Physical Point Simulation in 2+1 Flavor Lattice QCD

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Plan of talk

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§2. Reweighting method
§3. Parameters
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§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:

T.Boku, M.Sato, D.Takahashi, O.Tatebe	Tsukuba
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Physics plan

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

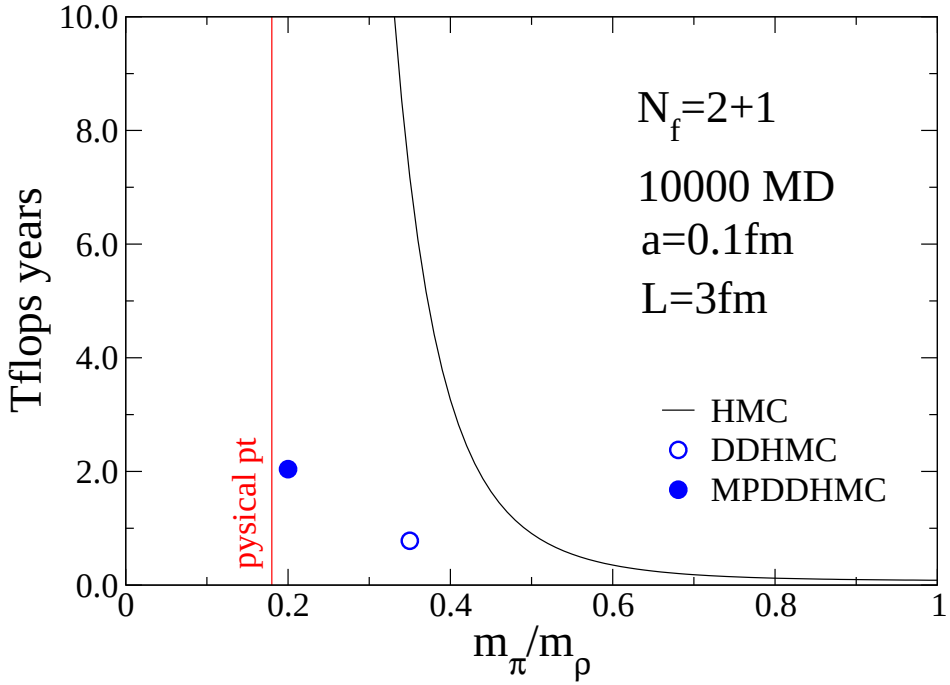
	PACS-CS	CP-PACS/JLQCD
gauge action	Iwasaki	Iwasaki
quark action	clover with $c_{\rm SW}^{\rm NP}$	clover with $c_{\rm SW}^{\rm NP}$
a[fm]	0.07,0.1,0.122	0.07,0.1,0.122
volume	$\gtrsim$ (3fm)^3	$\sim$ (2fm)^3
$m_{\rm ud}^{\rm AWI}$	physical point	64MeV
algorithm for ud	DDHMC with improvements	HMC
algorithm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

Why is physical point simulation necessary?

- difficult to trace chiral logs for chiral extrapolation
- ChPT is not always a good guiding principle
- need a proper treatment of resonances
- simulations with different up and down quark masses

$\Rightarrow$ there are two types of problems

(1) Computaional cost



successfully solved by (Mass-Preconditioned) DDHMC

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(2) Fine tuning on physical point

need 3 simulation points within a few MeV differenes around the physical point in 2+1 flavor case
$\Rightarrow$ demanding computational cost

try reweighting method both for ud and s quarks

§2. Reweighting method

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

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

reweighting factors

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

where $W[U](\rho_q) \equiv \frac{D_{\kappa'_{\rm q}}[U]}{D_{\kappa_{\rm q}}[U]}$

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

introduce a complex bosonic field η

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

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

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

Evaluation of $R_{\mathsf{S}}[U]$

assume $\det W[U](\rho_{\mathsf{S}})$ is positive

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

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

$$\begin{aligned} W^{-1}[U](\rho_{\mathsf{S}}) &= \frac{D_{\kappa_{\mathsf{S}}}[U]}{D_{\kappa'_{\mathsf{S}}}[U]} \\ &= 1-(1-\rho_{\mathsf{S}})\left(1-(D_{\kappa'_{\mathsf{S}}}[U])^{-1}\right) \\ &= 1-X[U](\rho_{\mathsf{S}}) \end{aligned}$$

where $|1-\rho_{\mathsf{S}}| \ll 1$
$\Rightarrow$ expansion of $W^{-1/2}[U](\rho_{\mathsf{S}})\eta$ in terms of $X[U](\rho_{\mathsf{S}})$

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. Parameters

simulation parameters

- original: $(\kappa_{\rm ud},\kappa_{\rm s})$=(0.137785,0.136600)
- 1000 MD time, still increasing
- 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

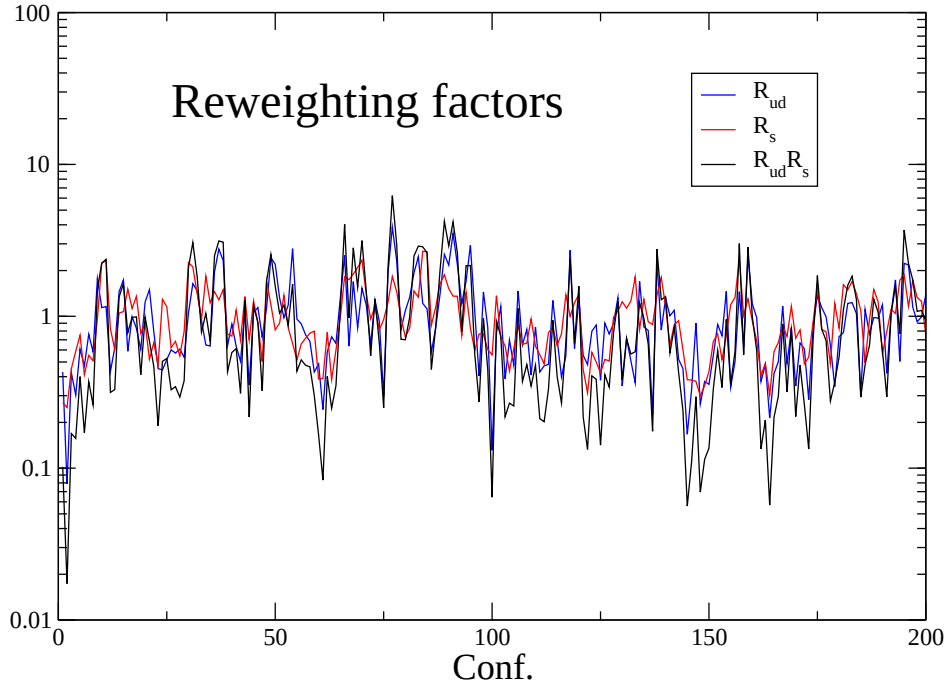
- target: $(\kappa'_{\rm ud},\kappa'_{\rm s})$=(0.137800,0.136645), (0.137800,0.136690)
- breakup intervals: $\Delta_{\rm ud} = (0.137800 - 0.137785)/2$,
  $\Delta_{\rm s} = (0.136690 - 0.136600)/4$
- $N_\eta = 10$ for stochastic estimation of $R_{\rm ud,s}$

§4. Preliminary Results

concentrate on $(\kappa'_{\mathrm{ud}}, \kappa'_{\mathrm{s}}) = (0.137800, 0.136645)$

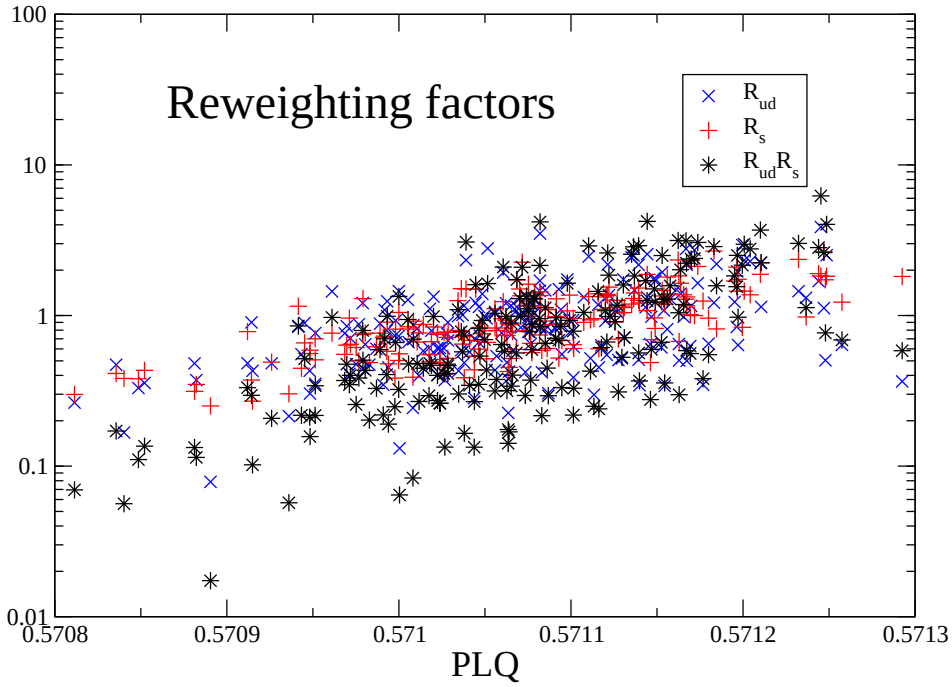
- results for $R_{\mathrm{ud,s}}$
- Reweighting for plaquette
- Reweighting for m_π, m_K, m_Ω
  (physical inputs for m_{ud}, m_{s}, a^{-1})
- hadron spectrum
- locate the physical point

Reweighting factors on each configuration



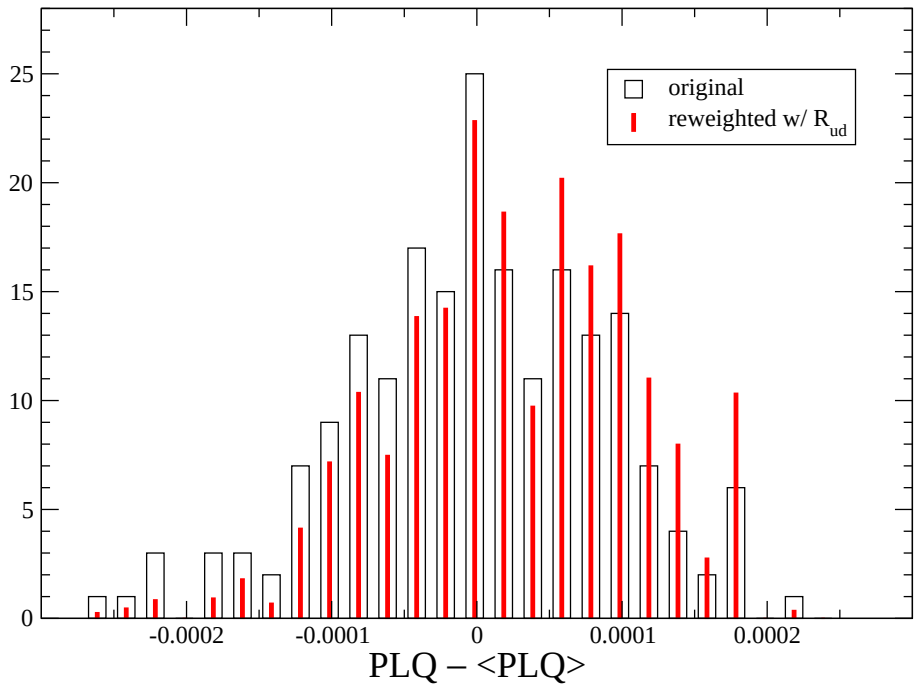
normalized with $\langle R_{\mathrm{ud,s}} \rangle = 1$

Reweighting factors vs. plaquette value



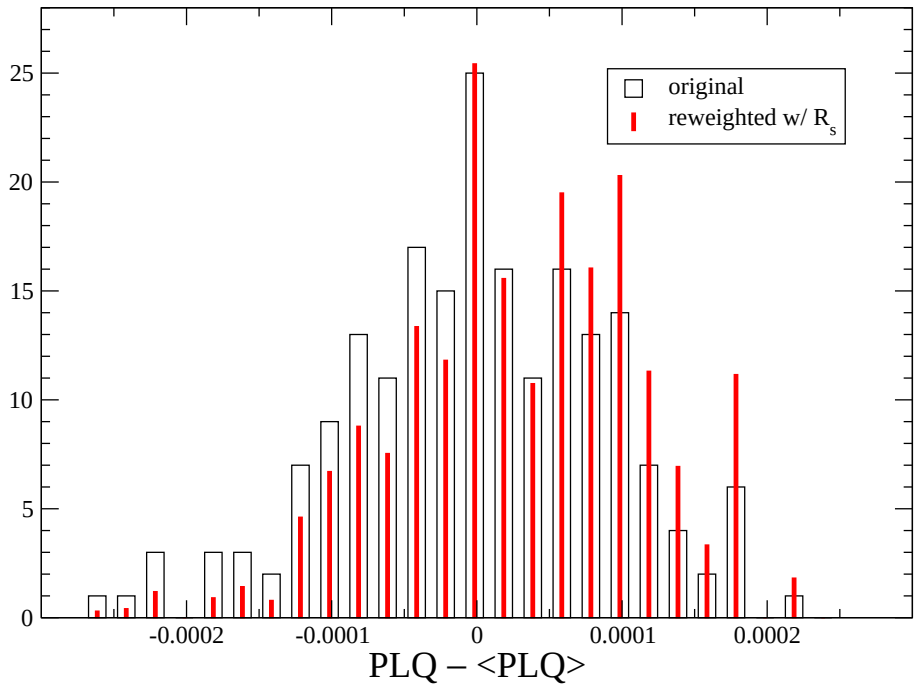
clear dependence

Plaquette histgram w/ and w/o R_{ud}



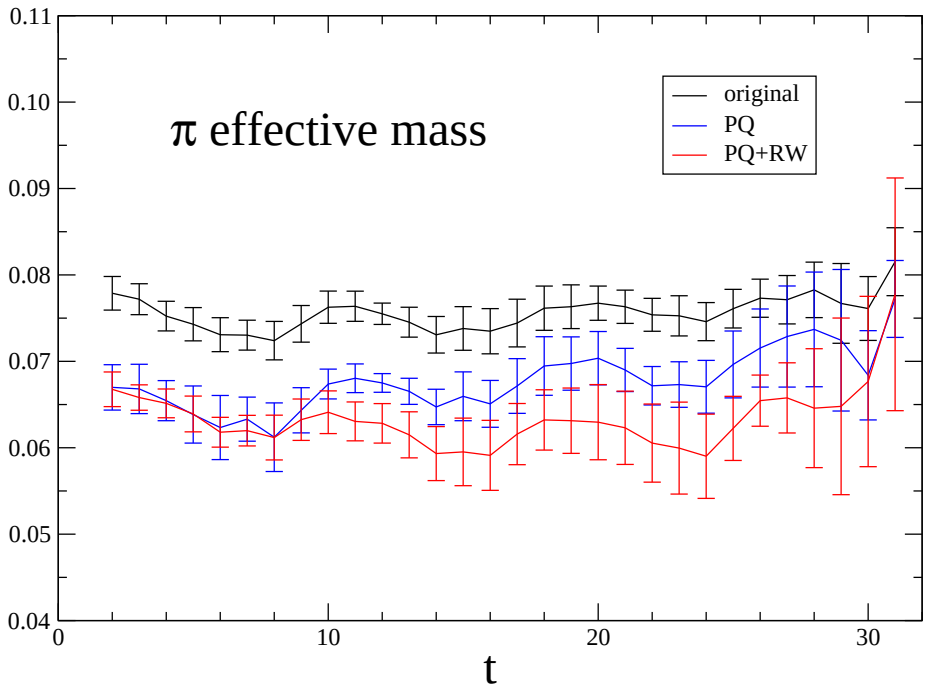
distribution is slightly moved toward larger values

Plaquette histgram w/ and w/o R_S



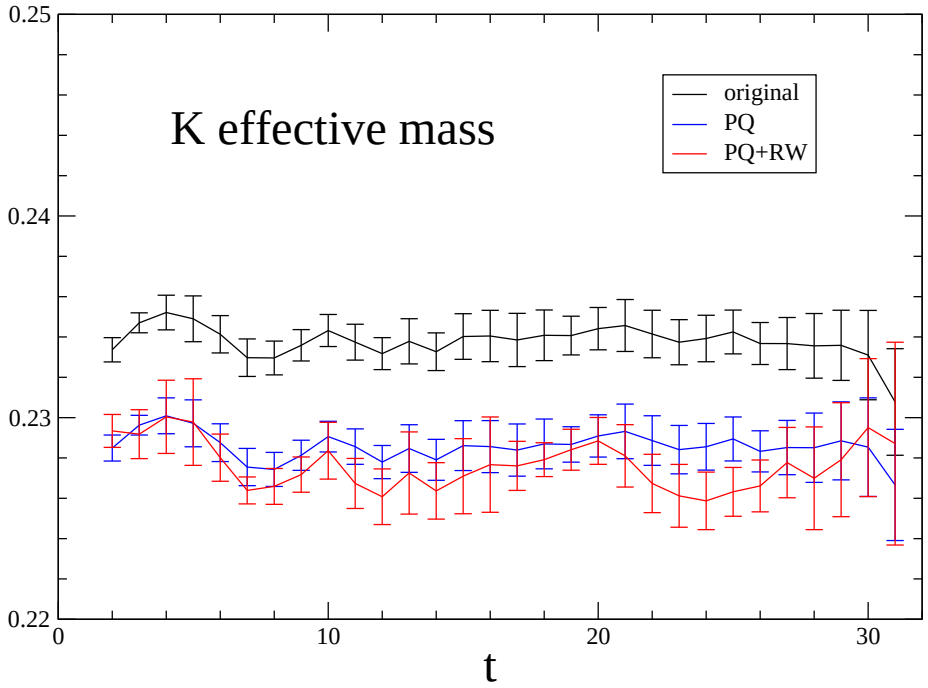
distribution is slightly moved toward larger values

π effective mass



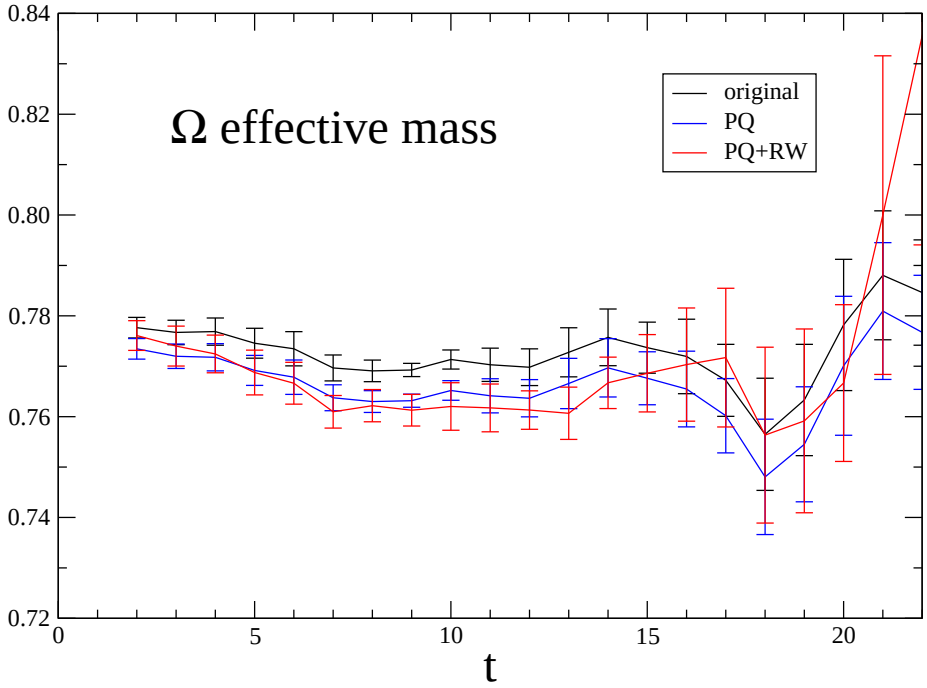
reweighting effects are observed

K effective mass



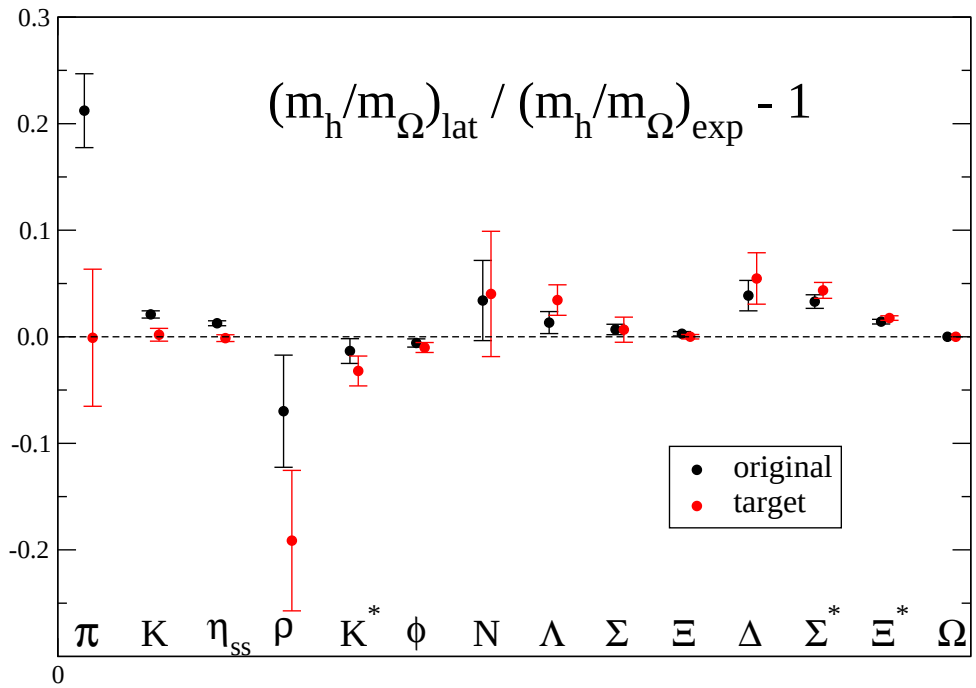
similar to π case

Ω effective mass



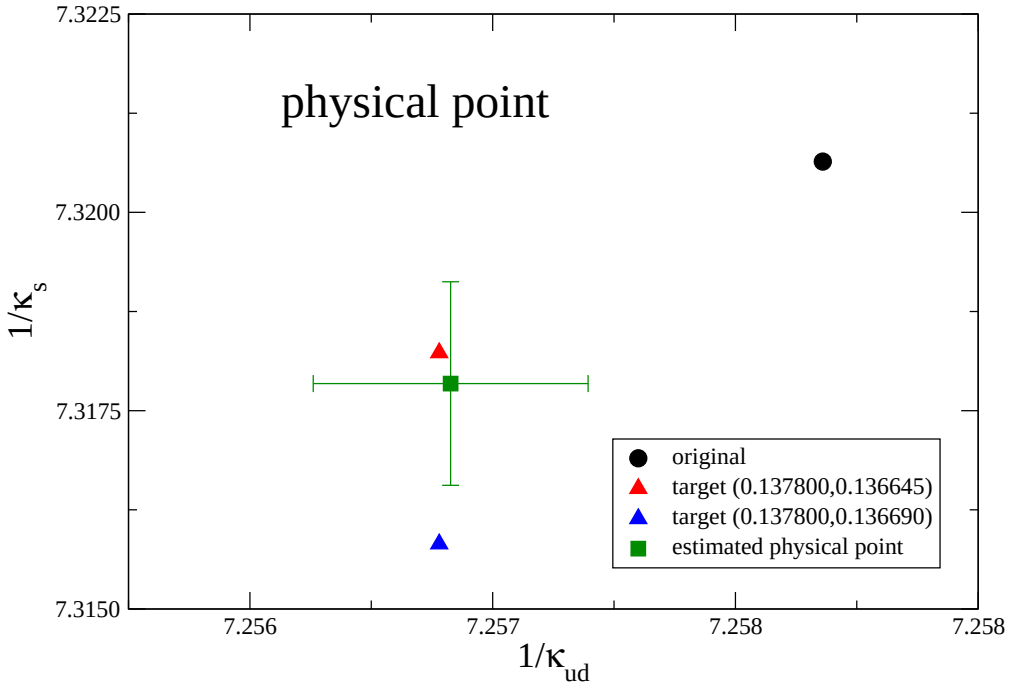
m_Ω is slightly decreased

Hadron spectrum in comparison with experiment



m_π/m_Ω, m_K/m_Ω are properly tuned

Locate the physical point



confirmed with three data point analysis

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

§5. Summary

- Chiral extrapolation is not necessary anymore
- $(6\text{fm})^3$ box simulation is under way
- starting point for precision measurements