1+1+1 Flavor QCD+QED Simulation at the Physical Point

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and

Advanced Institute for Computational Sciences (AICS)

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Before My Talk

What is Advanced Institute for Computational Science (AICS) ?

- Next-Generation Supercomputer (NGS) Project
- New Institute in Kobe
- Strategic Field Program for NGS

Next-Generation Supercomputer (NGS) Project

Overview of Project

- Development of 10 Pflops-class system in Kobe

  ⇒ named “K computer” by public competition
- Development of grand challenge applications in nano science and life science
- Buildup of a research center in computational science around the 10 Pflops-class system

  ⇒ Advanced Institute for Computational Science (AICS)
- Project period is from Japanese FY 2006 to 2012
- RIKEN is responsible for the computer development
- High Performance Computing Infrastructure (HPCI)

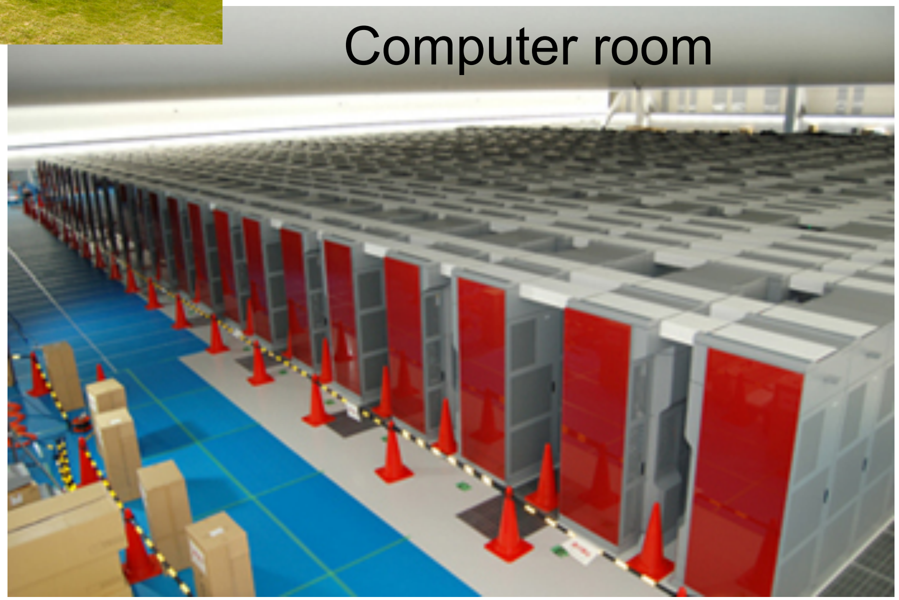
Site for K computer

450km (280miles)
west from Tokyo

Some Photo

Building

Logo



TOP500 CERTIFICATE

K computer, a Fujitsu System at the
RIKEN Advanced Institute for Computational Science (AICS), Kobe, Japan

is ranked

No. 1

among the World's TOP500 Supercomputers
with 8.162 PFlop/s Linpack Performance
on the TOP500 List published at the ISC'11 Conference, June 20, 2011

Congratulations from the TOP500 Editors

Hans Meuer, University of Mannheim
Erich Strohmaier, NERSC/Berkeley Lab
Jack Dongarra, University of Tennessee
Horst Simon, NERSC/Berkeley Lab

Advanced Institute for Computational Science

founded on July 1, 2010

Objectives

- Research and development of computational and computer science
- Operation of K computer
- Lead High Performance Computing (HPC) in Japan

Special emphasis on

- Strong collaboration between computational and computer scientists
- Research on future HPC systems after K computer
- Fostering young scientists with expertise in both computational and computer science

Research Division

launched on October 1, 2010

8 research teams lead by Principal Investigators (PI)

Computational Science	Field Theory	Y.Kuramashi
	Computational Molecular Science	T.Nakajima
	Computational Biophysics	Y.Sugita
	Computational Material Science	S.Yunoki
	Computational Climate Science	H.Tomita
Computer Science	System Software	Y.Ishikawa
	Programming Environment	M.Sato
	Processor	M.Taiji

Seeking Research Scientists

http://www.riken.go.jp/r-world/info/recruit/k111118_e_aics.html

Strategic Field Program

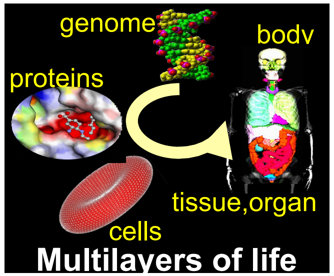
For strategic use of K computer

- Government selected 5 strategic fields in science and technology for importance from national view point
- For each field, Government also selected a core institute
- Each core institute is responsible for organizing research and supercomputer resources in the respective field and its community, for which they receive
  - priority allocation of K computer resources
  - funding to achieve the research goals

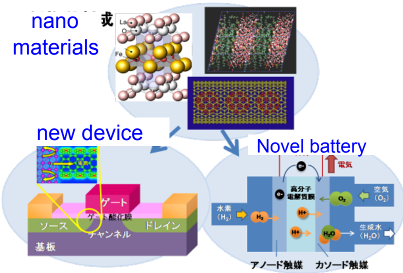
Strategic Fields and Core Institutes

strategic field

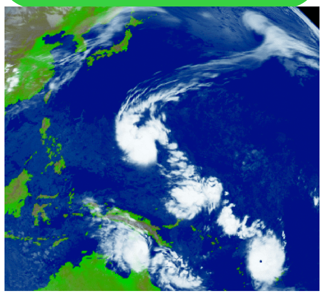
Life Science & Medicine



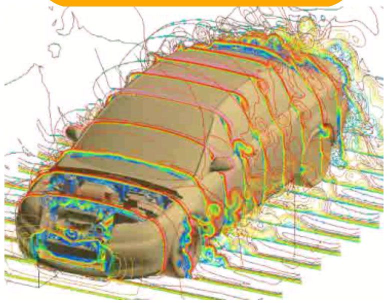
New materials & Energy



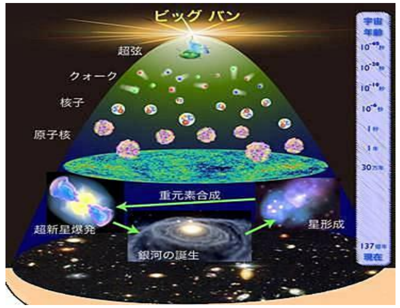
Global change prediction



Next generation engineering



Matter & Universe



core institute

RIKEN	Institute for Solid State Physics U. Tokyo	Earth Simulator Center JAMSTEC	Institute for Industrial Science U. Tokyo	Center for Comp. Science U. Tsukuba
Life science Community	materials science Community	Earth science Community	Engineering Community Industry	Basic science Community
Supercomputer resources	Supercomputer resources	Supercomputer resources	Supercomputer resources	Supercomputer resources

Plan of Talk

§1. Brief Introduction

§2. Hadron Spectrum

§3. Fine Tuning of Quark Masses

§4. 1+1+1 Flavor QCD+QED

§5. Summary

§1. Brief Introduction to Lattice QCD

QCD Lagrangian

$$\mathcal{L} = \frac{1}{4} F_{\mu\nu} F_{\mu\nu} + \sum_{q=u,d,s,c,b,t} \bar{q} \left[\gamma_\mu (\partial_\mu - i g A_\mu) + m_q \right] q$$

Only coupling const. g and quark masses m_q are free parameters

Why is numerical analysis necessary for strong interaction?

Too strong to investigate with perturbative analysis

Characteristic features (confinement etc.) are nonperturbative

Aiming at quantitative analyses on

- hierarchical structures made of quarks
- phase diagram and EOS under finite temperature/density

based on first principle (QCD Lagrangian) calculations

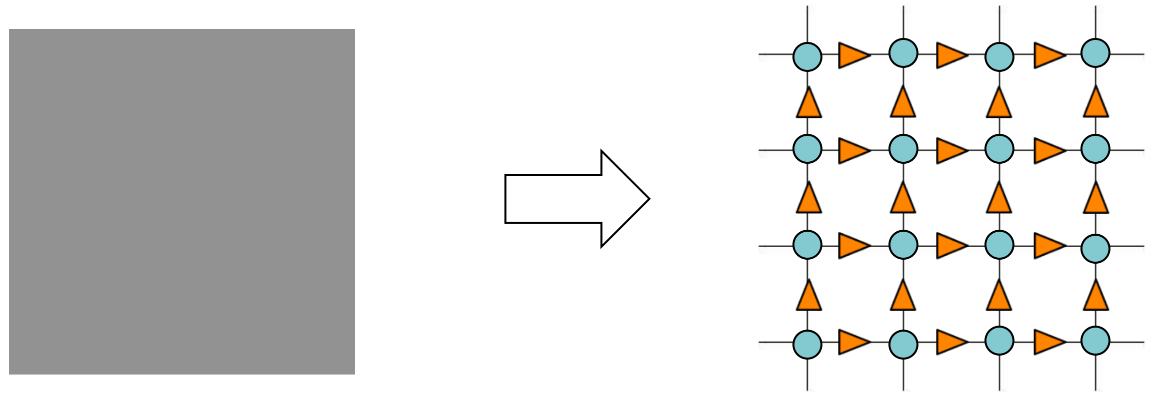
Numerical method (1)

Path integral in 4-dim.（space 3-dim. + time 1-dim.）continuum theory

$$\langle \mathcal{O}[A_\mu, q, \bar{q}] \rangle = \frac{1}{Z} \int \mathcal{D}A_\mu \mathcal{D}q \mathcal{D}\bar{q}\ \mathcal{O}[A_\mu, q, \bar{q}]\ \exp\left\{- \int d^4x \mathcal{L}[A_\mu, q, \bar{q}]\right\}$$

Similar to partition function in stat. mechanics ⇒ Monte Carlo method

Discretize 4-dim. space-time for finite degree of freedom ⇒ 4-dim. lattice



$q(x)$: quark field
$A_\mu(x)$: gauge field

● $q(n)$: quark field
▲ $U_\mu(n)$: SU(3) link variable

Numerical method (2)

Path integral on 4-dim. lattice

$$\langle \mathcal{O}[U_\mu, q, \bar{q}] \rangle = \frac{1}{Z} \int \prod_{n,\mu} dU_\mu dq d\bar{q}\; \mathcal{O}[U_\mu, q, \bar{q}]\; \exp\left\{ -\sum_n \mathcal{L}_{\mathrm{latt}}[U_\mu, q, \bar{q}] \right\}$$

Quark fields are Grassmann (anticommuting) numbers

⇒ analytically integrated

$$\langle \bar{\mathcal{O}}[U_\mu] \rangle = \frac{1}{Z} \int \prod_{n,\mu} dU_\mu\; \bar{\mathcal{O}}[U_\mu]\; \exp\left\{ -S_{\mathrm{latt}}^{\mathrm{eff}}[U_\mu] \right\}$$

Average over the configurations gives expectation value

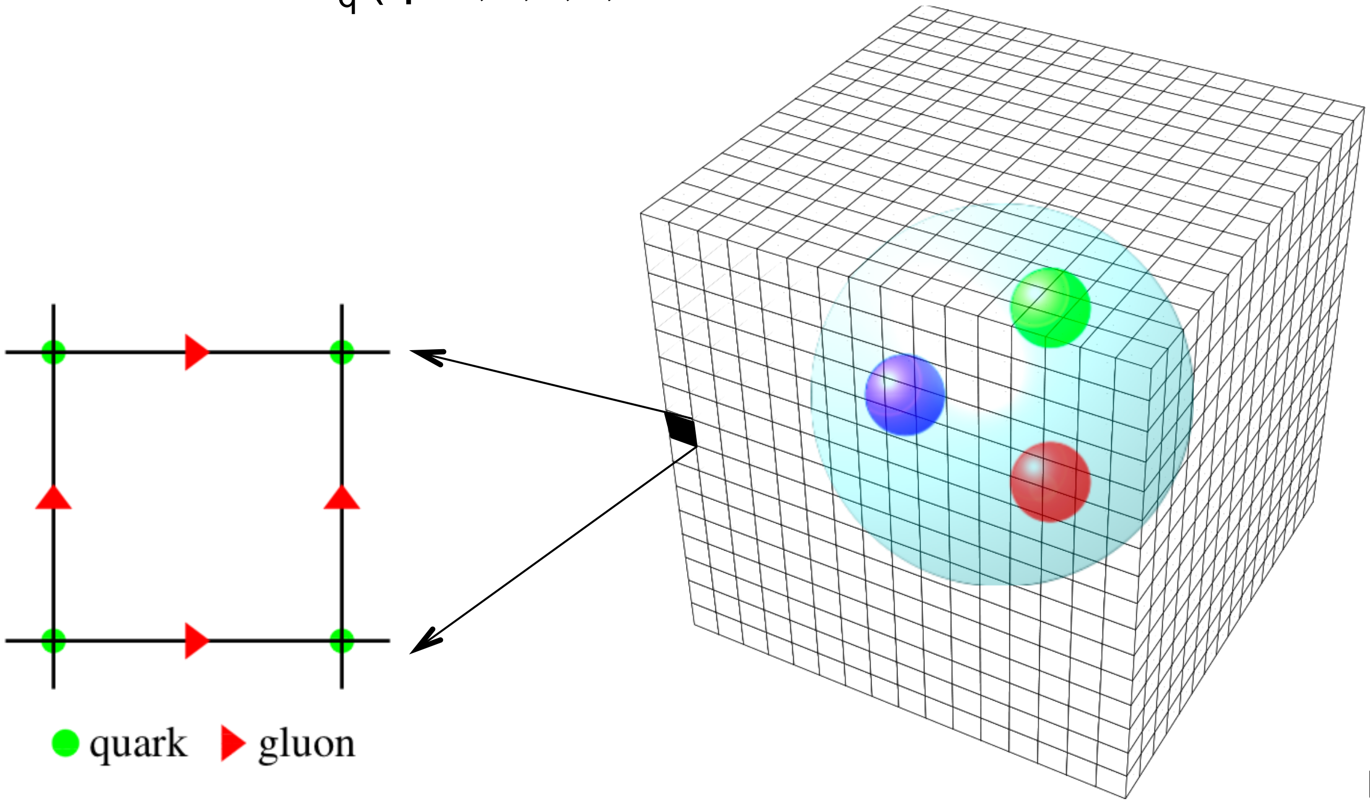
$$\langle \bar{\mathcal{O}}[U_\mu] \rangle = \frac{1}{N} \sum_{i=1}^{N} \bar{\mathcal{O}}[U_\mu^{(i)}] + O\left(\frac{1}{\sqrt{N}} \right)$$

statistical error

Simulation Parameters

Few parameters

- 4-dim. volume : V=NX・NY・NZ・NT
- lattice spacing : a (as function of bare coupling g)
- quark masses : m_q (q=u,d,s,c,b,t)



Major Systematic Errors

- Finite volume effects

  ⇒ larger V=NX·NY·NZ·NT

- Finite lattice spacing effects

  $\Lambda_{QCD} \ll 1/a$, currently $m_b > 1/a$

  ⇒ smaller a

- Quenched approximation (det D_q=1)

  ⇒ simulations including the effects of det D_q

- Chiral extrapolation

  ⇒ simulations at physical quark masses (physical point)

Need heavier computational cost to diminish the systematic errors

cost $\propto$ (physical vol.)$^{1.25}$·(lattice spacing)$^{-6\sim-7}$·(quark mass)$^{-2\sim-3}$

§2. Hadron Spectrum

Fundamental quantities both in physical and technical senses

<u>physical side</u>

physical input ⇒ $m_u, m_d, m_s, \ldots$ ⇒ reproduce hadron spectrum?

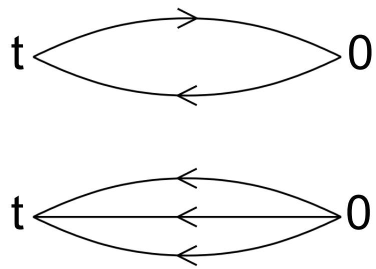
(ex. m_π, m_K, m_Ω) validity of QCD / determination of m_q

<u>technical side</u>

hadron correlators in terms of quark fields

$$\langle \mathcal{O}_h(t)\mathcal{O}_h^\dagger(0)\rangle \overset{t \gg 0}{\approx} C\exp\left(-m_h t\right)$$ ⇒ extract m_h by fit

quark diagrams from Wick contractions



meson

baryon

History of Hadron Spectrum Calculation

1981 first calculation of hadron masses in quenched approx.

Hamber-Parisi

demonstrate the possibility of first principle calculations

1996～2000 precision measurement in quenched approx.

CP-PACS

clear deviation from the experiment

2000～ initiate 2+1 flavor QCD simulations

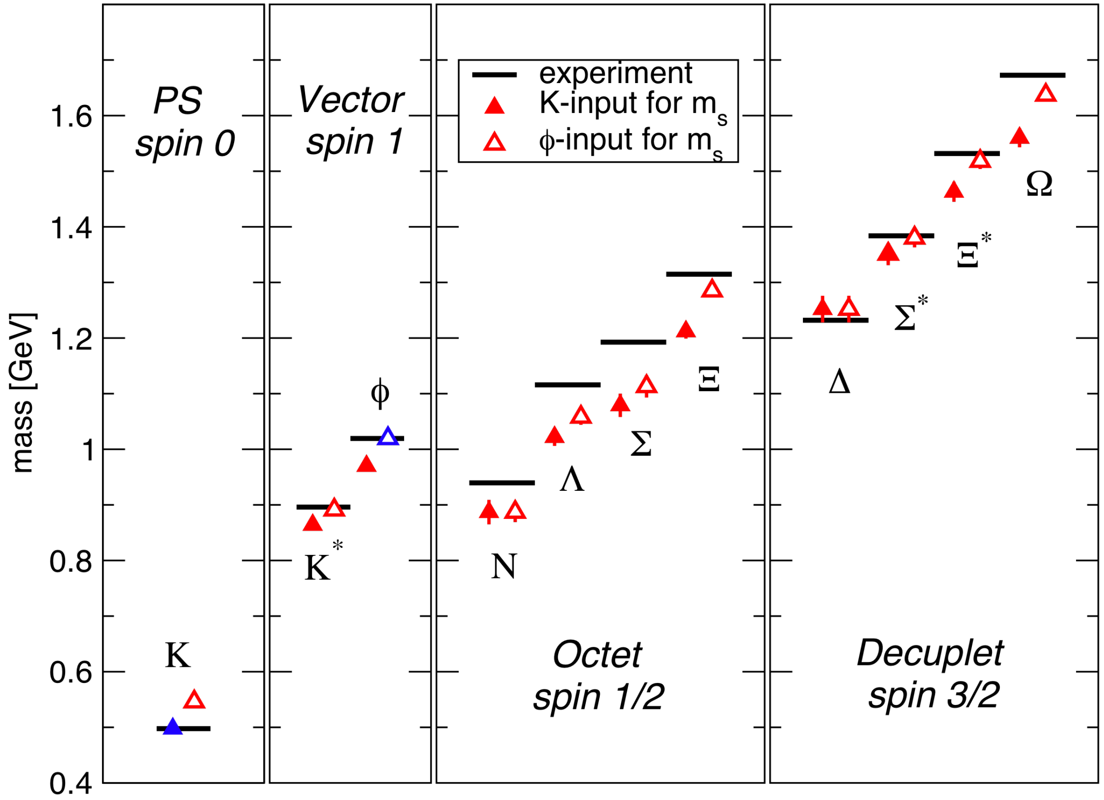
CP-PACS/JLQCD, MILC, …

incorporate det $D_{u,d,s}$ effects

reduce ud quark mass toward physical value

Hadron Spectrum in Quenched QCD

physical input m_π, m_K or m_φ, m_ρ $\Rightarrow$ m_u=m_d, m_s, a

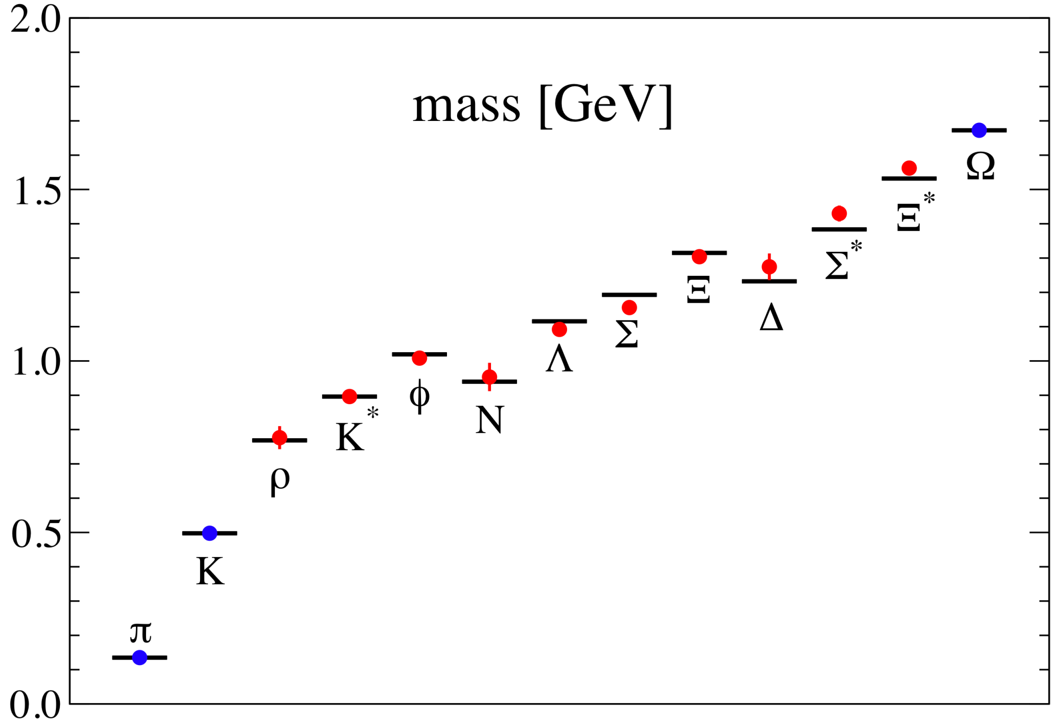


CP-PACS 00

～10% deviation from experimental values

Hadron Spectrum in 2+1 Flavor QCD

physical input m_π, m_K, m_Ω ⇒ m_u=m_d, m_s, a



PACS-CS 09

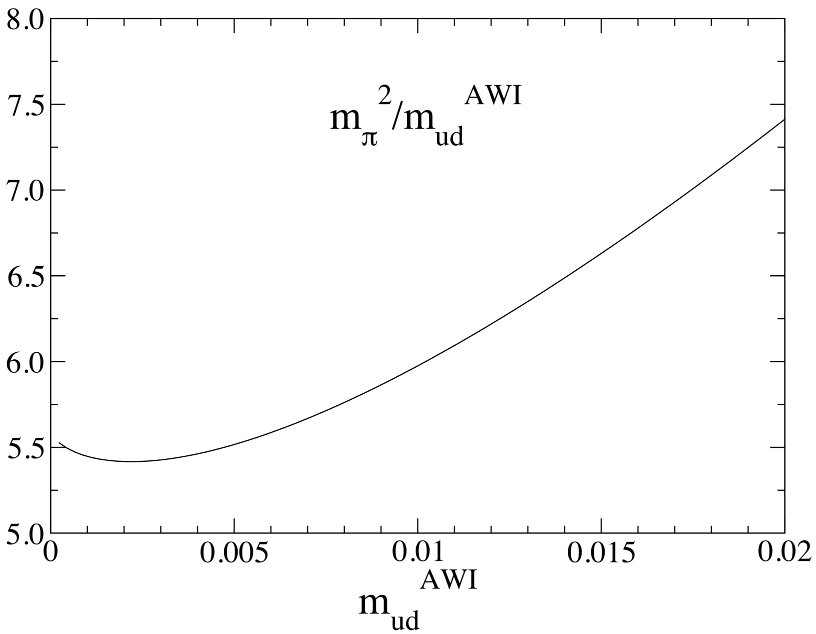
consistent within 2～3% error bars

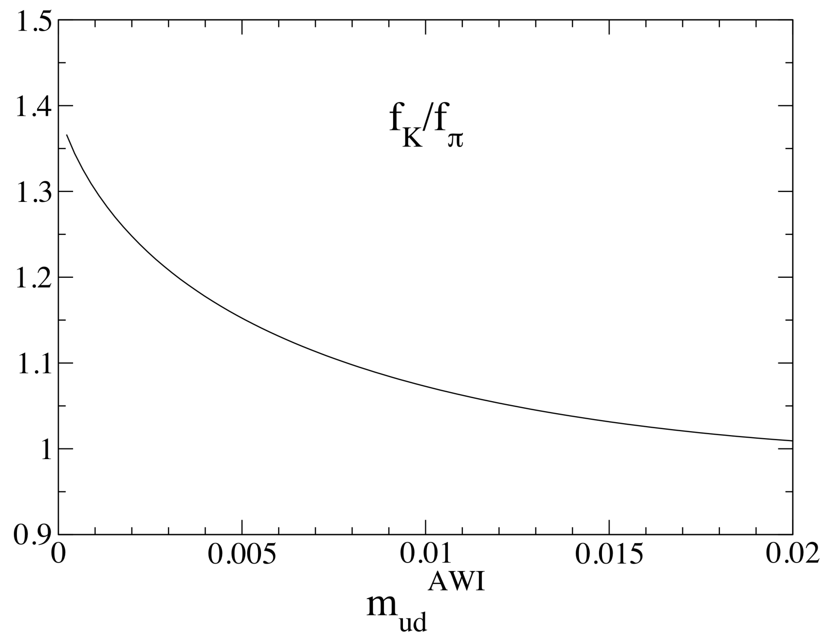
similar results are obtained by other groups

Chiral Behavior (1)

reduction of ud quark mass ⇒ check chiral properties as a by-product

Amorós-Bijnens-Talavera 01





logarithmic curvature expected from ChPT

Chiral Behavior (2)

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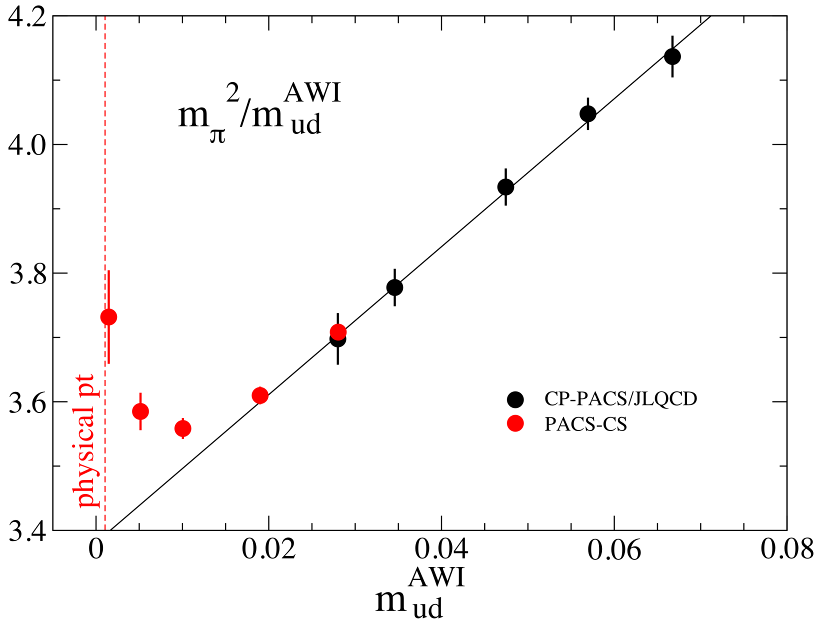
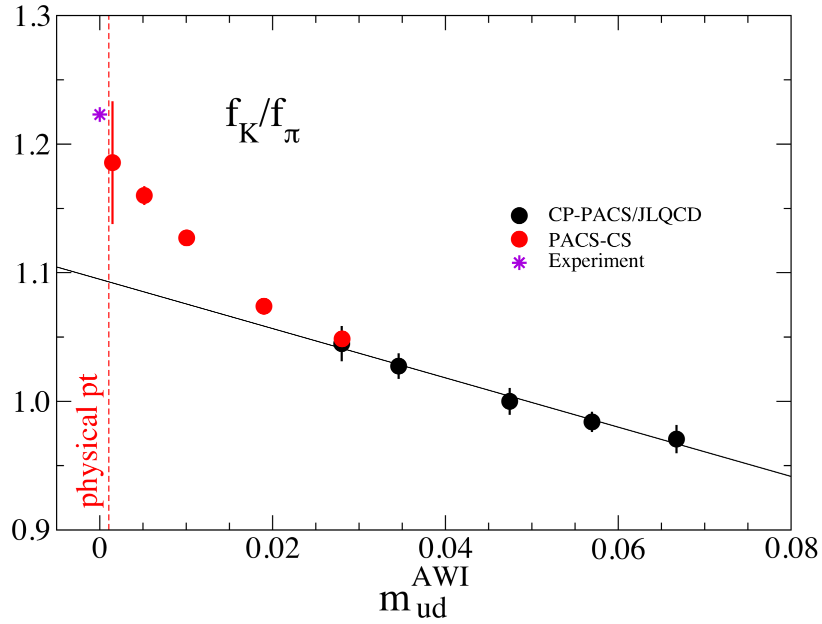




nontrivial curvature observed

ChPT fit gives reasonable LECs

What Next ?

- 2+1 (m_u=m_d≠m_s) flavor simulation at the physical point

  PACS-CS 10

  avoid chiral extraporation

- 1+1+1 (m_u≠m_d≠m_s) flavor simulation at the physical point
  - electromagnetic interactions

    quenched study: Eichten et al. 96, Blum et al. 07,10

    MILC@lat10, BMW@lat10
  - u-d quark mass difference

$K^0(d\bar{s})$ 497.6MeV

1%

$K^+(u\bar{s})$ 493.7MeV

- Direct treatment of resonances in lattice QCD

  decay width of resonance states

§3. Fine Tuning of Quark Masses

Reweighting method

original: $(\kappa_{ud},\kappa_s) \Rightarrow$ target: $(\kappa_{ud}{}^*,\kappa_s{}^*)$ assuming $\rho_q \equiv \kappa_q/\kappa_q{}^* \approx 1$

$$
\begin{aligned}
\langle \bar{\mathcal{O}}[U](\kappa^*_{\mathrm{ud}},\kappa^*_{\mathrm{s}})\rangle_{(\kappa^*_{\mathrm{ud}},\kappa^*_{\mathrm{s}})} &= \frac{\int \mathcal{D}U\,\bar{\mathcal{O}}[U](\kappa^*_{\mathrm{ud}},\kappa^*_{\mathrm{s}})|\det[D_{\kappa^*_{\mathrm{ud}}}[U]]|^2 \det[D_{\kappa^*_{\mathrm{s}}}[U]]\mathrm{e}^{-S_g[U]}}{\int \mathcal{D}U |\det[D_{\kappa^*_{\mathrm{ud}}}[U]]|^2 \det[D_{\kappa^*_{\mathrm{s}}}[U]]\mathrm{e}^{-S_g[U]}} \\
&= \frac{\int \mathcal{D}U\,\bar{\mathcal{O}}[U](\kappa^*_{\mathrm{ud}},\kappa^*_{\mathrm{s}})\left|\det\left[\frac{D_{\kappa^*_{\mathrm{ud}}}[U]}{D_{\kappa_{\mathrm{ud}}}[U]}\right]\right|^2 \det\left[\frac{D_{\kappa^*_{\mathrm{s}}}[U]}{D_{\kappa_{\mathrm{s}}[U]}}\right]|\det[D_{\kappa_{\mathrm{ud}}}[U]]|^2\det[D_{\kappa_{\mathrm{s}}}[U]]\mathrm{e}^{-S_g[U]}}{\int \mathcal{D}U\left|\det\left[\frac{D_{\kappa^*_{\mathrm{ud}}}[U]}{D_{\kappa_{\mathrm{ud}}}[U]}\right]\right|^2 \det\left[\frac{D_{\kappa^*_{\mathrm{s}}}[U]}{D_{\kappa_{\mathrm{s}}[U]}}\right]|\det[D_{\kappa_{\mathrm{ud}}}[U]]|^2\det[D_{\kappa_{\mathrm{s}}}[U]]\mathrm{e}^{-S_g[U]}} \\
&= \frac{\langle \bar{\mathcal{O}}[U](\kappa^*_{\mathrm{ud}},\kappa^*_{\mathrm{s}})R_{\mathrm{ud}}[U]R_{\mathrm{s}}[U]\rangle_{(\kappa_{\mathrm{ud}},\kappa_{\mathrm{s}})}}{\langle R_{\mathrm{ud}}[U]R_{\mathrm{s}}[U]\rangle_{(\kappa_{\mathrm{ud}},\kappa_{\mathrm{s}})}},
\end{aligned}
$$

Reweighting factors

$$
R_{\mathrm{ud}}[U] = \left|\det\left[W[U](\rho_{\mathrm{ud}})\right]\right|^2, \quad R_{\mathrm{s}}[U] = \det\left[W[U](\rho_{\mathrm{s}})\right]
$$

where

$$
W[U](\rho_q) \equiv \frac{D_{\kappa^*_{\mathrm{q}}}[U]}{D_{\kappa_{\mathrm{q}}}[U]}
$$

Evaluation of R_{ud}

Introduce a complex bosonic field η

$$
\begin{aligned}
R_{\rm ud}[U] &= \left|\det\left[W[U](\rho_{\rm ud})\right]\right|^2 \\
&= \langle \mathrm{e}^{-|W^{-1}[U](\rho_{\rm ud})\eta|^2+|\eta|^2}\rangle_\eta
\end{aligned}
$$

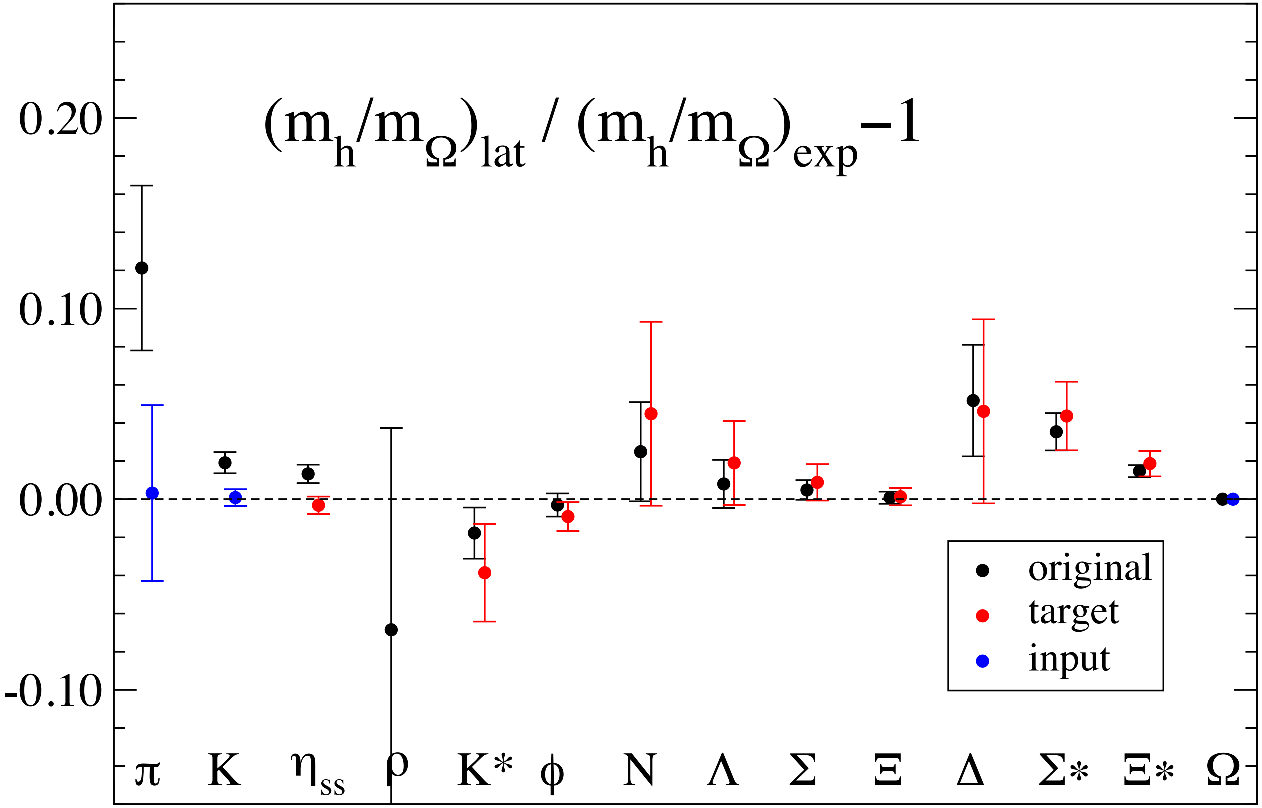
Given a set of $\eta^{(i)}$ ($i=1,\ldots,N_\eta$) with Gaussian distribution

$$
R_{\rm ud}[U] = \lim_{N_\eta\to\infty}\frac{1}{N_\eta}\sum_{i=1}^{N_\eta}\mathrm{e}^{-|W^{-1}[U](\rho_{\rm ud})\eta^{(i)}|^2+|\eta^{(i)}|^2}
$$

R_s is obtained in a similar way

Tuning to the Physical Point

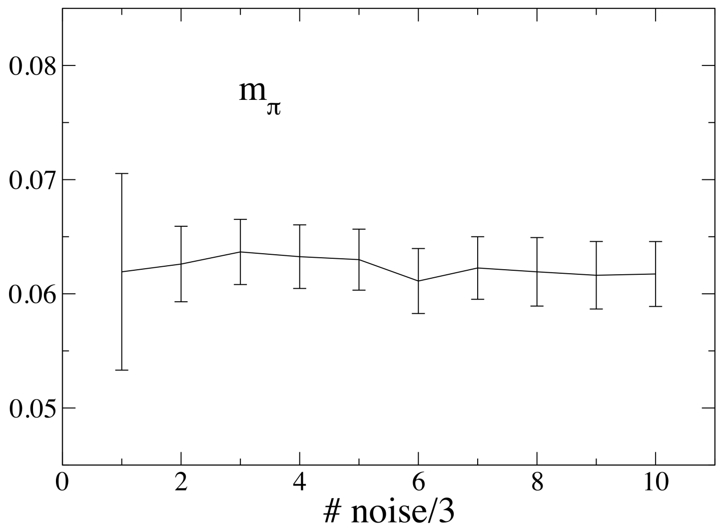
PACS-CS 10

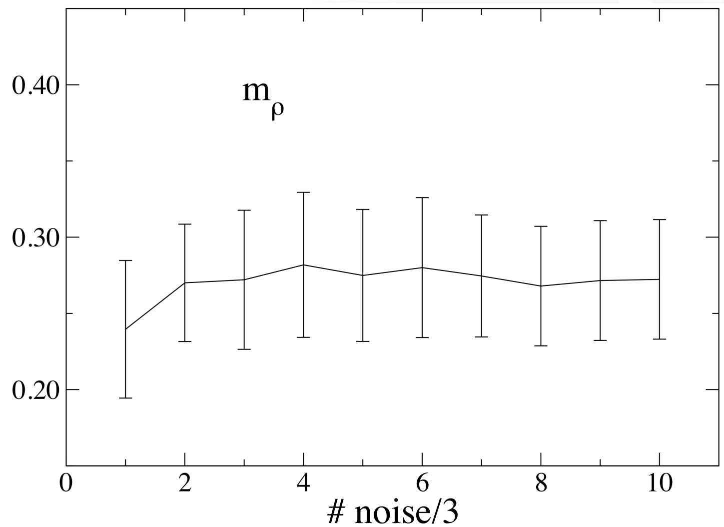


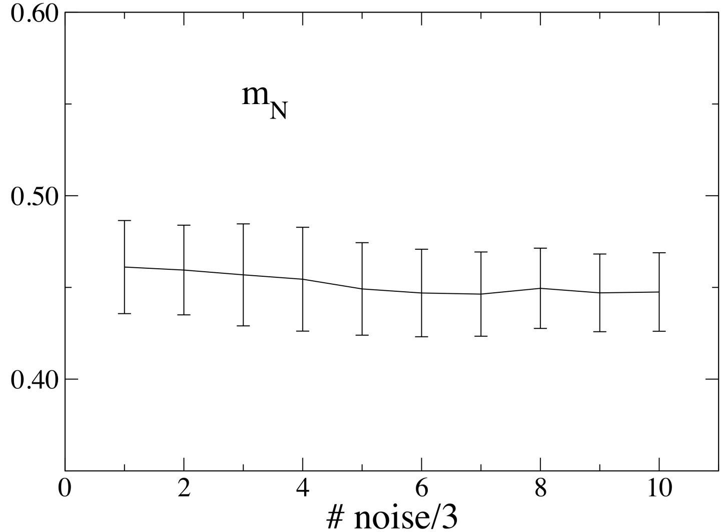
m_π/m_Ω, m_K/m_Ω are properly tuned

Δm_{ud}~1MeV, Δm_s~3MeV

N_η dependence

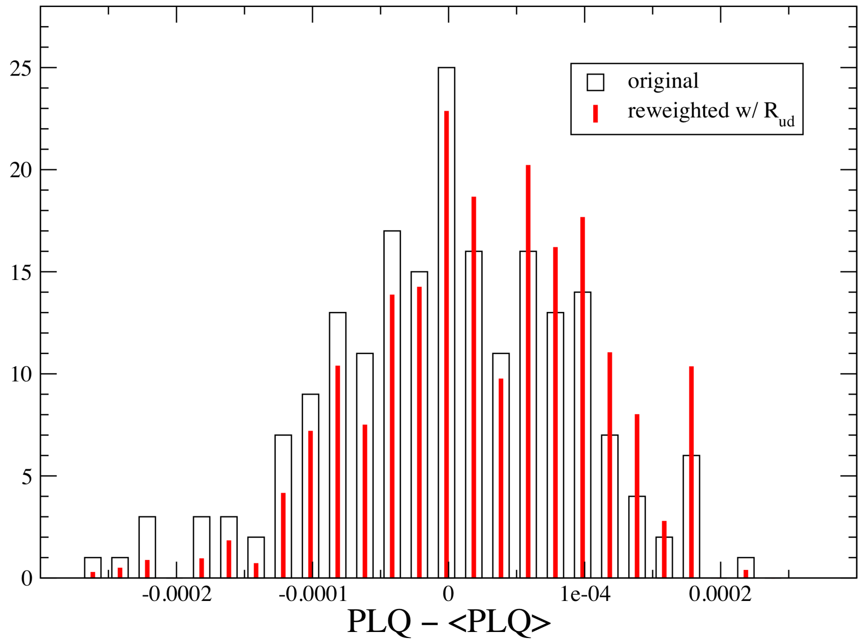


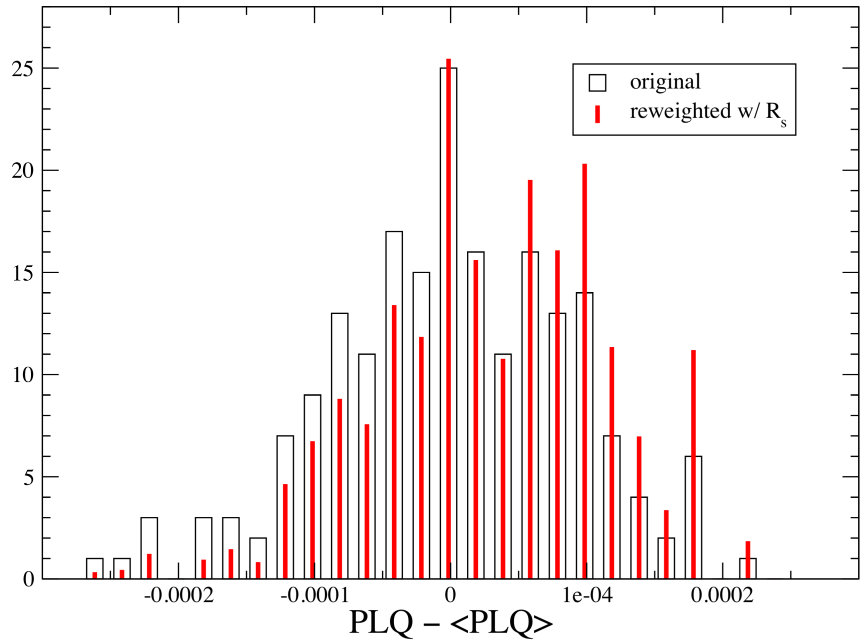




Look converged for $N_\eta \gtrsim 4$

Plaquette Histogram at Original and Target κ’s





Distribution is slightly moved toward larger values

Still almost degenerate

§4. 1+1+1 Flavor QCD+QED

Isospin symmetry breaking

- electromagnetic interactions

  $Q_u=+2/3e$, $Q_d=Q_s=-1/3e$, $e=\sqrt{4\pi/137}$

- u-d quark mass difference

  $m_u=m_d\neq m_s$ (2+1 flavor) $\Rightarrow$ $m_u\neq m_d\neq m_s$ (1+1+1 flavor)

Physical inputs:

$m_{\pi+}$(ud), m_{K0}(ds), m_{K+}(us), $m_{\Omega-}$(sss)

Outputs:

m_u, m_d, m_s, a(lattice spacing), m_n-m_p, …

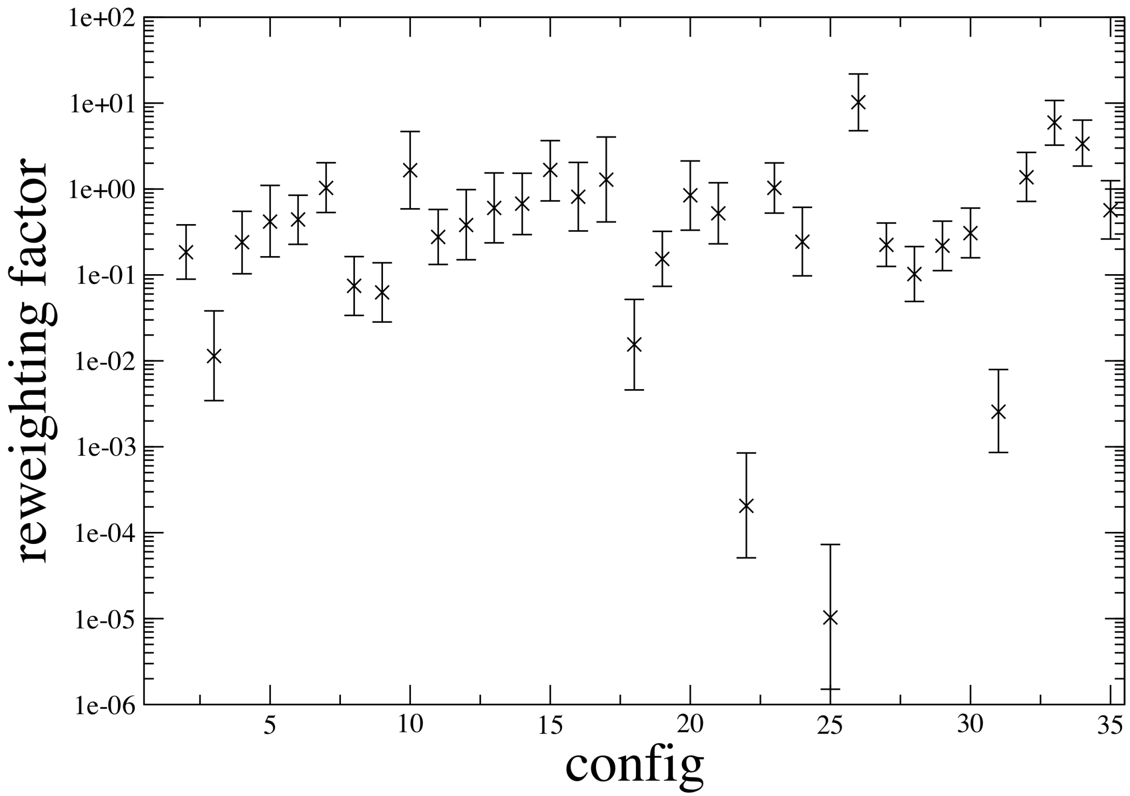
Strategy

- Generate 2+1 flavor QCD configs near the physical point
- Generate U(1) gauge configs independent of QCD ones
  - non-compact A_μ ⇒ compactification to $U_\mu^e=\exp(iQ_q A_\mu)$
- Incorporate EM effects by reweighting method
  - $Q_u=0 \Rightarrow Q_u=+2/3e$ for u quark
  - $Q_{d,s}=0 \Rightarrow Q_{d,s}=-1/3e$ for d, s quark
- Tune $(\kappa_u,\kappa_d,\kappa_s)$ to the physical point such that $m_{\pi+}$(ud), m_{K0}(ds), m_{K+}(us), $m_{\Omega-}$(sss) are reproduced

In the following, all the results are preliminary

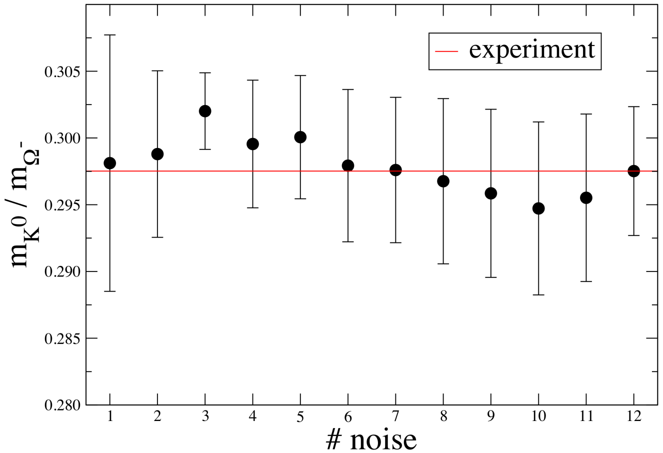
Reweighting factor

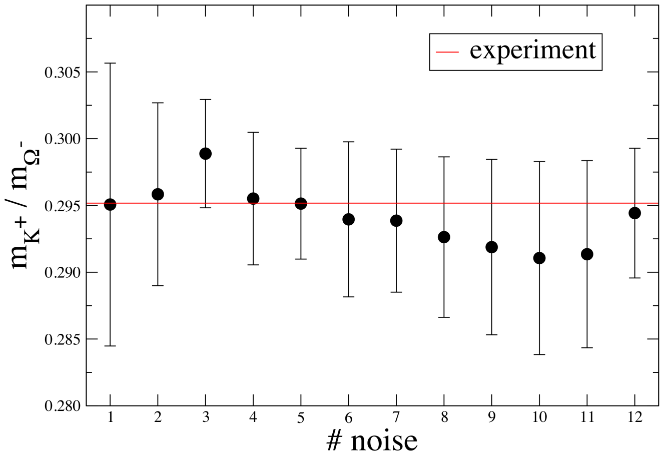
$$R_{\mathrm{uds}}[U_\mu] = \det\left[\frac{D_{\kappa_{\mathrm{u}}^*}[U_\mu\exp(iQ_uA_\mu)]}{D_{\kappa_{\mathrm{u}}}[U_\mu]}\frac{D_{\kappa_{\mathrm{d}}^*}[U_\mu\exp(iQ_dA_\mu)]}{D_{\kappa_{\mathrm{d}}}[U_\mu]}\frac{D_{\kappa_{\mathrm{s}}^*}[U_\mu\exp(iQ_sA_\mu)]}{D_{\kappa_{\mathrm{s}}}[U_\mu]}\right]$$

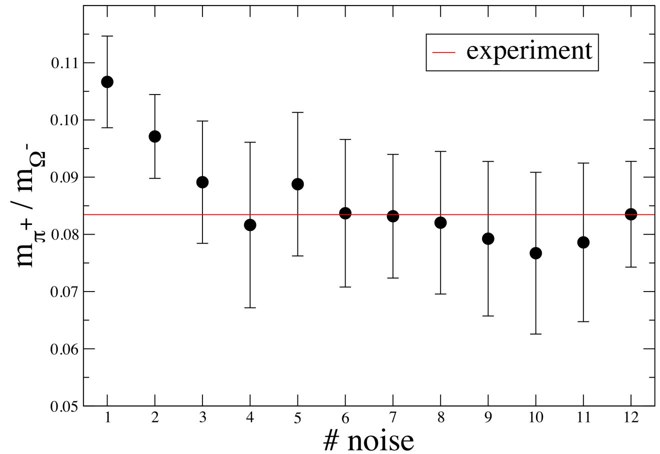


N_η dependence

Physical inputs: $m_{\pi+}(ud)$, $m_{K0}(ds)$, $m_{K+}(us)$, $m_{\Omega-}(sss)$

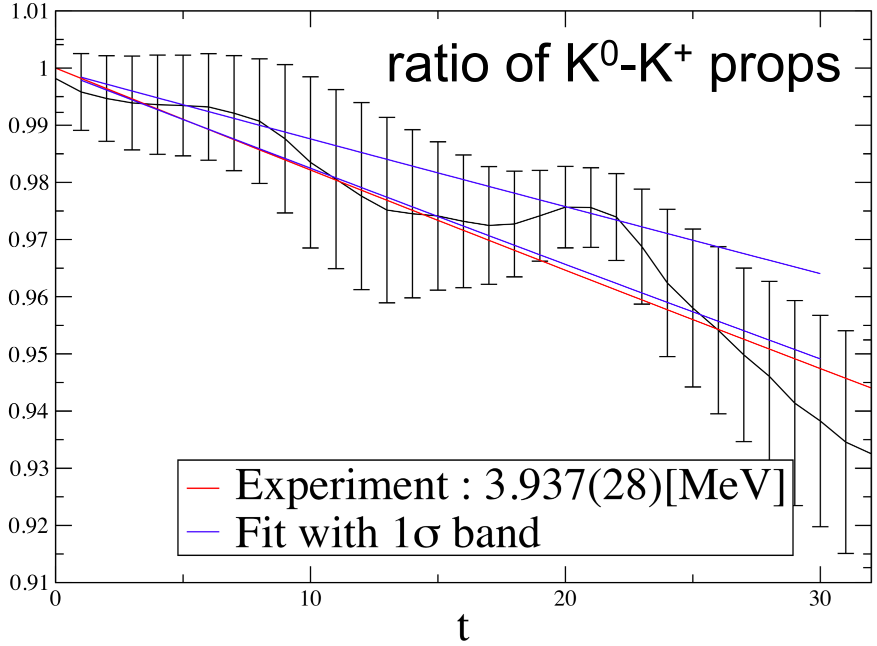


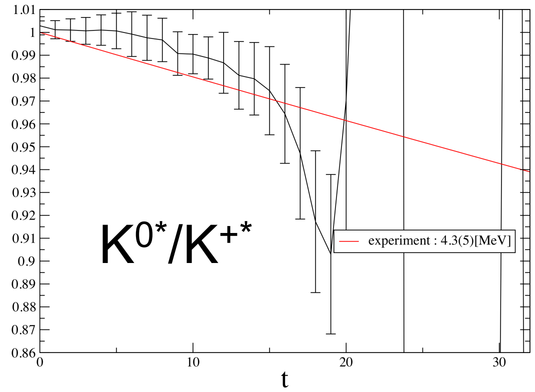


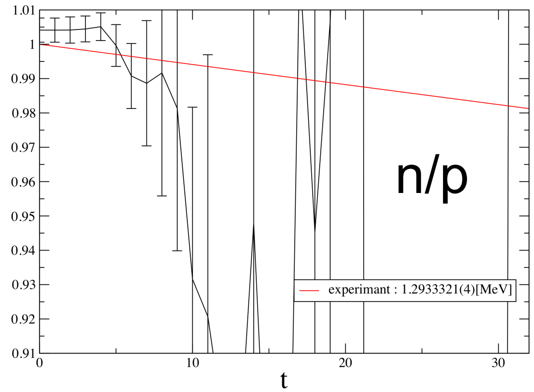


Look converged for $N_\eta \gtrsim 4$ or 5

Mass Splittings among Isospin Multiplets







Quark Masses with NP Renormalization Factor

Physical inputs:

$m_{\pi+}(ud)$=139.7(15.5) [MeV] exp: 139.6 [MeV]

$m_{K0}(ds)$=497.6(8.1) [MeV] exp: 497.6 [MeV]

$m_{K+}(us)$=492.4(8.1) [MeV] exp: 493.7 [MeV]

$m_{K0}(ds)-m_{K+}(us)$=3.21(57) [MeV] exp: 3.937(28) [MeV]

Quark Masses in MSbar at μ=2 GeV:

m_u=1.97(67) [MeV]

m_d=4.31(83) [MeV]

m_s=90.32(67) [MeV]

$(m_u+m_d)/2$=3.14(72) [MeV]

m_u/m_d=0.457(93)

$2m_s/(m_u+m_d)$=28.8(6.6)

§5. Summary

- 2+1 ($m_u = m_d \neq m_s$) flavor QCD ⇒ 1+1+1 ($m_u \neq m_d \neq m_s$) flavor QCD+QED
- Incorporate QED effects by reweighting method
- Next step is to enlarge the lattice volume