Physical Point Simulation in 2+1 Flavor Lattice QCD

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based on PRD81(2010)074503

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Plan of talk

§1. The PACS-CS project
§2. Reweighting method
§3. Simulation and reweighting parameters
§4. Results
§5. Summary

§1. The PACS-CS project

Parallel Array Computer System for Computational Sciences

operation started on 1 July 2006 at CCS in U.Tsukuba

collaboration members

physicists:

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computer scientists:

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Physics plan

aim: 2+1 flavor QCD simulation at the physical point

	PACS-CS	CP-PACS/JLQCD
gauge action	Iwasaki	Iwasaki
quark action	clover with $c_{\rm SW}^{\rm NP}$	clover with $c_{\rm SW}^{\rm NP}$
a[fm]	$\gtrsim 0.1$	0.07,0.1,0.122
volume	$\gtrsim (3\text{fm})^3$	$\sim (2\text{fm})^3$
$m_{\rm ud}$	physical point	64MeV
algorithm for ud	DDHMC with improvements	HMC
algorithm for s	UV-filtered exact PHMC	exact PHMC

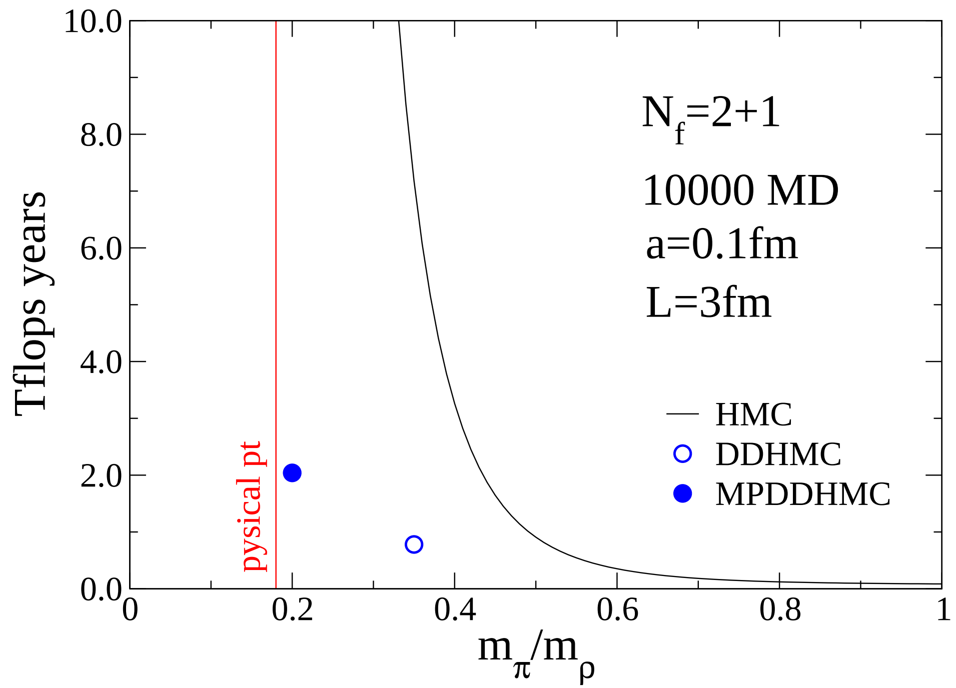
strategy: physical point $\Rightarrow$ enlarge volume $\Rightarrow$ smaller a

Why physical point simulation?

- difficult to trace chiral logs for chiral extrapolation
- ChPT is not always a good guiding principle
- direct treatment of resonances based on phase shift
  $\rho \to \pi\pi$ decay: PRD76(2007)094506, LATTICE2010
- simulations with different up and down quark masses

$\Rightarrow$ there exist two types of problems

(1) Computational cost



drastic reduction with (Mass-Preconditioned) DDHMC

PRD79(2009)034503

(2) Fine-tuning to physical point

physical point is known a posteriori, unfortunately
need 3 simulation points within a few MeV differences around the physical point in 2+1 flavor case
$\Rightarrow$ demanding computational cost

try reweighting method both for ud and s quarks
whose masses are slightly (and unfortunately) off the physical point

§2. Reweighting method

original:$(\kappa_{\mathrm{ud}}, \kappa_{\mathrm{s}})$ $\Rightarrow$ target:$(\kappa^*_{\mathrm{ud}}, \kappa^*_{\mathrm{s}})$ assuming $\rho_q \equiv \kappa_q/\kappa^*_q \approx 1$

$$\langle \mathcal{O}[U](\kappa^*_{\mathrm{ud}}, \kappa^*_{\mathrm{s}})\rangle_{(\kappa^*_{\mathrm{ud}}, \kappa^*_{\mathrm{s}})} = \frac{\langle \mathcal{O}[U](\kappa^*_{\mathrm{ud}}, \kappa^*_{\mathrm{s}}) R_{\mathrm{ud}}[U] R_{\mathrm{s}}[U]\rangle_{(\kappa_{\mathrm{ud}}, \kappa_{\mathrm{s}})}}{\langle R_{\mathrm{ud}}[U] R_{\mathrm{s}}[U]\rangle_{(\kappa_{\mathrm{ud}}, \kappa_{\mathrm{s}})}}$$

reweighting factors

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

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

Evaluation of $R_{\rm ud}[U]$

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 the Gaussian distribution

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

Evaluation of $R_\mathrm{s}[U]$

assume $\det W[U](\rho_\mathrm{s})$ is positive

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

Taylor expansion for $W^{-1/2}[U](\rho_\mathrm{s})\eta$

$$
\begin{aligned}
W^{-1}[U](\rho_\mathrm{s}) &= \frac{D_{\kappa_\mathrm{s}}[U]}{D_{\kappa_\mathrm{s}^*}[U]} \\
&= 1-(1-\rho_\mathrm{s})\left(1-(D_{\kappa_\mathrm{s}^*}[U])^{-1}\right) \\
&= 1-X[U](\rho_\mathrm{s})
\end{aligned}
$$

where $|1-\rho_\mathrm{s}| \ll 1$

$\Rightarrow$ expansion of $W^{-1/2}[U](\rho_\mathrm{s})\eta$ in terms of $X[U](\rho_\mathrm{s})$

Additional technique Hasenfratz-Hoffmann-Schaefer

determinant breakup: divide $(\kappa_q^* - \kappa_q)$ into N_B subintervals

$$\kappa_q \Rightarrow \kappa_q + \Delta_q \Rightarrow \ldots \Rightarrow \kappa_q + (N_B - 1)\Delta_q \Rightarrow \kappa_q^*$$
$$\text{with } \Delta_q = (\kappa_q^* - \kappa_q)/N_B$$

$$\det\left[W^{-1}[U](\rho_{\mathrm{q}})\right] = \det\left[W^{-1}[U]\left(\frac{\kappa_q + \Delta_q}{\kappa_q}\right)\right] \times \det\left[W^{-1}[U]\left(\frac{\kappa_q + 2\Delta_q}{\kappa_q + \Delta_q}\right)\right] \times \ldots \times \det\left[W^{-1}[U]\left(\frac{\kappa_q^*}{\kappa_q + (N_B - 1)\Delta_q}\right)\right],$$

reduce fluctuations of the reweighting factors

§3. Simulation and reweighting parameters

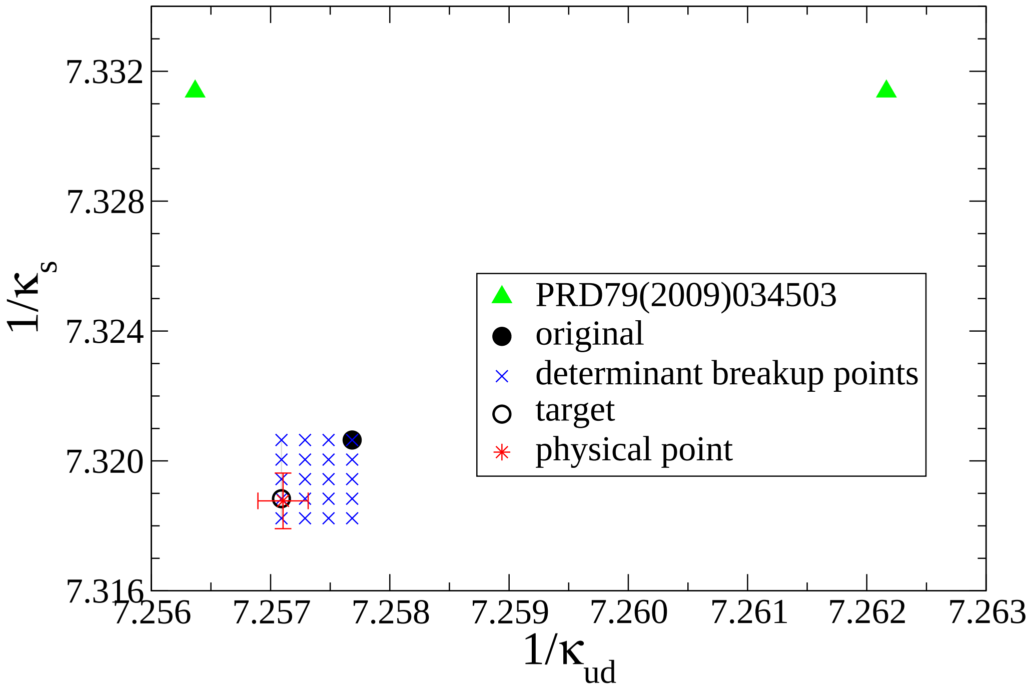
simulation parameters

- original: $(\kappa_{\rm ud},\kappa_{\rm s})$=(0.137785,0.136600)
- 2000 MD time
- MP^{2}DDHMC for ud quark with 8^4 block, $\rho_1 = 0.9995$, $\rho_2 = 0.99$
- UV-filtered PHMC for s quark with $N_{\rm poly} = 220$

reweighting parameters

- target: $(\kappa^*_{\rm ud},\kappa^*_{\rm s})$=(0.13779625,0.13663375)
- breakup intervals: $\Delta_{\rm ud} = (0.13779625 - 0.13778500)/3$,
  $\Delta_{\rm s} = (0.13663375 - 0.13660000)/3$
- $N_\eta = 10$ for stochastic estimation of $R_{\rm ud,s}$

location of the physical point



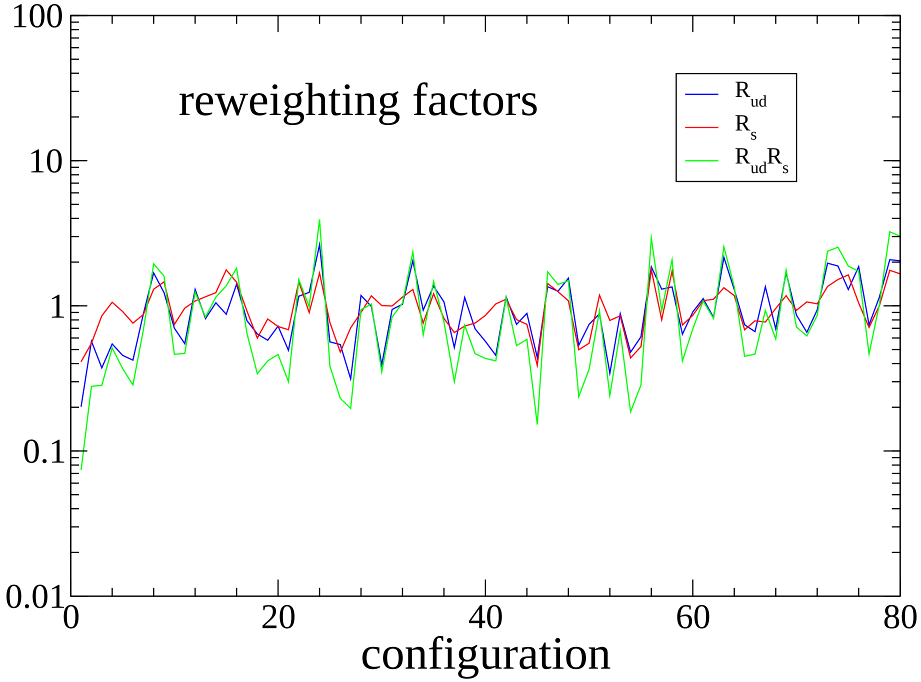
original and target points are fairly close

$\Delta m_{\rm ud} \sim$ 1MeV, $\Delta m_{\rm s} \sim$ 3MeV

§4. Results

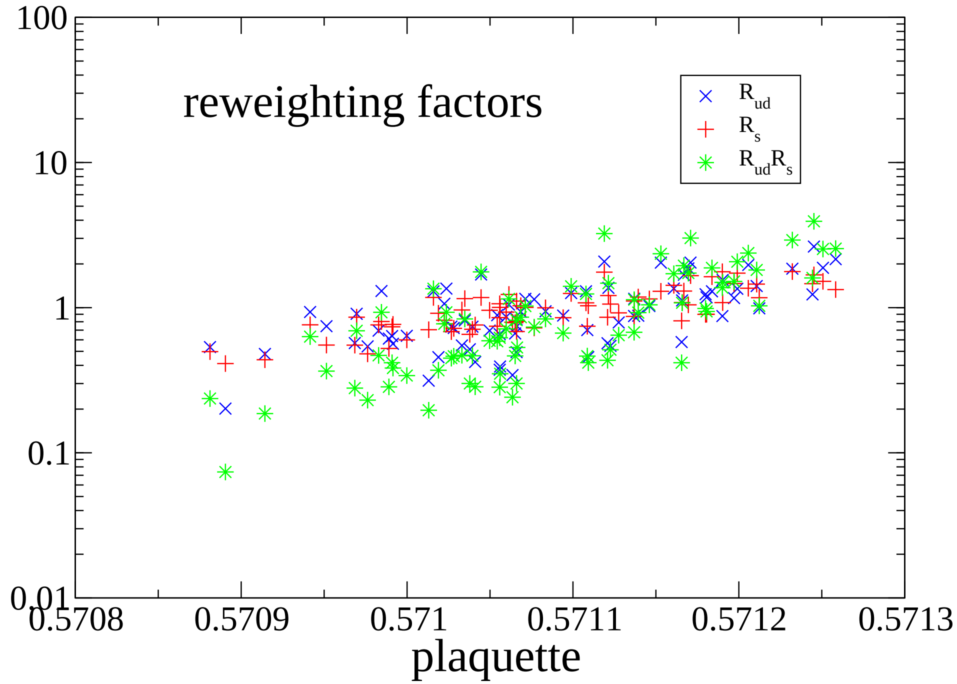
- results for $R_{\mathrm{ud,s}}$
- reweighting for plaquette
  N_η and N_B dependences
- effective masses for m_π, m_K, $m_{\eta_{\mathrm{ss}}}$
  reweighting and partially quenching effects
- hadron spectrum

Reweighting factors on each configuration



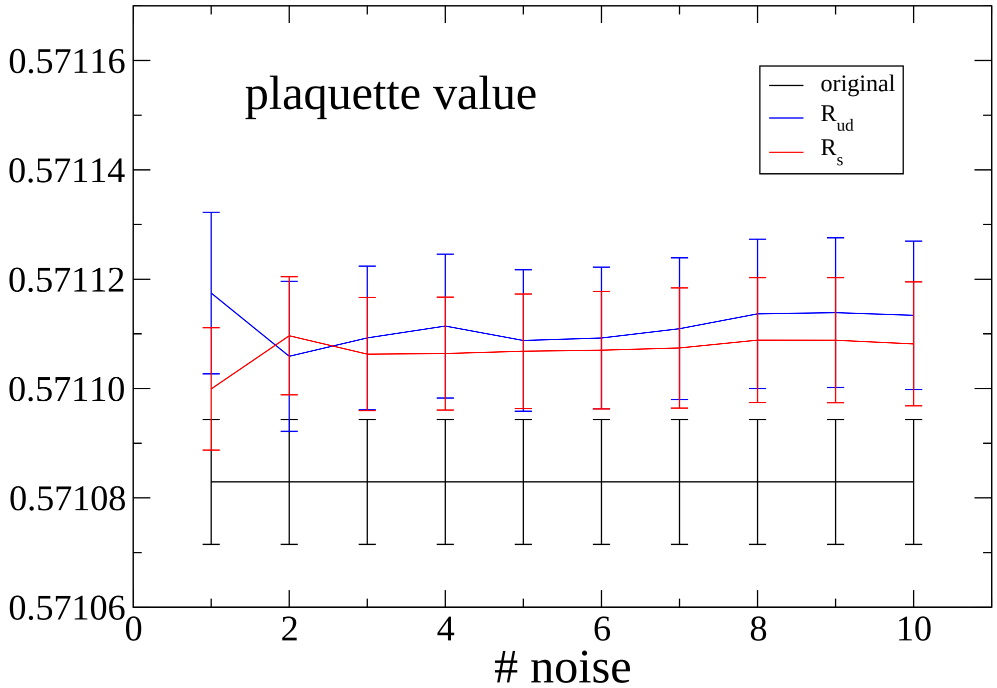
normalized with $\langle R_{\text{ud,s}} \rangle = 1$

Reweighting factors vs. plaquette value



clear dependence as expected

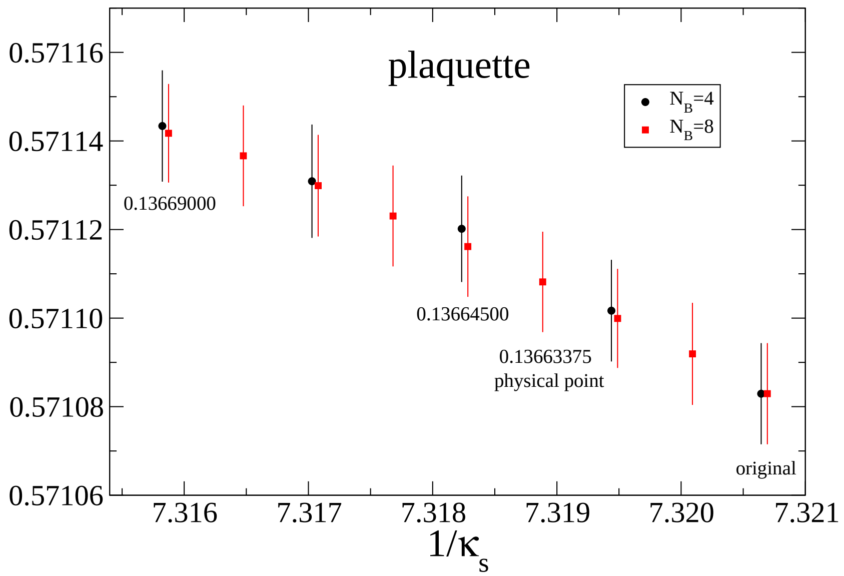
N_η dependence of reweighted plaquette value

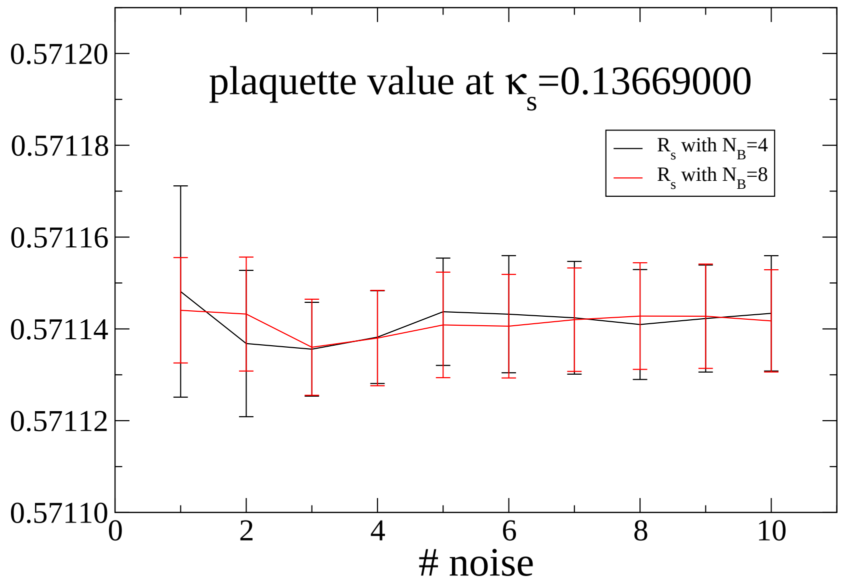


look converged for $N_\eta \gtrsim 4$

N_B dependence of reweighted plaquette value

test for $R_\mathrm{S}[\kappa_\mathrm{S} = 0.13660000 \to \kappa_\mathrm{S}^* = 0.13669000]$ with $N_B = 4$ and 8

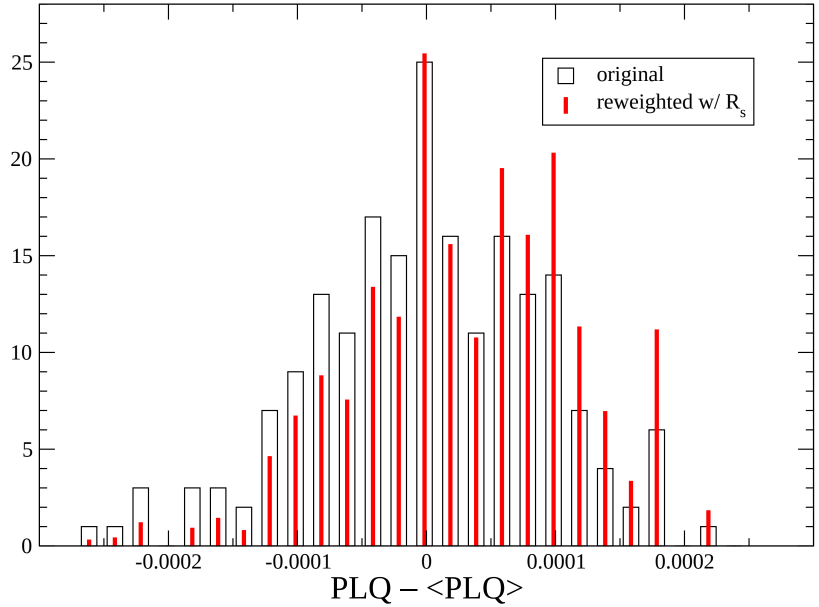




consistent even at $\kappa_\mathrm{S}^* = 0.13669000$

Plaquette histogram w/ and w/o R_s

test for $R_\mathrm{s}[\kappa_\mathrm{s} = 0.13660000 \to \kappa_\mathrm{s}^* = 0.13664500]$ with $N_B = 2$



distribution is slightly moved toward larger values

still almost degenerate

comments on Hasenfratz-Hoffmann-Schaefer's work

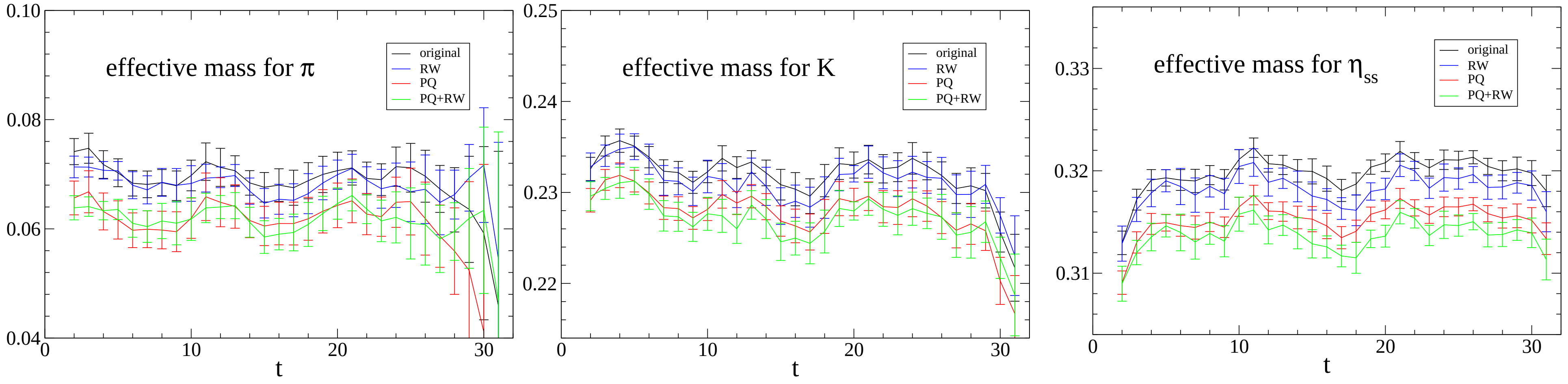
– 2 flavor Wilson-clover on a 16^4, $(1.85\ \text{fm})^4$ lattice
– reweighting from $m_{\text{ud}} \approx 20$ MeV to $m_{\text{ud}} \approx 5$ MeV
to explore ϵ-regime

could be possible thanks to their small lattice volume
(smaller volume $\Rightarrow$ broader distribution)

our usage is restricted to fine-tuning for small $\Delta m_{\text{ud,s}}$

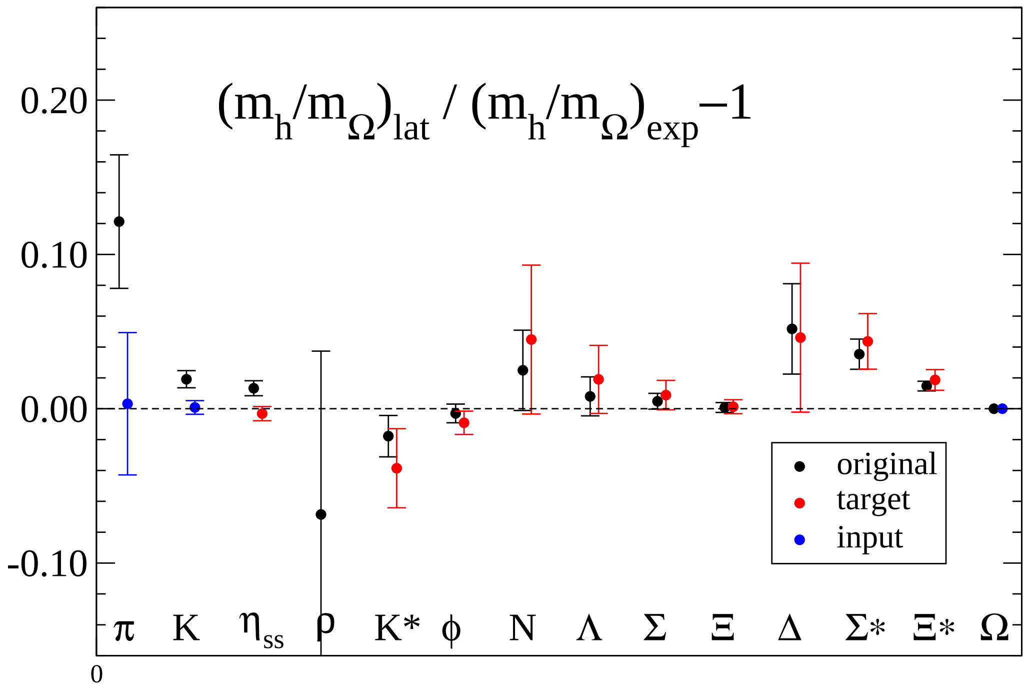
PS effective masses

reweighting effect, partially quenching effect and their sum



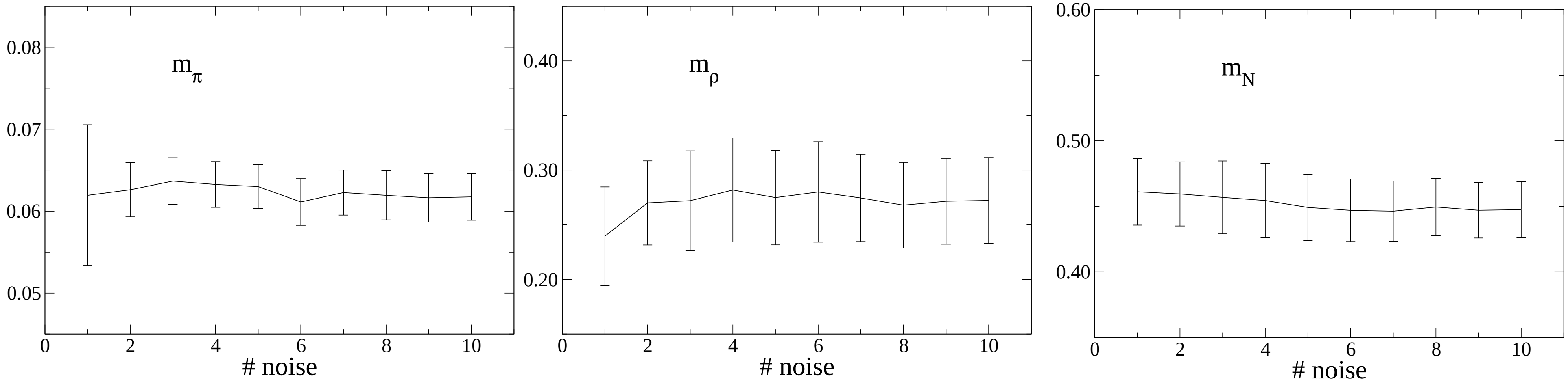
both effects reduces the PS meson masses

Hadron spectrum in comparison with experiment



m_π/m_Ω, m_K/m_Ω are properly tuned

N_η dependence of hadron masses



look converged for $N_\eta \gtrsim 4$ as in the plaquette case

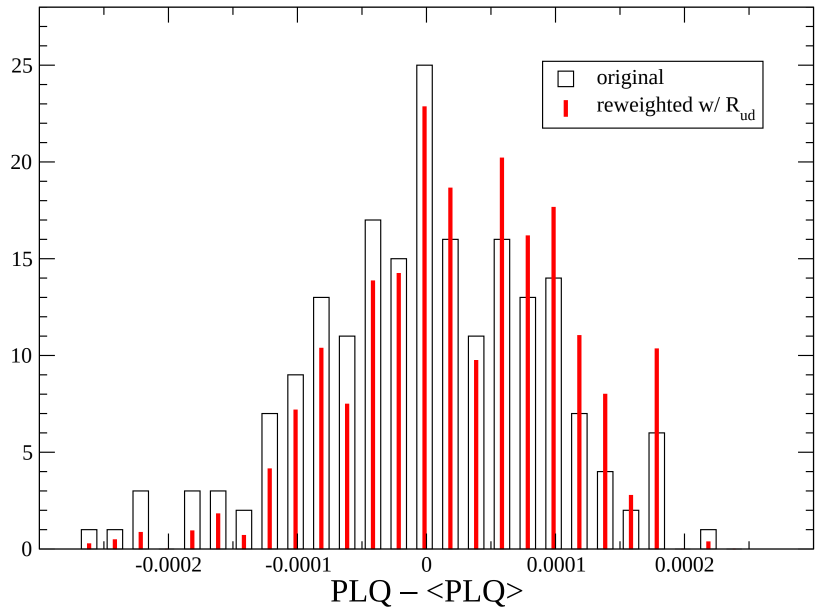
§5. Summary

- fine-tuning of $m_{\mathrm{ud,s}}$ to the physical point with reweighting technique
- starting point for precision measurements
- $(6\mathrm{fm})^3$ box simulation is under way

BACKUP

Plaquette histogram w/ and w/o $R_{\rm ud}$

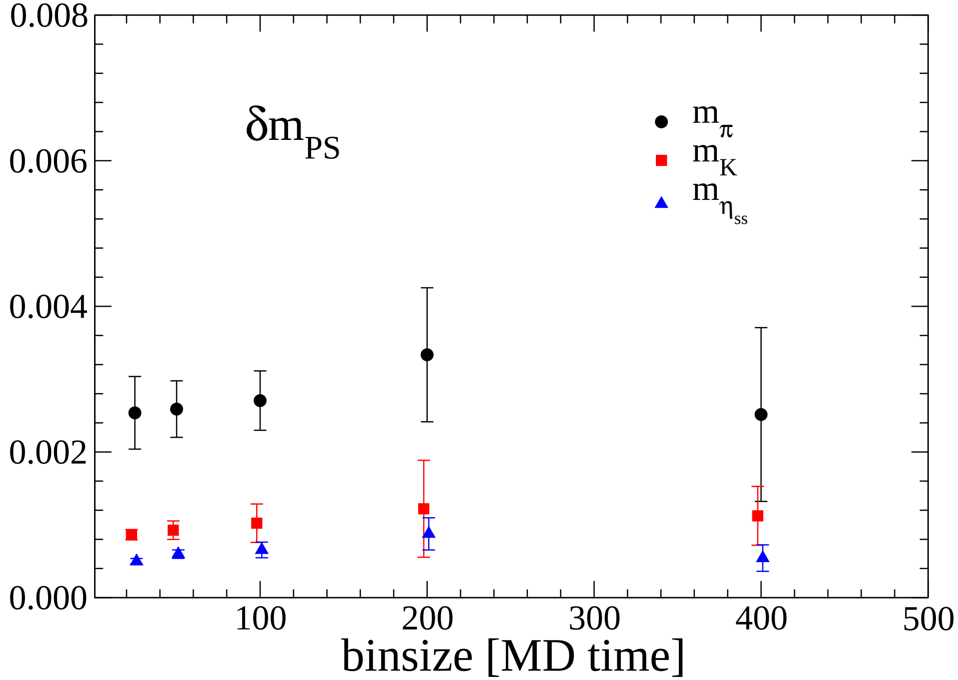
test for $R_{\rm ud}[\kappa_{\rm ud} = 0.13778500 \rightarrow \kappa^*_{\rm ud} = 0.13780000]$ with $N_B = 2$



distribution is slightly moved toward larger values

similar behavior as strange case

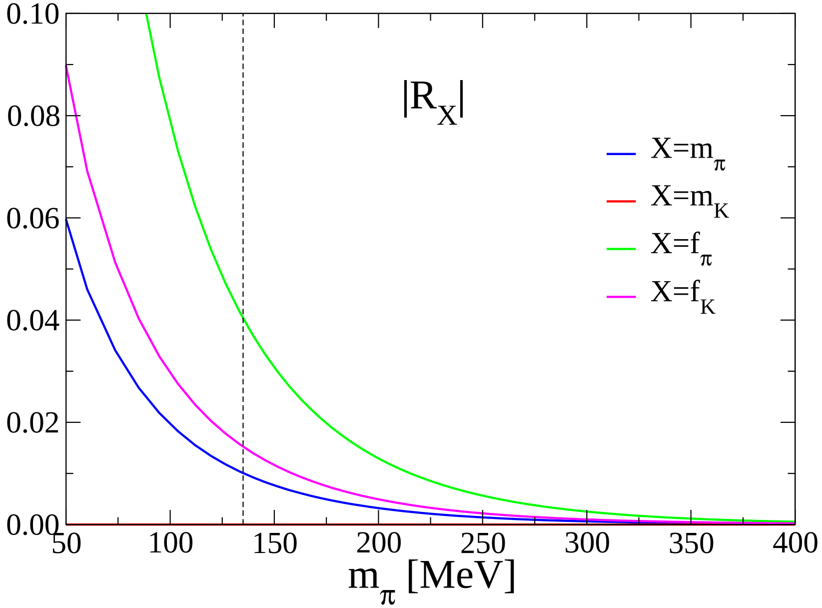
Jackknife analysis on PS meson masses



autocorrelation is rather small

Finite size effects based on ChPT

Colangero-Dürr-Haefeli, NPB721(2005)136



$R_{m_{\text{PS}}} > 0$ and $R_{f_{\text{PS}}} < 0$

at most a few % at the physical point

$\rho \to \pi\pi$ decay based on phase shift

Lüscher, NPB354(1991)531

$$\begin{pmatrix} \langle \mathcal{O}_{\pi\pi}(t)\mathcal{O}^\dagger_{\pi\pi}(0)\rangle & \langle \mathcal{O}_{\pi\pi}(t)\mathcal{O}^\dagger_{\rho}(0)\rangle \\ \langle \mathcal{O}_{\rho}(t)\mathcal{O}^\dagger_{\pi\pi}(0)\rangle & \langle \mathcal{O}_{\rho}(t)\mathcal{O}^\dagger_{\rho}(0)\rangle \end{pmatrix} \Rightarrow E_{\text{eigen}} \Rightarrow \text{phase shift}$$

group	Ref.	#flavor	m_π [MeV]	$g_{\rho\pi\pi}$
CP-PACS	PRD76(07)094506	2	330	6.25(67)
QCDSF	LAT08	2	240–810	5.3(+2.1)(−1.5)
ETMC	LAT10	2	290–480	6–7 ($m_{\text{ud}} \to 0$)
PACS-CS	LAT10	2+1	410	5.24(51)
BMW	LAT10	2+1	200,340	5.5(2.9),6.6(3.4)

physical value: $g^{\text{ph}}_{\rho\pi\pi} = 5.98(2)$ from Γ^{ph}_ρ