partial \mu} (\mu = 0) \cdot \mu + \ldots
  \]

- Calculate
  \[
  \frac{d^2 \beta_c(\mu)}{d\mu^2} \bigg|_{\mu=0} \Rightarrow \frac{d^2 T_c(\mu)}{d\mu^2} \bigg|_{\mu=0}
  \]

- Simulation
  - P4-improved KS
  - $N_f = 2$ [m$_{ud}=0.01, 0.02$]
  - $16^3 \times 4$
Analytic continuation from Imaginary to Real $\mu$

- Determinant real for Imaginary $\mu$, hence amenable to Monte Carlo
- Fit observables in polynomials of $\mu$
- Analytically continue in $\mu$

$$\beta_c(\mu) = \beta_c(0) + c(\mu)^2$$

$\Rightarrow$

$$i\mu_I \Rightarrow \mu$$

From Ph. Forcrand et al hep-lat/0205016
Conclusions and prospects

- Visible shift from quenched to full QCD simulations
  - Important effects observed in physical observables
  - Crucial for consistent predictions from lattice QCD
- Development of lattice fermion with exact chiral symmetry
  - Both conceptual and practical advantages
  - Need $O(10)$ times more computer power; awaits next generation of computers for full QCD
- Notable progress in
  - Study of finite chemical potential
- Require further effort to understand
  - K meson decays
- Expect substantial progress by the next PaNic onference with next generation of computers
  - QCDOC/APENEXT
  - Development of clusters