16 December 2002

Present and Future of Lattice QCD

Akira Ukawa Center for Computational Physics University of Tsukuba

overview

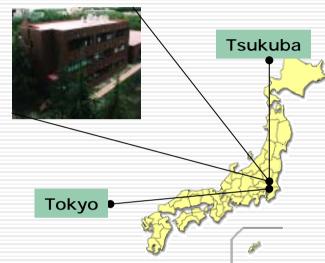
- hadron spectrum and fundamental constants of QCD
- topics in hadron physics
- □ issues and progress with chiral symmetry
- weak interactions of hadrons
- QCD thermodynamics
- conclusions and prospects



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







Quantum Chromodynamics

Quantum Chromodynamics (QCD)

Fundamental theory of quarks and gluons and their strong interactions

$$S_{QCD} = \frac{1}{8\pi\alpha_s} Tr(F_{\mu\nu}F_{\mu\nu}) + \sum_f \overline{\psi}_f (\gamma_\mu \cdot (\partial_\mu - iA_\mu) + m_f) \psi_f$$
$$\langle O(A,\overline{\psi},\psi) \rangle = \frac{1}{Z} \int dAd\,\overline{\psi}d\,\psi O(A,\overline{\psi},\psi) e^{-S}$$

1 coupling constant and6 quark masses

Knowing

 $m_u, m_d, m_s, m_c, m_b, m_t$

 α_{s}

will allow full understanding of strong interactions "Yukawa's dream(1935) in modern form"



Lattice QCD

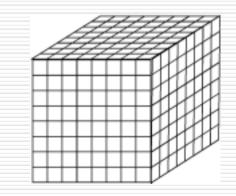
Powerful mean to calculate the QCD Feyman path integral

$$S_{QCD} = \frac{1}{\alpha_s} \sum_{p} tr(UUUU) + \sum_{f} \overline{\psi}_f (\gamma \cdot U + m_f) \psi_f$$
$$\langle O(U, \overline{\psi}, \psi) \rangle = \frac{1}{Z} \int dU d \overline{\psi} d \psi O(U, \overline{\psi}, \psi) e^{-S}$$

From computational point of view

- Relatively simple calculation
 - Uniform mesh
 - Single scale
- Requires much computing power due to
 - 4-dim. Problem
 - Fermions essential
 - Physics is at lattice spacing a=0
- Precision required(<a few % error in many cases)

lattice spacing aQCD scale parameter $\Lambda_{_{QCD}}$



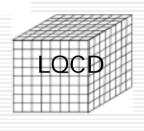


Hadron spectrum and Fundamental constanst of QCD

Strong coupling constant

 $m_{\mu}, m_{d}, m_{s}, m_{c}, m_{h}, m_{t}$

Quark masses



Hadron physics

 $\alpha_{\rm c}$

- eta' meson mass and U(1) problem
- exotic states glueball, dibaryon, hybrids,...
- hadronic matrix elements proton spin, sigma term,
- structure functions/form factors

 $\int dx x^{n-1} F(x,q^2) = \left(\ln q^2 \right)^{-\gamma_n} \left\langle N \left| O_n \right| N \right\rangle$

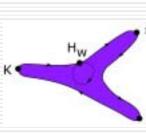
Finite-temperature/ density behavior

- order of transition
- critical temperature/density
- equation of state

Physics of quark-gluon plasma

Weak interaction matrix elements

• K meson amplitudes B_K K $\pi\pi$ decays



 B meson amplitudes f_B, B_B, form factors

CKM matrix and CP violation

plasma phase

End point

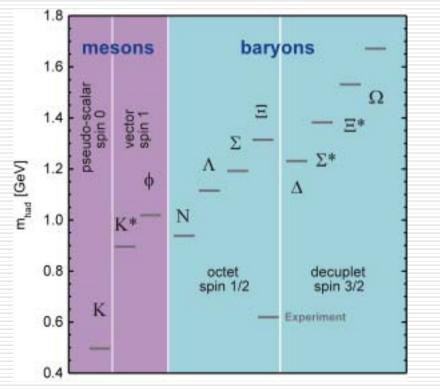
hadron phase

Physics subjects 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
 - 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>3fm
 - Finite quark mass mq 0
 - Finite lattice spacing a 0

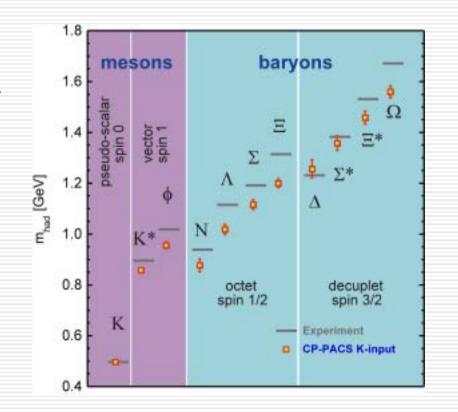


Experimental spectrum

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)

use m_{π}, m_{ρ} for fixing a and m_{ud} use m_{K} for fixing m_{s}



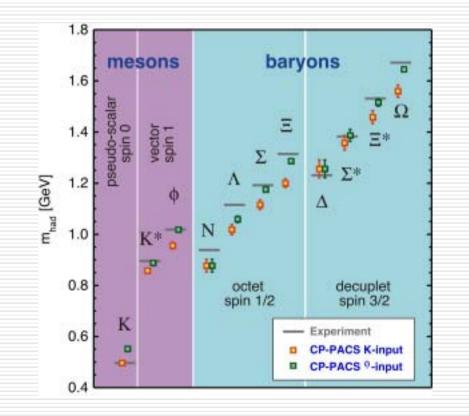
Calculated quenched spectrum

Input dependence in quenched QCD

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

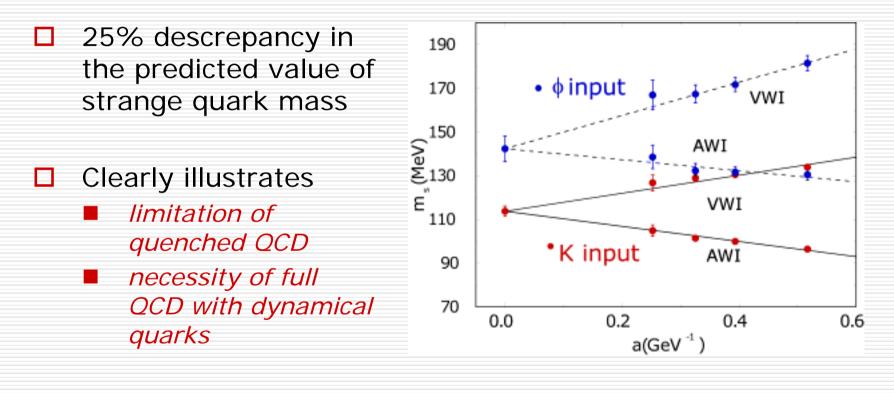
> use m_K for fixing m_s use m_{ϕ} for fixing m_s

predictions in quenched QCD suffer from uncertainties depending on input



Calculated quenched spectrum

Strange quark mass in quenched QCD



 $m_{s}(\overline{MS}, 2GeV) = \begin{cases} 142^{+28}_{-6} MeV & \phi \text{ meson mass input} \\ 114^{+8}_{-6} MeV & K \text{ meson mass input} \end{cases}$

QCD simulation with dynamical quarks

m < 1 GeV

m >1GeV

Spectrum of quarks

- 3 light quarks (u,d,s)
 D Need dynamical simulation
- 3 heavy quarks (c,b,t) □ Quenching sufficient
- Dynamical quark simulation (full QCD)
 - costs 100-1000 times more computing power
 - Algorithm for *odd number of quarks* now available

$\square \quad Two-flavor full QCD (since around 1996) \qquad N_f = 2$

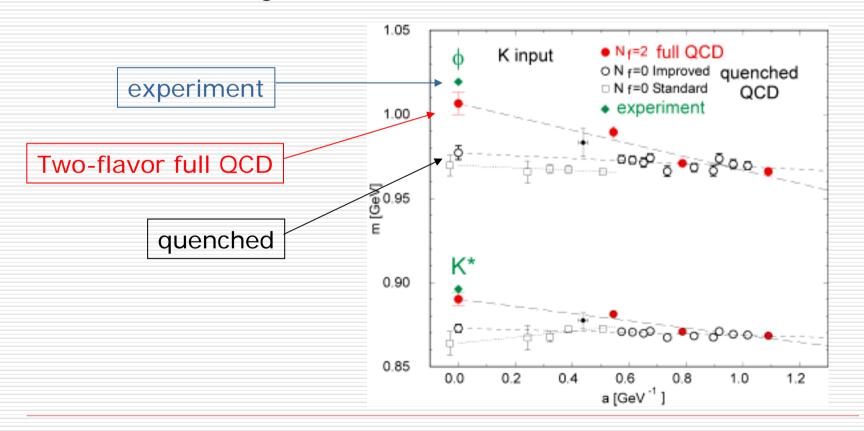
- u and d quarkdynamical simulations quarkquenched approximation
- Number of studies: SESAM/UKQCD/MILC/CP-PACS/JLQCD
- **D** Three-flavor full QCD (since around 2000) $N_f = 2+1$

s quark also treated dynamically

Extensive studies have begun : MILC/CP-PACS-JLQCD

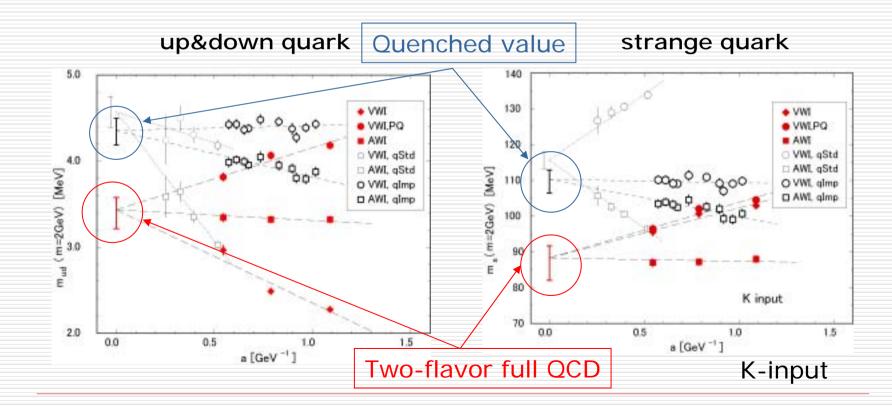
Sea quark effects in the spectrum

- K*-K and -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

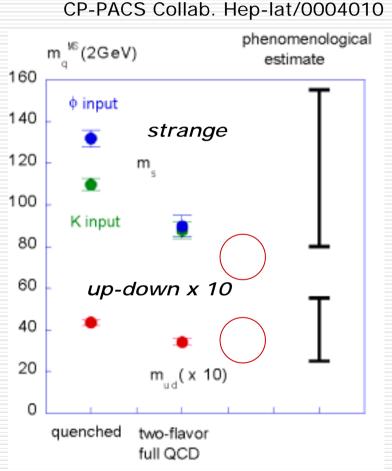


MS(2GeV)Light quark masses (u, d, s) m_a

Significant sea quark effects

- Large uncertainty (~ 20%) depending on input in quenched theory
- Sizable decrease (~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?

Heavy quark masses (c, b)

Charm quark mass

- J. Rolf and S. Sint Lattice01
 - Fully non-perturbative determination in the continuum in quenched QCD

$$m_c^{\overline{MS}}(m_c) = 1.314(45)GeV$$

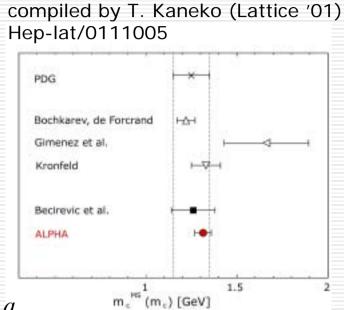
Bottom quark mass

- Not straightforward since $m_b > 1/a$
- Use

$$M_{B} = m_{b}^{pole} + \underbrace{E_{b}}_{binding \ energy}$$

$$\begin{cases} M_{B}, E_{B} \quad Monte \ Carlo \\ \delta m \quad pert. \ theory \end{cases}$$

G. Gimenez et al ('00)



$$m_b^{\overline{MS}}(m_b) = 4.27(9)GeV$$

radiative corrections

Strong coupling constant $\alpha_s(\mu)$

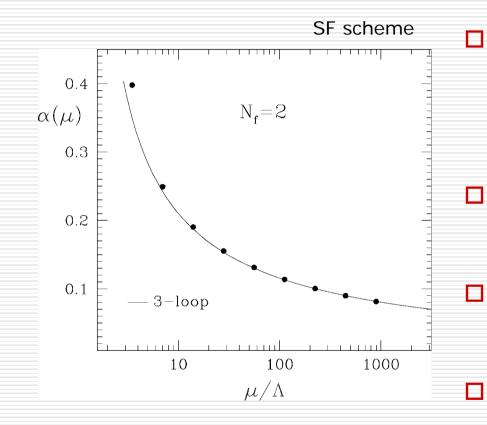
Another fundamental parameter of QCD

- 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 Shcrodinger functional finite-size technique

Scale dependence of $\alpha_s(\mu)$



M. Della Morte et al hep-lat/0209023

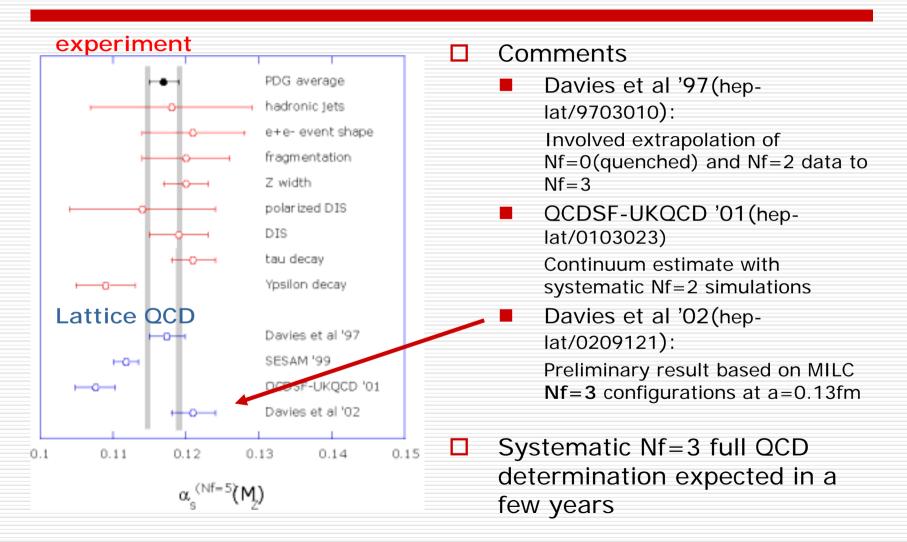
Non-perturbative determination by Alpha Collaboration for twoflavor full QCD (Lattice02)

Indicates perturbative evolution for p>a few GeV

Similar results for quenched QCD ('94)

Physical scale yet to be determined

Determination of $\alpha_s^{\overline{MS}} (M_z)^{N_f=5}$



Topics in hadron physics

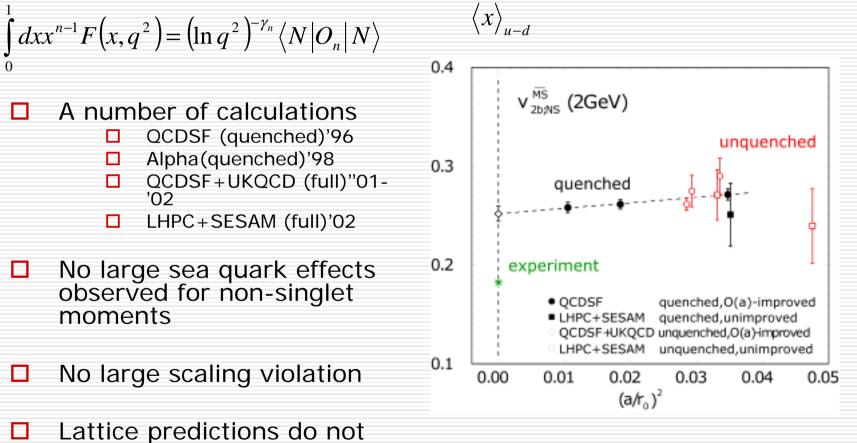
- Progress in hadron spectroscopy
 - Eta' meson mass and U(1) problem
 - Glueballs
 - Multiquark states
 - Excited string states etc

Hadron structure

- Moments of nucleon structure functions
- Form factors
- Hadron scattering amplitudes
 - Scattering length
 - Phase shift

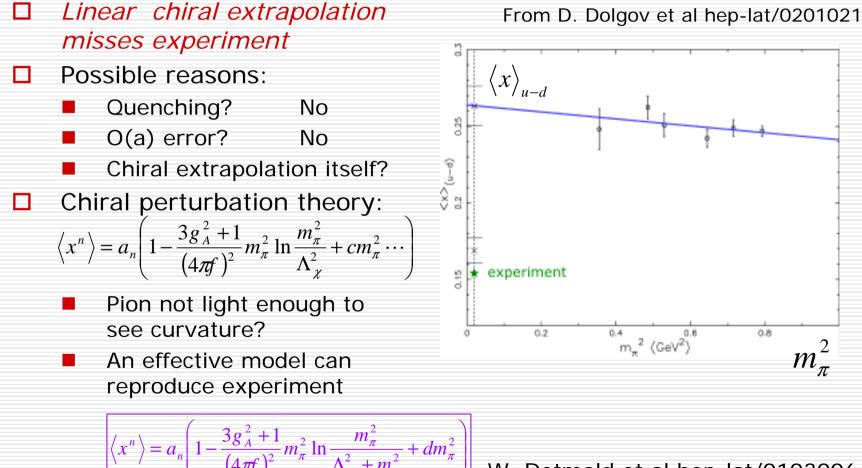
 $I=2 \pi \pi$ channel Ishizuka et al 2002

Moments of nucleon structure functions (I)



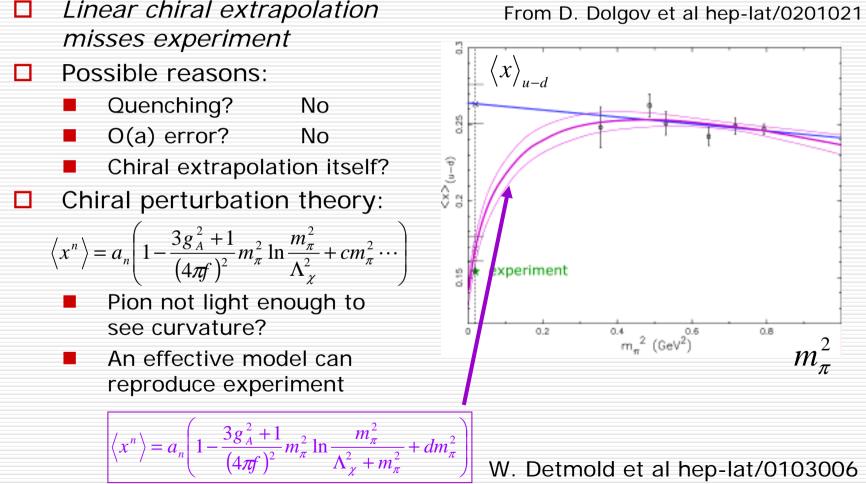
Lattice predictions do not agree with experiment Compiled in M. Goeckeler et al hep-lat/0209160

Moments of nucleon structure functions (II)



W. Detmold et al hep-lat/0103006

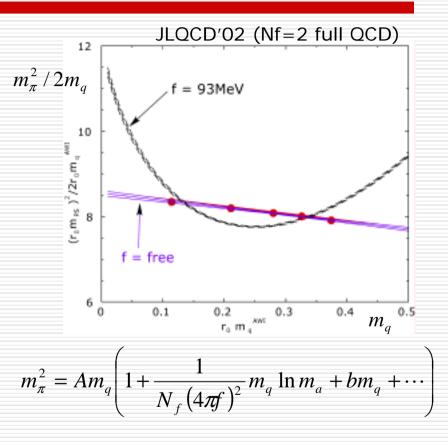
Moments of nucleon structure functions (II)



From D. Dolgov et al hep-lat/0201021

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

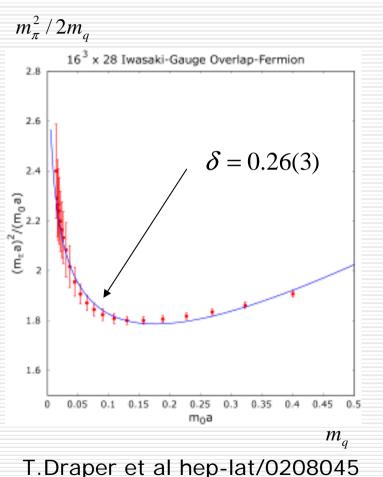
$$m_{\pi}^2 = Am_0(1 - \delta \ln m_0 + bm_0 + \cdots)$$

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

- $\square m_{\pi} \sim 170 \text{MeV} (T. \text{ Draper et al})$
- Similar results from other chiral formalisms



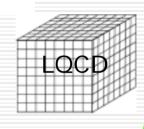


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Strong coupling constant

 $m_{\mu}, m_{d}, m_{s}, m_{c}, m_{h}, m_{t}$

Quark masses



Hadron physics

 $\alpha_{\rm s}$

- eta' meson mass and U(1) problem
- exotic states glueball, dibaryon, hybrids,...
- hadronic matrix elements proton spin, sigma term,
- structure functions/form factors

 $\int dx x^{n-1} F(x,q^2) = \left(\ln q^2 \right)^{-\gamma_n} \left\langle N \left| O_n \right| N \right\rangle$

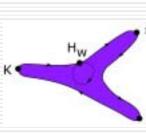
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K meson amplitudes
 B_K
 K ππ decays



plasma phase

color super

CEL7

End point

hadron phase

 B meson amplitudes f_B, B_B, form factors

CKM matrix and CP violation

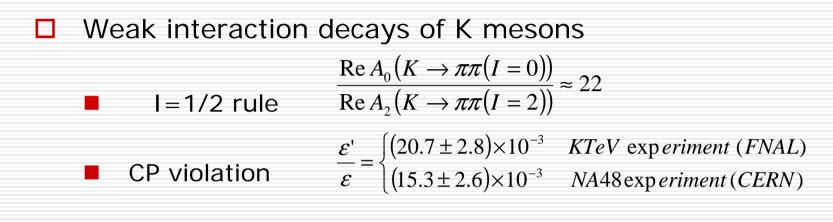
Weak amplitudes of hadrons

- 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 decay
- Constraints on the CKM mixing matrix
 - Neutral K and B meson mixings
 - B meson decay form factors



QCD matrix element



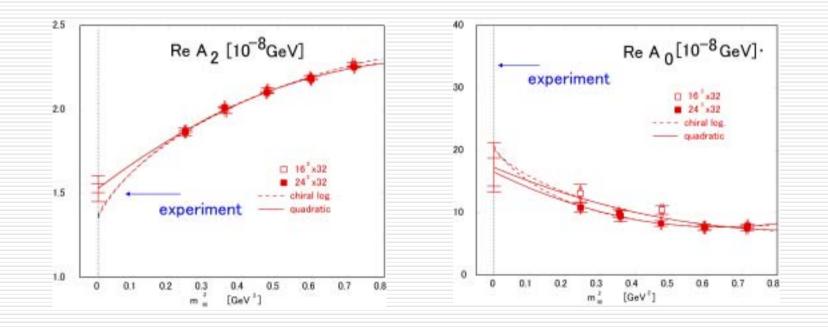


- Crucial numbers to verify the Standard Model understanding of CP violation
- Chiral symmetry crucial because of the chiral structure of weak interactions
- Two large-scale calculations using domain-wall QCD
 - RIKEN-BNL-Columbia
 - CP-PACS

- T. Blum et al hep-lat/0110124
- J. Noaki et al hep-lat/0108013



- 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)



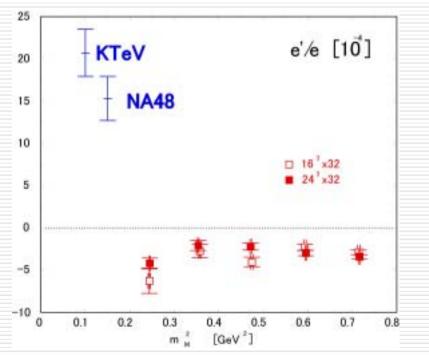
CP violation parameter ',

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



- 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

$$\frac{\varepsilon'}{\varepsilon} = \frac{\omega}{\sqrt{2}|\varepsilon|} \left[\frac{\operatorname{Im} A_2}{\operatorname{Re} A_2} - \frac{\operatorname{Im} A_0}{\operatorname{Re} A_0} \right]$$



Constraints on the CKM matrix



QCD matrix element

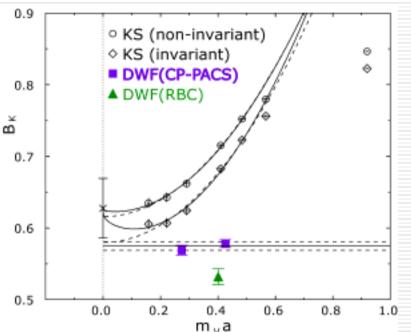
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Lattice results for B_K

- 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

 $\hat{B}_{K} = 0.87^{+0.06}_{-0.13}$

Current best estimate:



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

CP-PACS hep-lat/0105020 RBC hep-lat/0110075

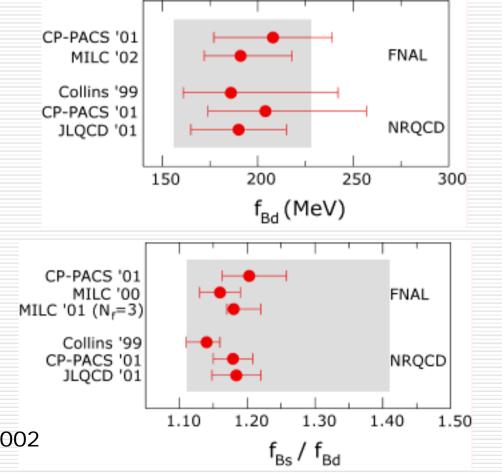
RG-invariant B parameter



- 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:
 - $f_{B_d} = 198(30)_{-34}^{+0} MeV$
 - $f_{B_d} / f_{B_s} = 1.16(5)^{+24}_{-0}$

N. Yamada at Lattice2002

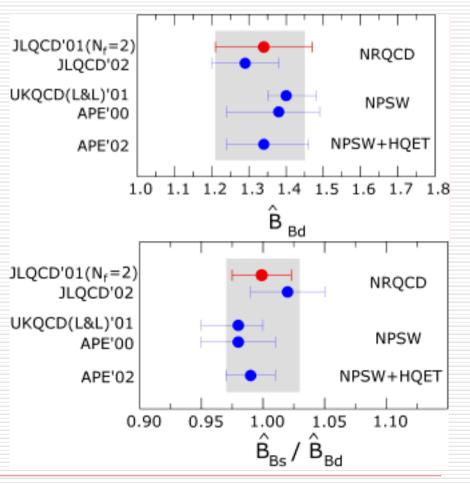
Compilation by N. Yamada at Lattice02





- Still mostly quenched (only one calculation in full QCD)
- Sea quark effects small
- Uncertainty with chiral extrapolation is small
- Current best estimate:
 - $B_{B_d} = 1.33(12)$
 - $B_{B_d} / B_{B_s} = 1.00(3)$

N. Yamada at Lattice2002



Compilation by N. Yamada at Lattice02

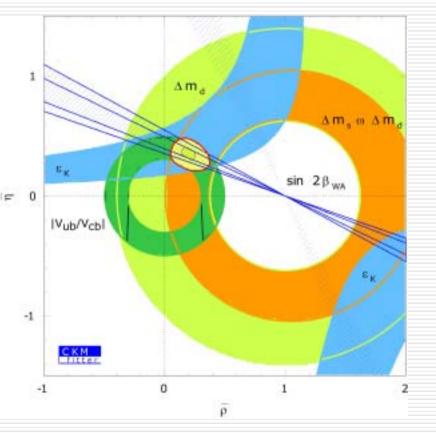
Summary of lattice results for CKM matrix

 $\hat{B}_{K} = 0.87^{+0.06}_{-0.13}$ $f_{B_{d}} \sqrt{B_{B_{d}}} = 0.227(37)^{+0}_{-34} GeV$ $\xi = 1.16(5)^{+24}_{-0}$

Cf. numbers used in the figure left

$$\hat{B}_{K} = 0.87^{+0.06}_{-0.13}$$
$$f_{B_{d}} \sqrt{B_{B_{d}}} = 0.227(28)GeV$$
$$\xi = 1.16^{+3}_{-5}$$

status 2002 http://www.ckmfitter.in2p3.fr/



Better control of chiral extrapolation needed

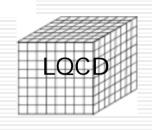
Subjects of lattice QCD

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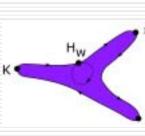
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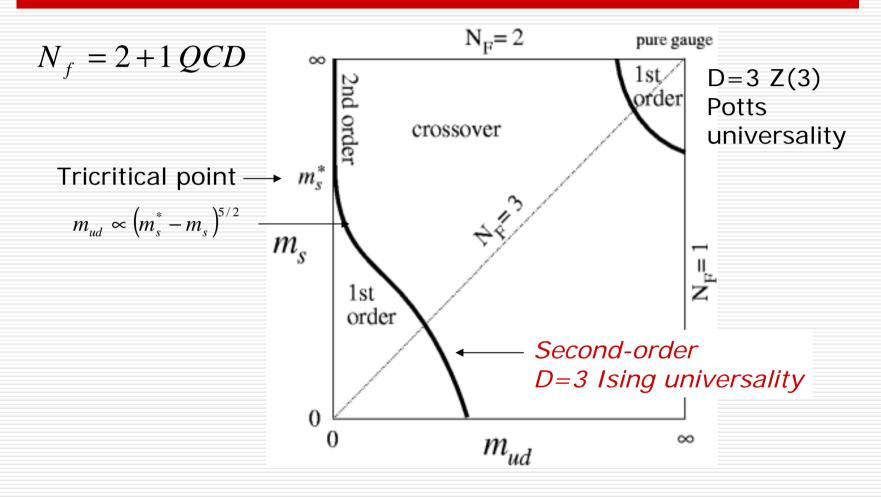
- **Status for T>0 and \mu=0**
 - Expected phase diagram
 - Recent results
- **D** Progress toward $\mu \neq 0$
 - Reweighting
 - Taylor expansion
 - Analytic continuation

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 $\mu=0$



Where is the physical point?

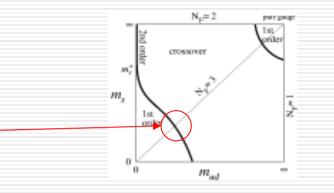
Nature of the 2nd order endline

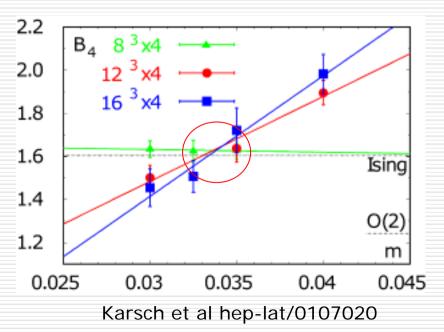
- Existence of the endline well established JLQCD/Bielefeld/Columbia
- Binder cumulant test to distinguish universality class

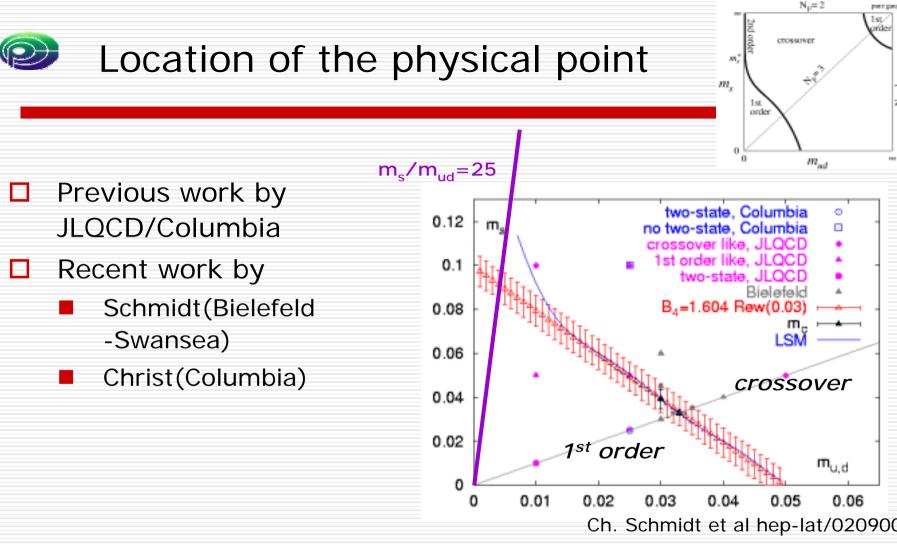
$$B_{4} = \frac{\left\langle \left(\delta \overline{\psi} \psi\right)^{4} \right\rangle}{\left\langle \left(\delta \overline{\psi} \psi\right)^{2} \right\rangle^{2}}$$

Clear evidence of Ising universality as predicted by S. Gavin et al

S. Gavin et al hep-ph/9311350







Cross-over at the physical point indicated

with the KS fermion simulations

NB first-order with Wilson fermion; old controversy still remains

41

Progress with finite chemical potential

Difficulties with finite density:

- Monte Carlo methods fail for comlex quark determinant for
 - μ**≠**0

- New developments:
 - Reweighting method to move from $\mu=0$ to $\mu \neq 0$

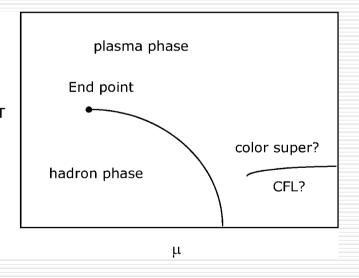
Butapest (Fodor et al)

- Taylor expansion around μ=0 Bielefeld-Swansea
- analytic continuation from Imµ ≠0 to Reµ≠0

Forcrand et al/Lombardo et al

$$Z_{QCD} = \int dU \det D(\mu) e^{-\beta S_{gluon}}$$

Schematic phase diagram (assuming cross-over at T=0)



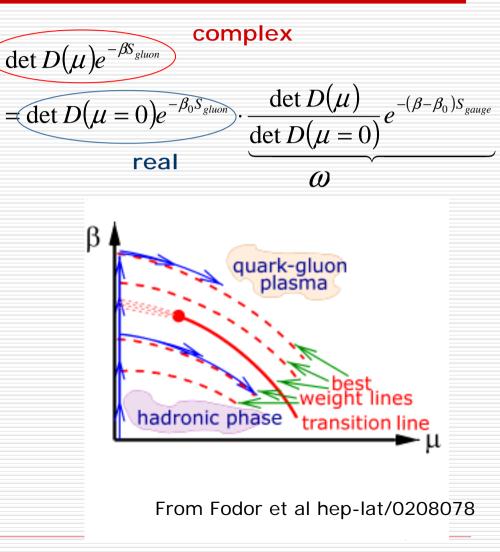
O Reweighting in chemical potential μ

Fodor-Katz strategy

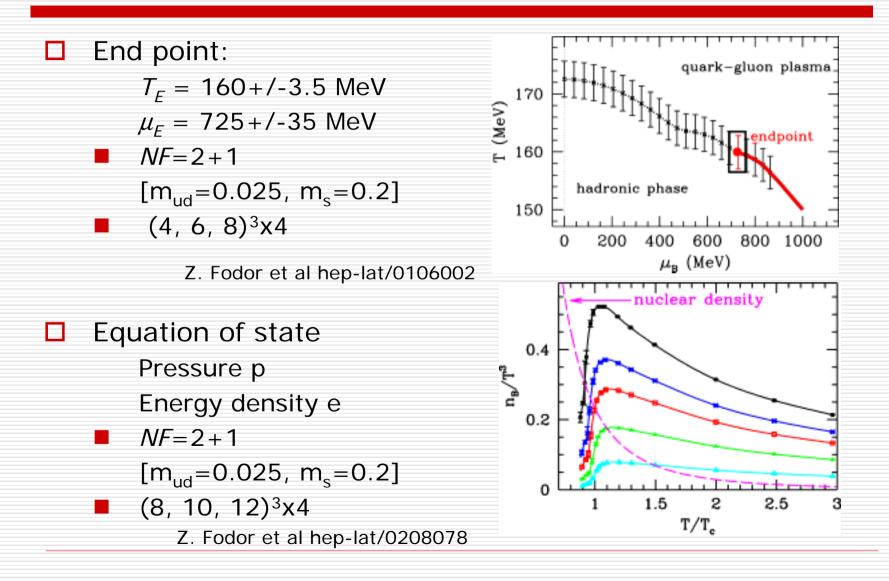
- Z.Fodor et al hep-lat/0104001
 - Reweight in β and μ such that width of ω is minimal
 - Turned out to work for small volume;

 $\mu a \leq \left(N_t \cdot N_s^3\right)^{-1/4}$

Use Lee-Yang zero analysis to locate the end-point E



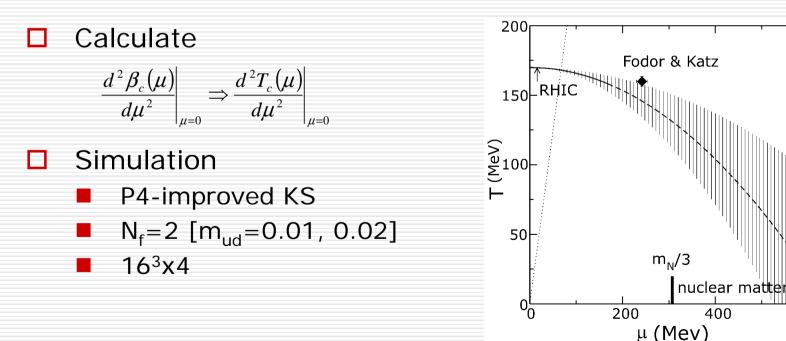




O Taylor expansion in chemical potential μ

S. Ejiri et al heo-lat/0209012 C. R. Allton et al hep-lat/0204010

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

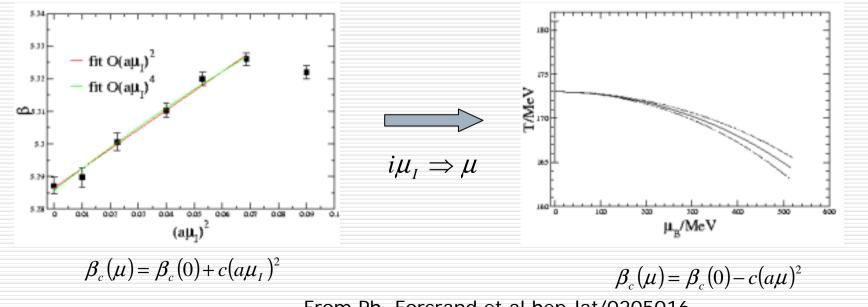


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Provide the set of th

- Determinant real for Imaginary μ, hence amenable to Monte Carlo
 M. Alford et al hep-lat/
- \square Fit obervables in polynomials of μ
- Analytically continue in μ

M. Alford et al hep-lat/9807039 Ph. Forcrand et al hep-lat/020501 M. D'Elia et al hep-lat/0209146



Future direction of lattice QCD

From 2-flavor QCD to 3-flavor QCD

- Dynamical treatment of all light quarks (u, d, s)
- "Light" light quarks
- Non-perturbative improvement coefficients and renormalization factors

Polynomial HMC algorithm

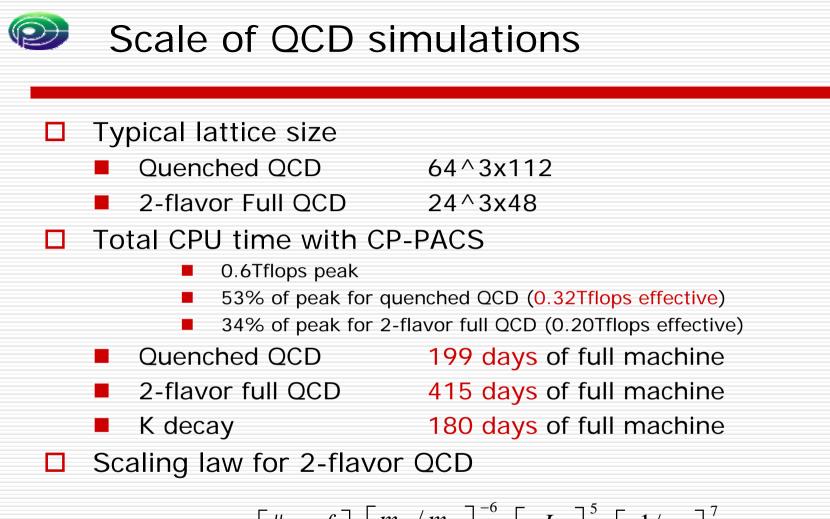
$$\frac{m_{\pi}}{m_{\rho}} \approx 0.6 \left(m_{\pi} \approx 500 MeV \right)$$
$$\Rightarrow \frac{m_{\pi}}{m_{\rho}} \approx 0.4 \left(m_{\pi} \approx 300 MeV \right)$$

O(a²) continuum extrapolation

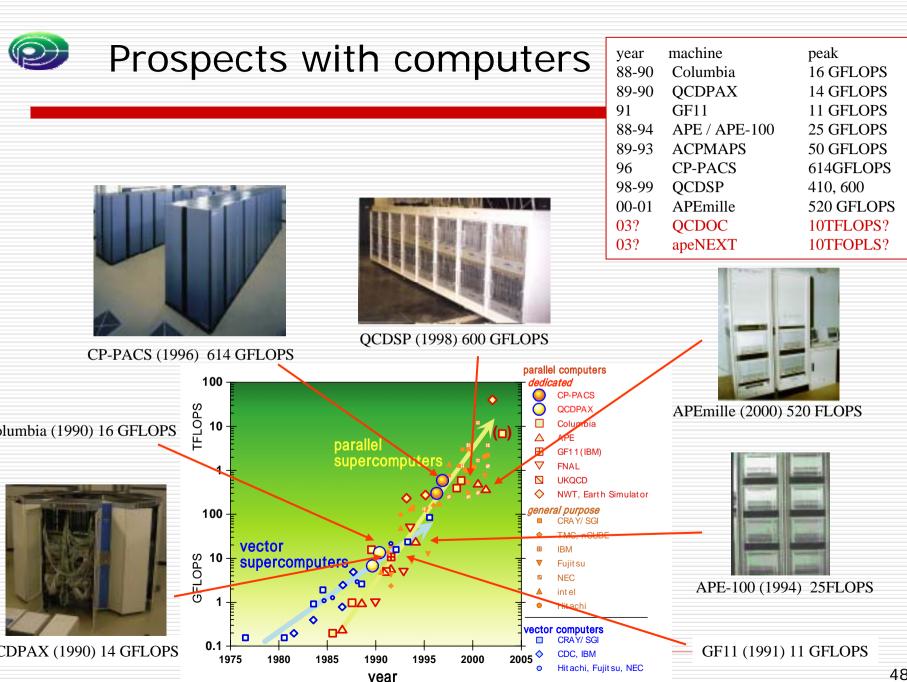
- From non-chiral to chiral action for quark
 - Domain-wall/overlap/perfect actions

Truly realistic and exact simulation of QCD

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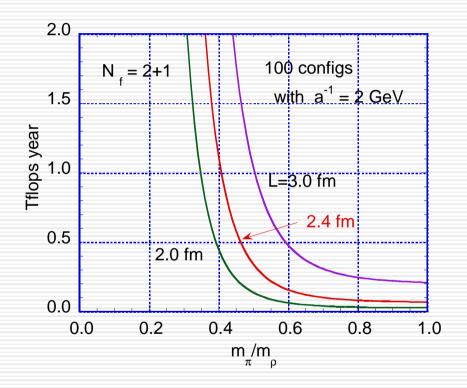


$$\#FLOP's = C \cdot \left[\frac{\#conf}{1000}\right] \cdot \left[\frac{m_{\pi}/m_{\rho}}{0.6}\right]^{-0} \cdot \left[\frac{L}{3fm}\right]^{5} \cdot \left[\frac{1/a}{2GeV}\right]^{7} Tflops \cdot year$$
$$C \approx 2.8$$



Prospects toward 3-flavor simulations

- Polynomial HMC algorithm
- Assumption for Scaling law for 3flavor QCD
 - FLOPS=1.5*(2flavor case)
- O(5-10)Tflops
 computer needed for
 L=2.4fm simulations





QCDOC/apeNEXT (fall 2003) machines well suited for the job

Worldwide prospects



Regional developments and competition

- Asia-Pacific Mini-Workshop on lattice QCD (23-24 Jan 03) China/Taiwan/Korea/Australia/Japan/
- International collaboration
 - Sharing of resources

International Workshop on Lattice Data Grid (19-20 Dec 02)

Exchange of people



Visible shift from quenched to full QCD simulations with dynamical quarks

- 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



- Full QCD simulations with dynamical up, down and strange quark
 - Already underway with staggered quark action
 - Simulations with Wilson quark action will follow
- Definitive prospect toward exact QCD predictions with realistic quark spectrum over the next few years
 - Firm numbers to our phenomenology/experiment colleagues
 - Quantitative understanding of the full range of strong interactions
 - 1935 meson theory (Yukawa)
 - 1951 strangeness (Gell-Mann-Nishijima)
 - 1961 chiral symmetry and pion(Nambu-Jona-Lasinio)
 - 1973 QCD and asymptotic freedom(Gross-Wilczek-Politzer)
 - 1974 Lattice QCD(Wilson)
 - 1981 Monte Carlo simulation of QCD(Creutz-Jacobs-Rebbi)