Status of the 2+1 Flavor Wilson-Clover Simulation of QCD by PACS-CS Collaboration

Y.Kuramashi (Univ. of Tsukuba)
for PACS-CS collaboration

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Plan of talk

§**1.** History of hadron spectrum calculation

§**2.** The PACS-CS project

§**3.** Lüscher's domain-decomposed HMC(LDDHMC) algorithm

§**4.** Simulation details

§**5.** Hadron effective masses(preliminary)

§**6.** Chiral extrapolations(preliminary)

§**7.** Summary

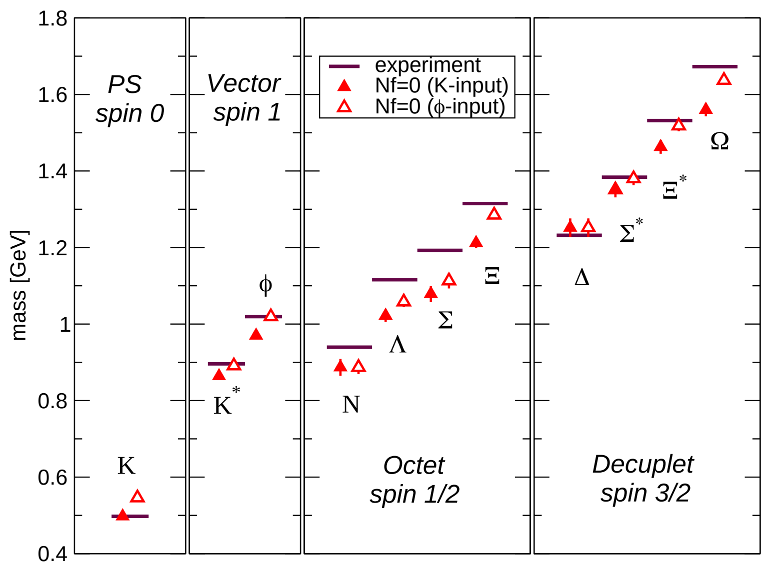
§1. History of hadron spectrum calculation

$N_f = 0$ CP-PACS collab., PRD67(2003)034503

plaquette gauge action + Wilson quarks

$a = 0.05 - 0.10$fm, $L \approx 3$fm, $m_\pi \gtrsim 300$MeV

clear deviation from the experimental values

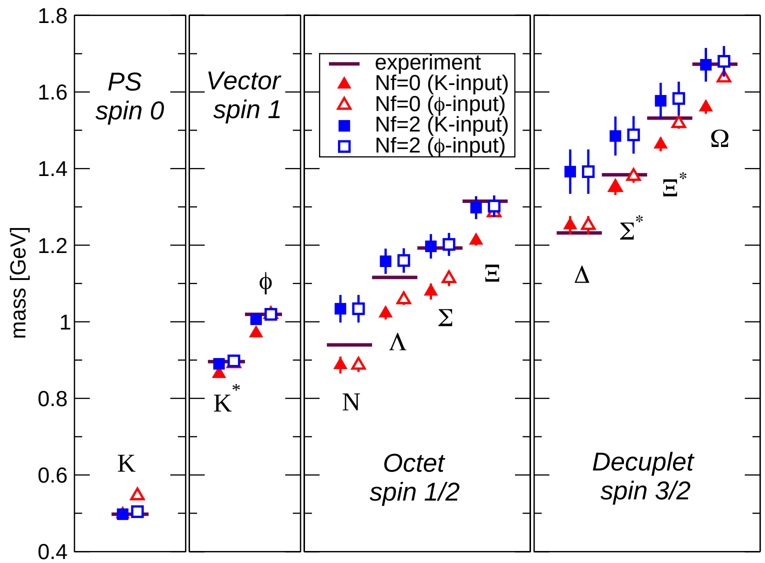


$N_f = 2$ CP-PACS collab., PRD65(2002)054505

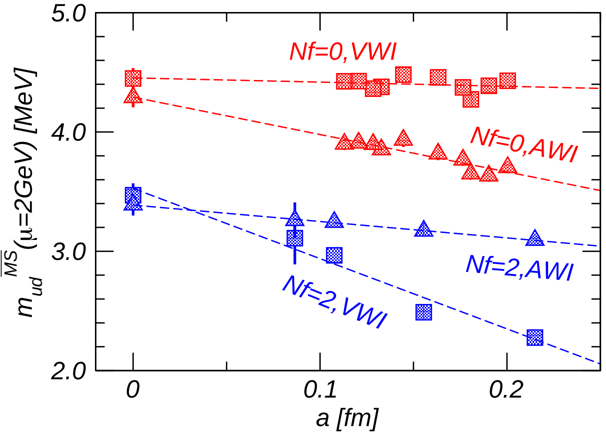
Iwasaki gauge action + clover quarks with c_{SW}^{PT}

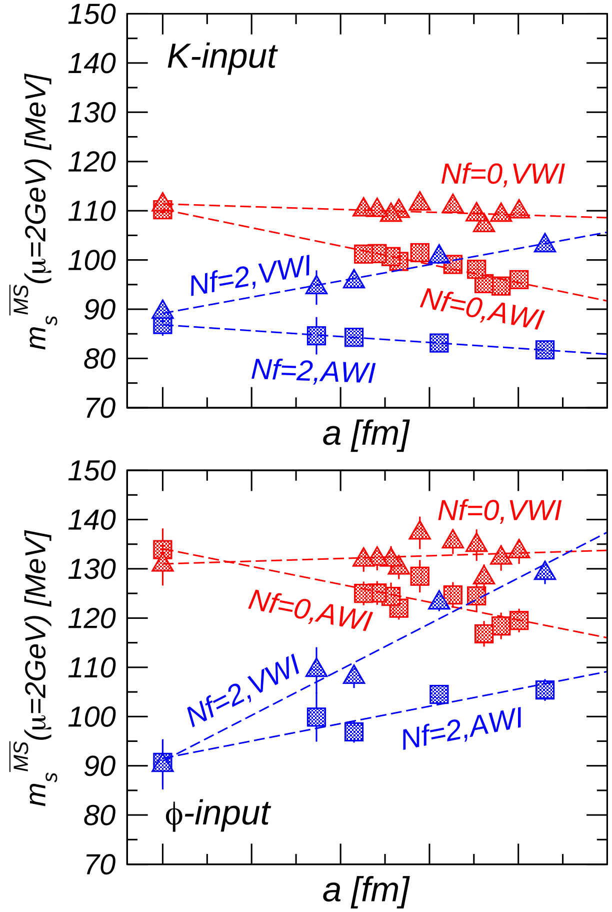
$a = 0.086 - 0.215$fm, $L \approx 2.4$fm, $m_\pi \gtrsim 500$MeV

better agreement with the experimental values for meson sector



clear dynamical quark effects on the quark masses



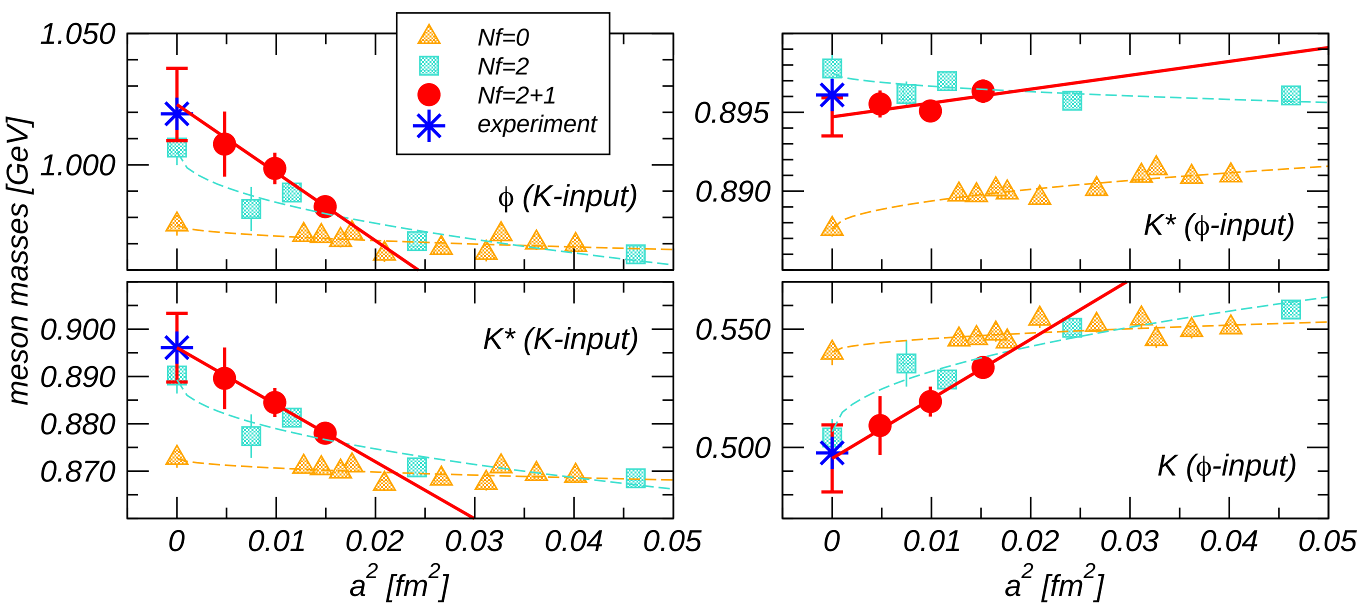


$\underline{N_f = 2+1}$ CP-PACS-JLQCD collabs., in preparation

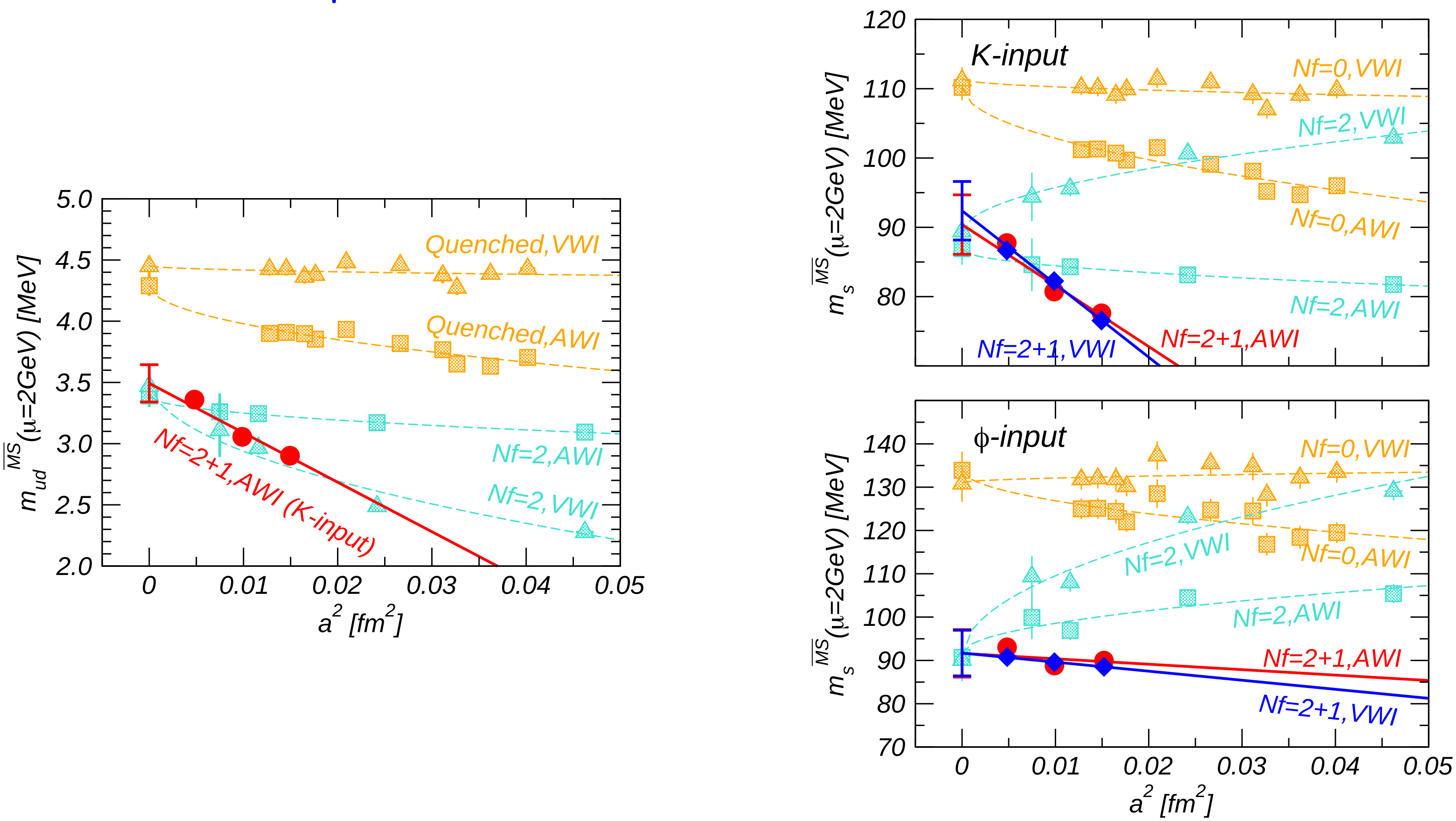
Iwasaki gauge action + clover quarks with $c_{\rm SW}^{\rm NP}$

$a = 0.07 - 0.122$fm, $L \approx 2$fm(too small for baryons), $m_\pi \gtrsim 600$MeV

statistically comparable with the $N_f = 2$ results



same for the quark masses



present situation of the hadron spectrum calculation

$N_f = 0$: clear deviation from the experimental values

$N_f = 2$: confirm the dynamical quark effects
especially on the quark masses

$N_f = 2 + 1$: succeeded in including the dynamical strange quark
$L \approx 2$fm and $m_\pi \gtrsim 600$MeV

→ 2+1 flavor simulation toward the physical point with a larger volume on PACS-CS

§2. The PACS-CS project

Parallel Array Computer System for Computational Sciences

operation started on 1 July 2006

PACS-CS specifications

#nodes	2560($16 \times 16 \times 10$)
peak speed	14.3Tflops
node	single CPU + memory + HDD + 8GBEthernet ports
CPU	Intel LV Xeon EM64T, 2.8GHz, 1MB L2 cache
memory	2GB/node (5.12TB/system)
network	3 dimensional hyper-crossbar uses dual GBEthernet/link
network performance	250MB/s/direction 750MB/s/node (3 dim. simultaneous send/receive)
local HDD	160GB$\times$2 (RAID-1) (410TB$\times$2/system)
#racks	59 racks
OS	Linux, Score
programming	Fortran, C, C++, MPI for communication

collaboration members

physicists:

S.Aoki, N.Ishii, N.Ishizuka, D.Kadoh, K.Kanaya, Y.Kuramashi, K.Sasaki, Y.Taniguchi, A.Ukawa, N.Ukita, T.Yoshié	Tsukuba
K-I.Ishikawa, M.Okawa	Hiroshima
T.Izubuchi	Kanazawa

computer scientists:

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

Physics plan for PACS-CS

simulation details for the previous CP-PACS-JLQCD results

– Iwasaki gauge action + clover quarks with $c_{\mathrm{SW}}^{\mathrm{NP}}$

– three lattice spacing : $a = 0.122$fm, 0.1fm, 0.07fm

– fixed physical volume $\sim (2\mathrm{fm})^3$

– light quark masses down to $m_{\mathrm{ud}}^{\mathrm{AWI}} \approx 64\mathrm{MeV}$ $(m_{\mathrm{PS}}/m_{\mathrm{V}} \sim 0.6)$

– conventional HMC for up-down quarks

– exact PHMC for strange quark

simulation details for the PACS-CS project

– Iwasaki gauge action + clover quarks with $c_{\rm SW}^{\rm NP}$

– three lattice spacing : $a = 0.122$fm, 0.1fm, 0.07fm

– fixed physical volume $\sim$ (3fm)^3

– light quark masses down to $m_{\rm ud}^{\rm AWI} < 10$MeV ($m_{\rm PS}/m_{\rm V} \sim 0.3$)

– LDDHMC with replay trick for up-down quarks

– UV-filtered exact PHMC for strange quark

complete the Wilson-clover $N_f = 2+1$ program

§3. Lüscher's domain-decomposed HMC algorithm

Wilson Dirac matrix

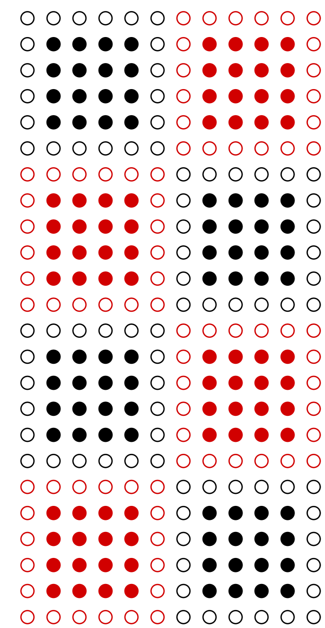
$$D \;=\; \frac{1}{2}\left\{\gamma_\mu(\bar{\nabla}^*_\mu + \bar{\nabla}_\mu) - \bar{\nabla}^*_\mu \bar{\nabla}_\mu\right\} + m_0$$

geometric separation of UV and IR modes

$$D = \begin{pmatrix} D_\Omega & D_{\partial\Omega} \\ D_{\partial\Omega^*} & D_{\Omega^*} \end{pmatrix} \begin{matrix} \} & \Omega \\ \} & \Omega^* \end{matrix}$$

the quark determinant becomes

$$\det D = \det D_\Omega \det D_{\Omega^*} \times \det R$$



$$\det D_\Omega \det D_{\Omega^*} = \prod_{\text{blocks } \Lambda} \det D_\Lambda$$

$$R \;:\; \partial\Omega^* \to \partial\Omega^*$$
$$R \;=\; 1 - P_{\partial\Omega^*} D_\Omega^{-1} D_{\partial\Omega} D_{\Omega^*}^{-1} D_{\partial\Omega^*}$$

R^{-1} takes a simple form

$$R^{-1} \;=\; 1 - P_{\partial\Omega^*} D^{-1} D_{\partial\Omega^*}$$

the pseudofermion action becomes

$$S_{\text{pf}} = \sum_{\text{blocks } \Lambda} \phi_\Lambda^\dagger \frac{1}{(D_\Lambda^\dagger D_\Lambda)} \phi_\Lambda + \phi_{\partial\Omega^*}^\dagger \frac{1}{(R^\dagger R)} \phi_{\partial\Omega^*}$$

separation of UV and IR modes

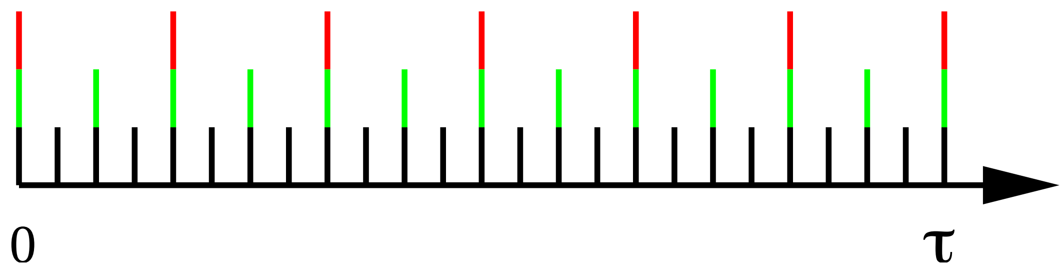
molecular dynamics driving force

$$\frac{d}{d\tau}U(x,\mu) = \Pi(x,\mu)U(x,\mu)$$
$$\frac{d}{d\tau}\Pi(x,\mu) = -F_G(x,\mu) - F_\Lambda(x,\mu) - F_R(x,\mu)$$

leap-frog integration step-sizes are chosen to be

$$\delta\tau_G||F_G|| \sim \delta\tau_\Lambda||F_\Lambda|| \sim \delta\tau_R||F_R||$$

multiple time scale integration scheme



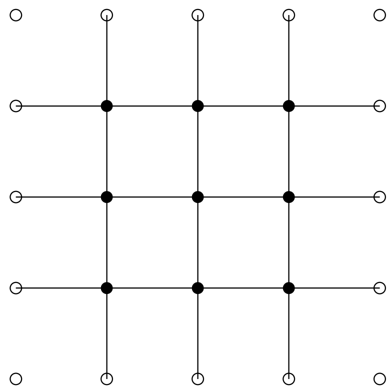
good points

– F_Λ can be calculated independently without communication
  suitable for PC clusters

– blocks provide a safe infrared cutoff on the spectrum of D_Λ
  $\lesssim(1\text{fm})^4$ is preferred

defect

– a sizable fraction of the link variables are not updated
  need a random translation of the gauge field after each trajectory



§4. Simulation details

– Iwasaki gauge action + clover quarks with $c_{\rm SW}^{\rm NP}$
– $\beta = 1.9$ ($a = 0.1$fm, $a^{-1} = 2.0$GeV), lattice size=$32^3 \times 64$
– $\kappa_s = 0.13640$, $N_{\rm poly} = 180$ for PHMC
– ud quarks: block size=8^4, $\delta\tau_\Lambda = \tau/(N_1 N_2)$, $\delta\tau_R = \tau/N_2$
– s quark: not domain-decomposed, $\delta\tau_s = \tau/(N_1 N_2)$
– SAP+GCR for IR part, SSOR+GCR for UV part
– tolerance: $|\text{residual}|/|\text{source}| \le \epsilon$, $\epsilon = 10^{-9}$(force), $10^{-14}(H)$

$\kappa_{\rm ud}$	0.13727	0.13754	0.13770	0.13776	0.13781
$m_{\rm ud}^{\rm AWI}$[MeV]	45	24	12	9	6
N_0, N_1, N_2	4,4,14	4,4,20	4,4,16	4,4,26	4,4,12
τ	0.5	0.5	0.25	0.25	0.075
trajs	–	4600	3300	–	1400
$\tau_{\rm int}[P]$	–	12.5(4.2)	7.7(2.3)	–	–

τ dependence

instabilities are avoided by making τ shorter with $\delta\tau = \tau/N_2$ fixed

good points

– more frequent random translation of the gauge field
  prefereable for LDDHMC

– acceptance probability is kept fixed
  (smaller $\delta\tau$ with τ fixed $\rightarrow$ wastefully high acceptance probability)

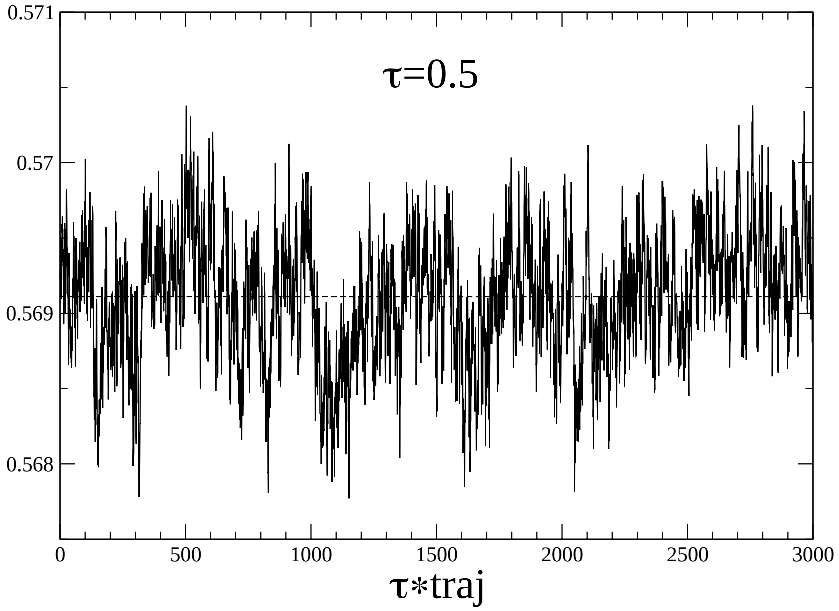
concern

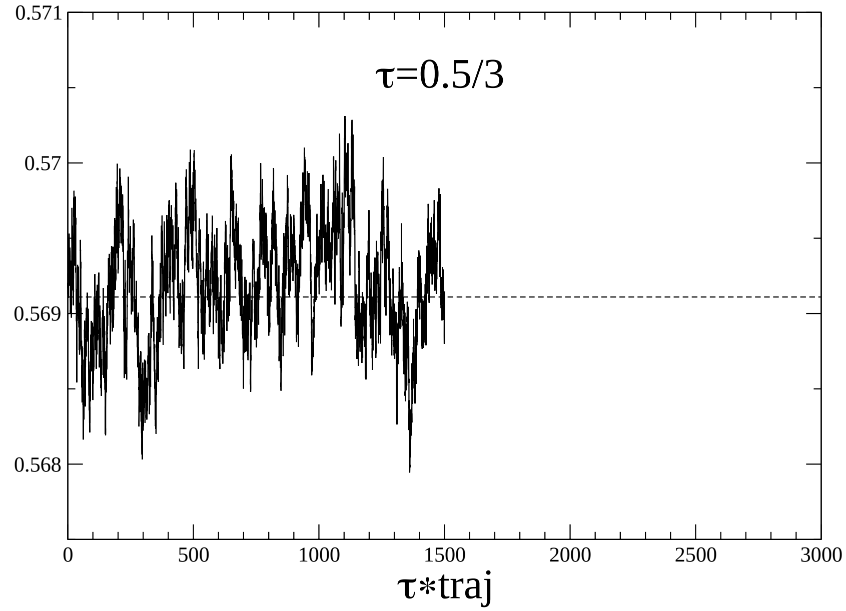
– autocorrelation $\propto 1/\tau$? (random walk) check of τ dependence

- $\kappa_{\mathrm{ud}} = 0.1370$ ($m_{\mathrm{PS}}/m_{\mathrm{V}} \simeq 0.6$)
- lattice size$=16^3 \times 32$
- $\kappa_s = 0.1364$, $N_{\mathrm{poly}} = 130$ for PHMC
- other parameters are same as the production run

τ	0.5	0.5/3
N_0, N_1, N_2	4,4,6	4,4,2
trajs	6000	9000

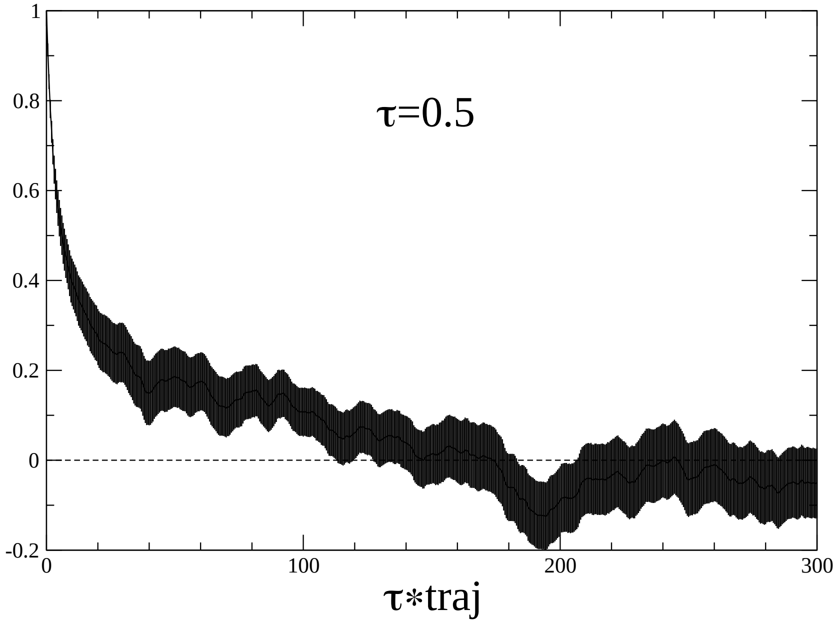
plaquette history



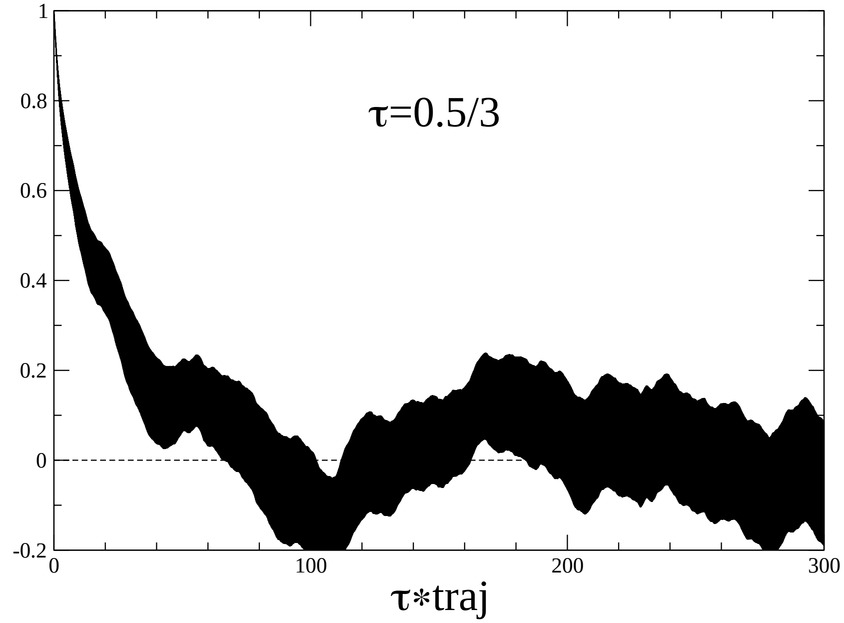


fluctuations are quite similar as a function of MD time

normalized autocorrelation function



$\tau_{\mathrm{int}}[P] = 24(9)$

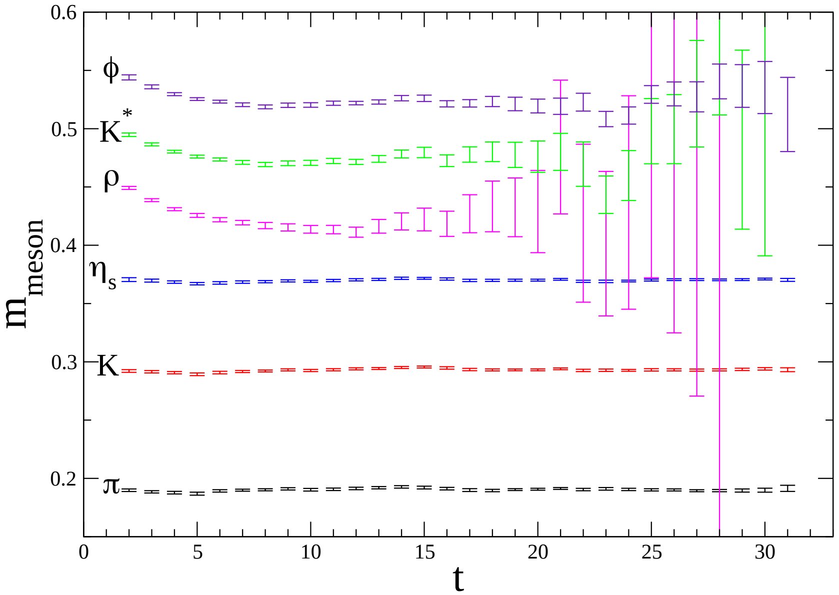


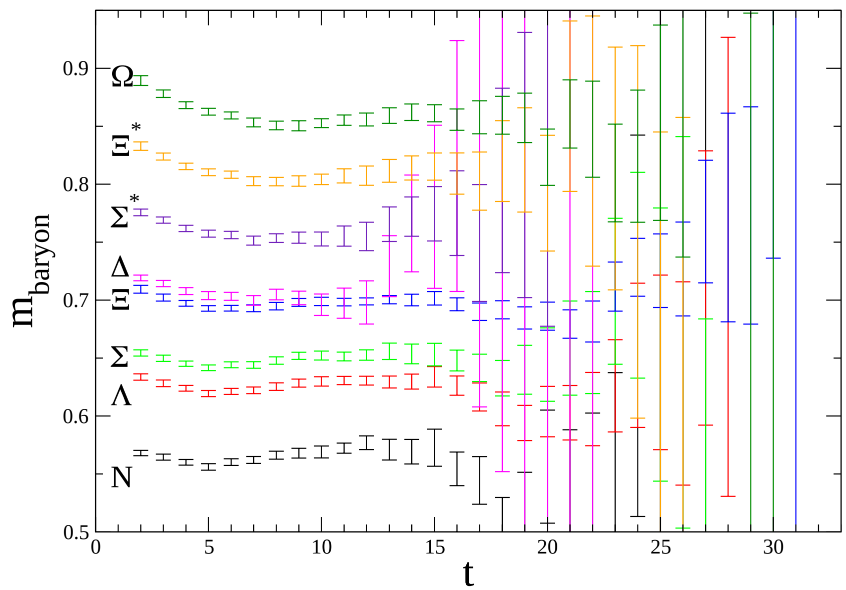
$\tau_{\mathrm{int}}[P] = 20(8)$

$\tau_{\mathrm{int}}[P]$ are comparable with each other

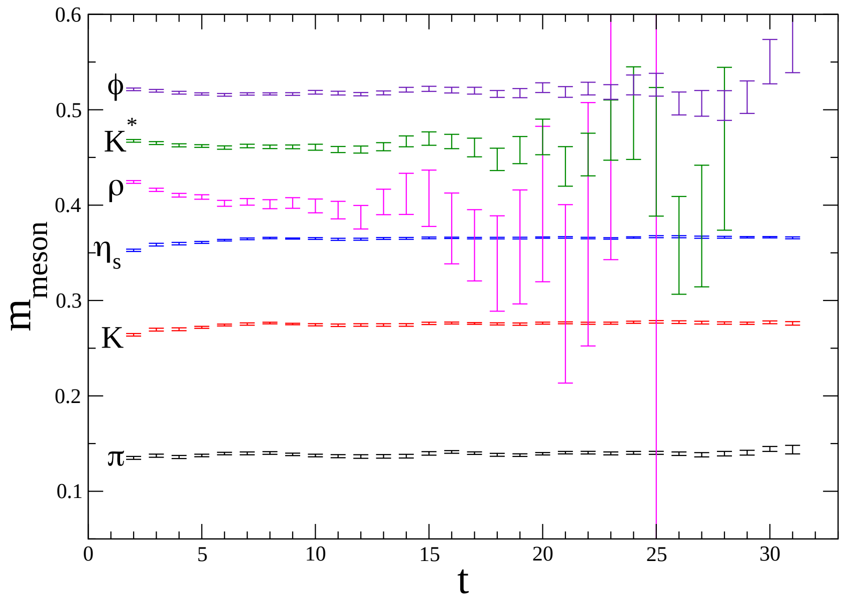
§5. Hadron effective masses(preliminary)

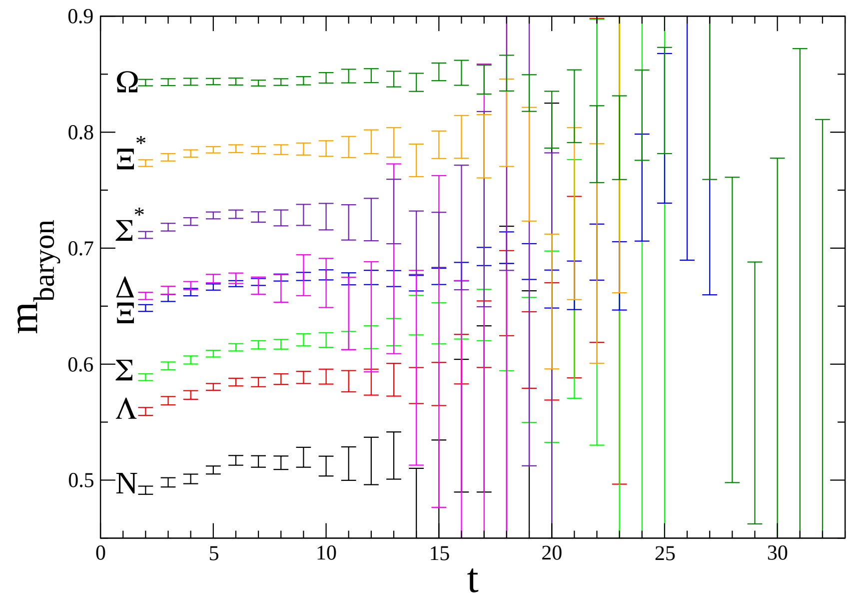
$\kappa_{ud} = 0.13754(m_{ud}^{AWI} = 24\text{MeV})$



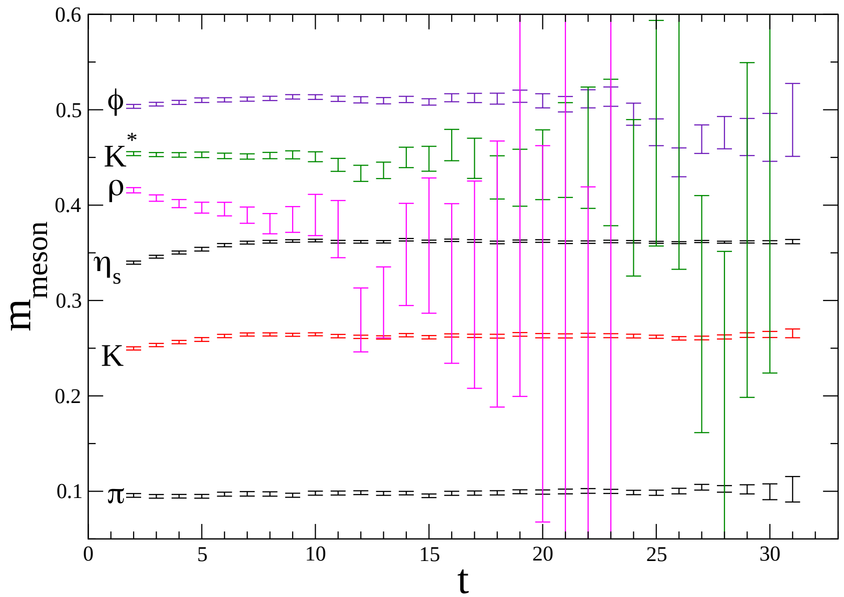


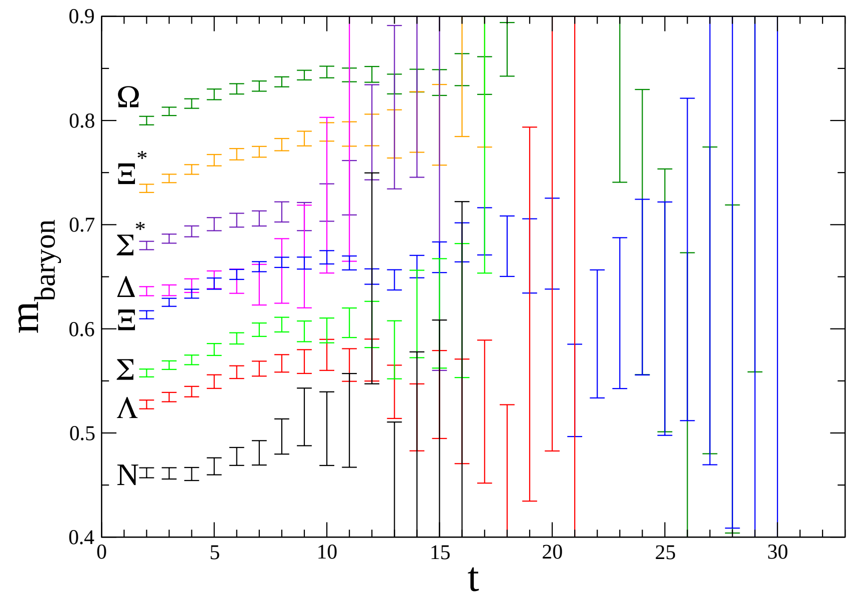
$\kappa_{\mathrm{ud}} = 0.13770(m_{\mathrm{ud}}^{\mathrm{AWI}} = 12\mathrm{MeV})$





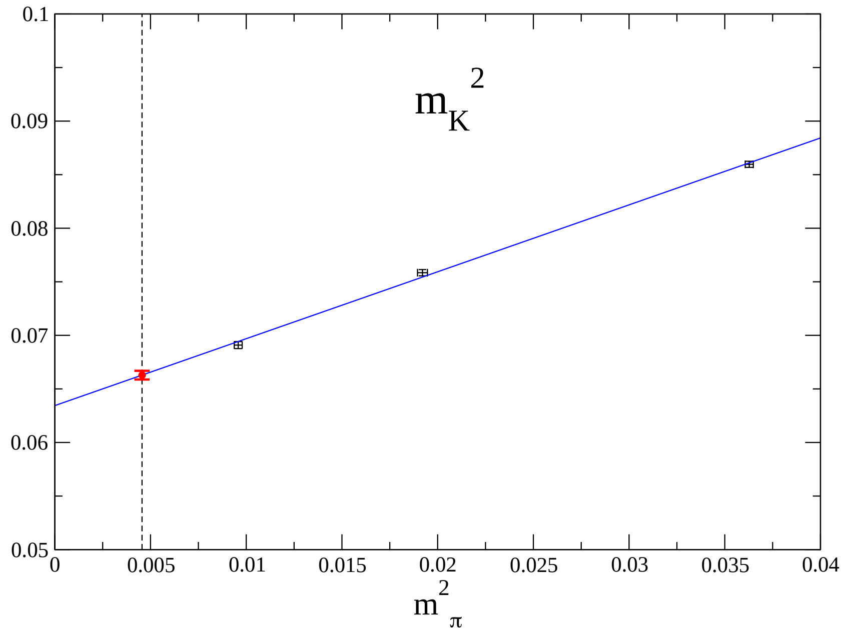
$\kappa_{\rm ud} = 0.13781(m_{\rm ud}^{\rm AWI} = 6\text{MeV})$

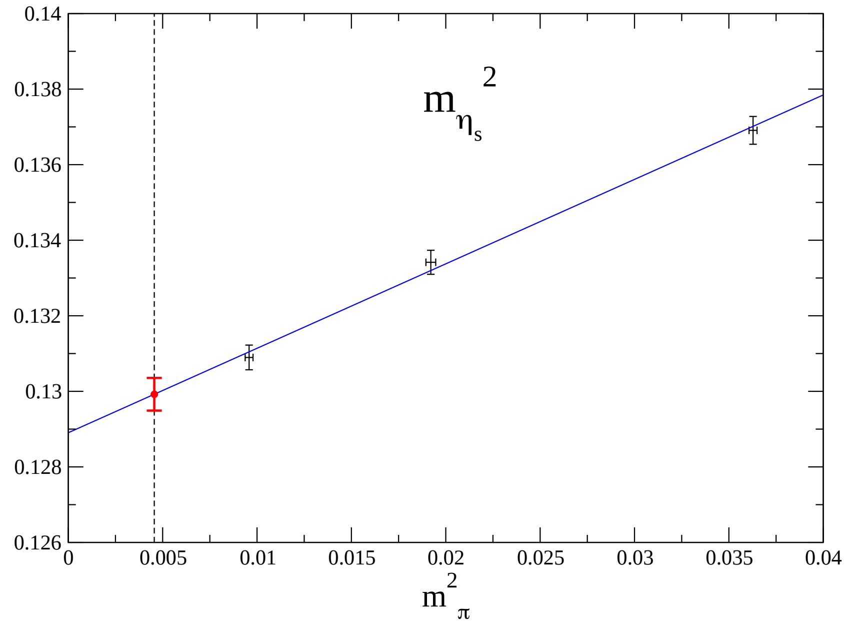




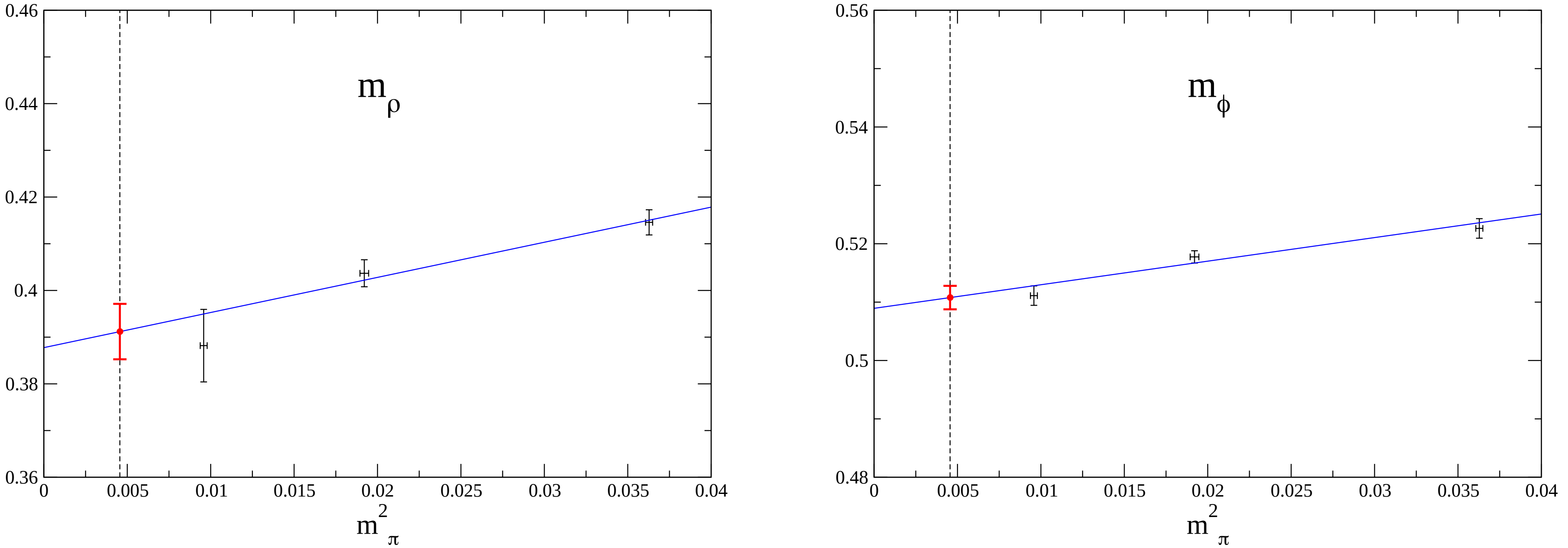
§6. Chiral extrapolations(preliminary)

pseudoscalar meson

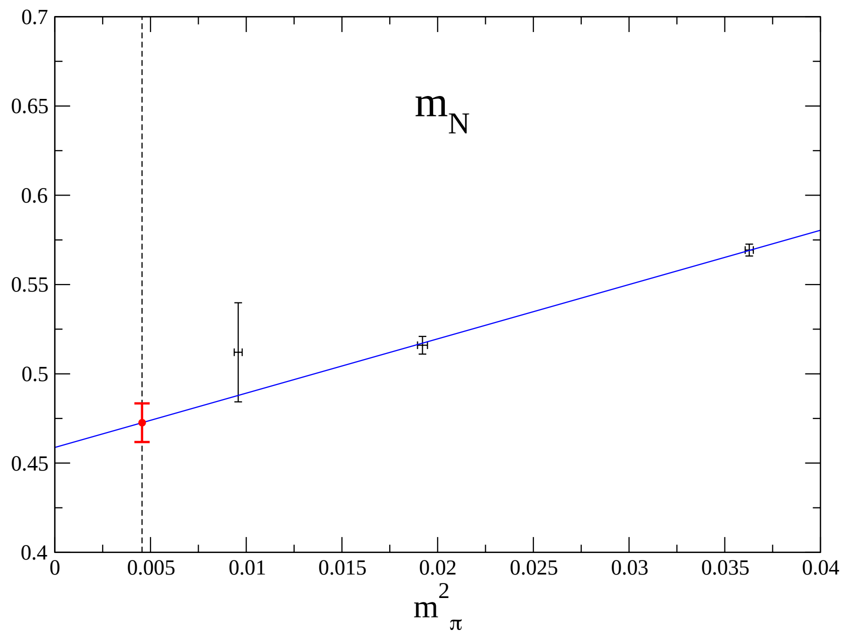


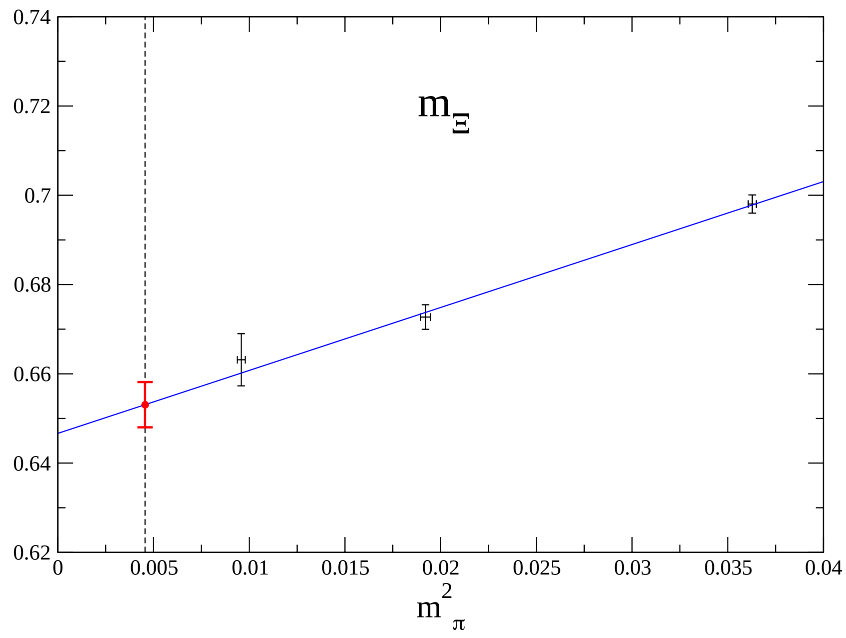


vector meson

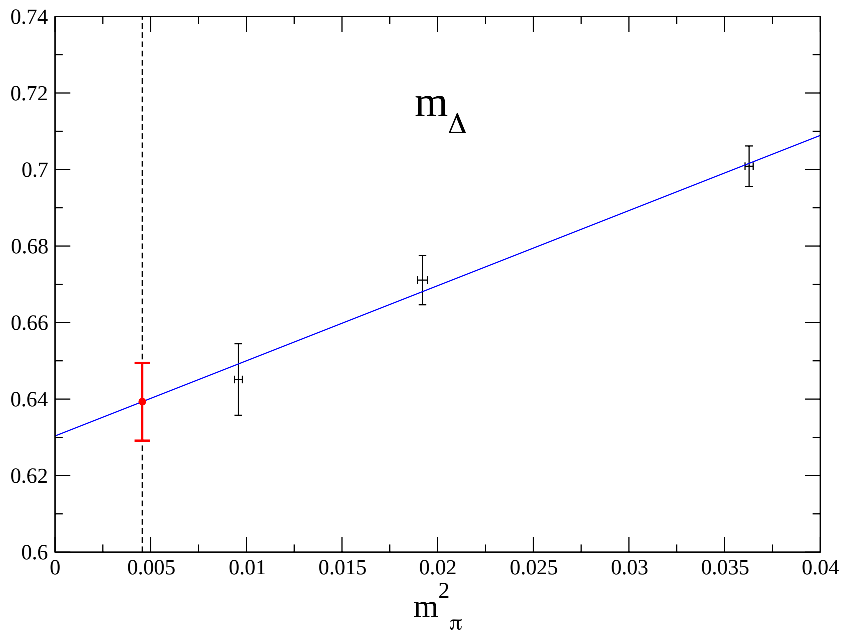


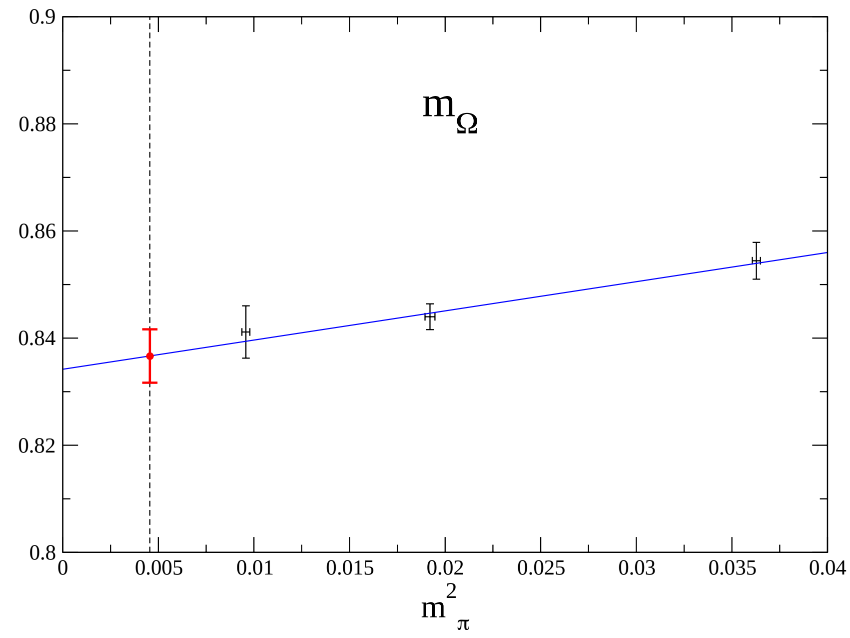
octet baryon

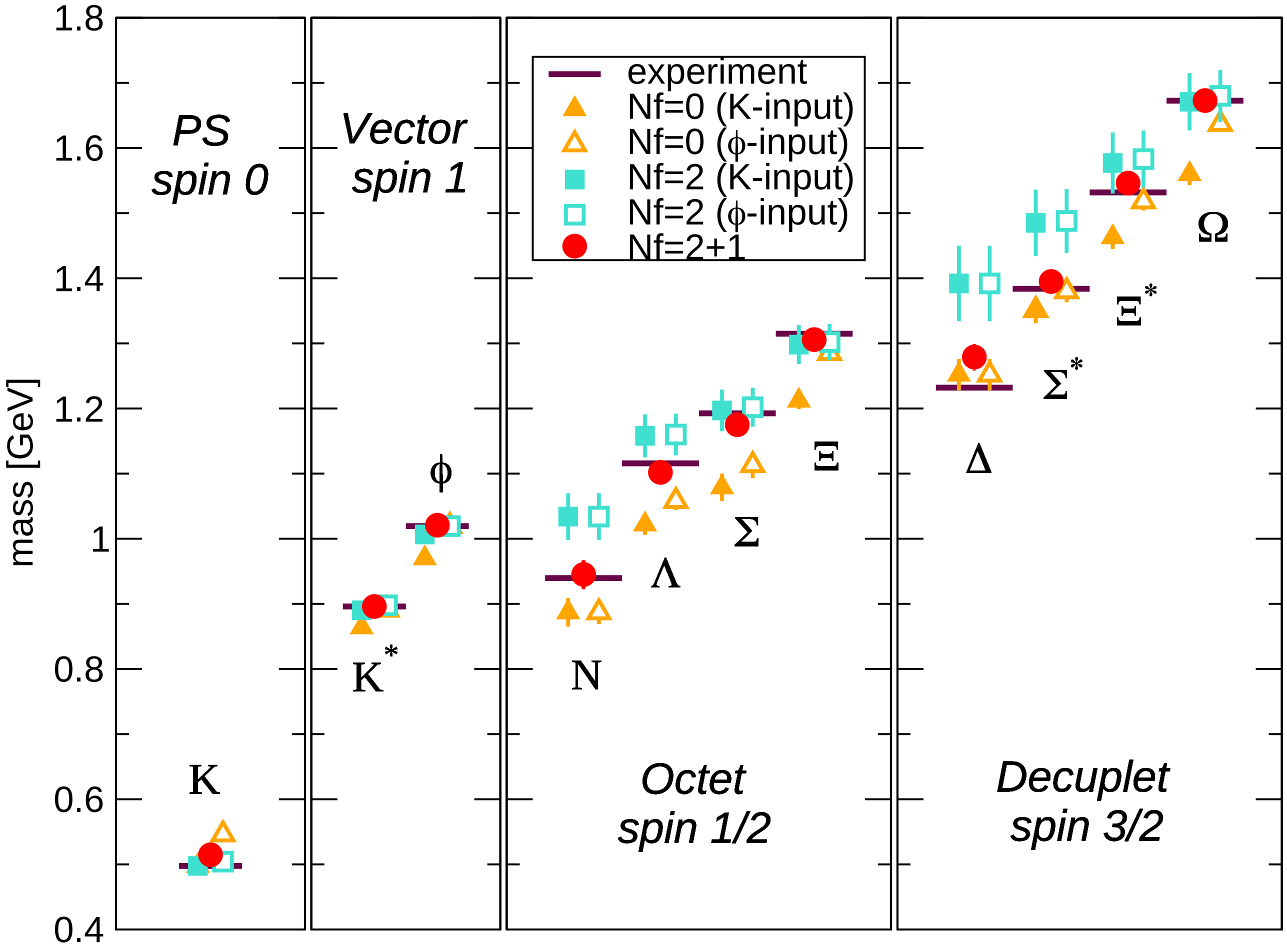




decuplet baryon

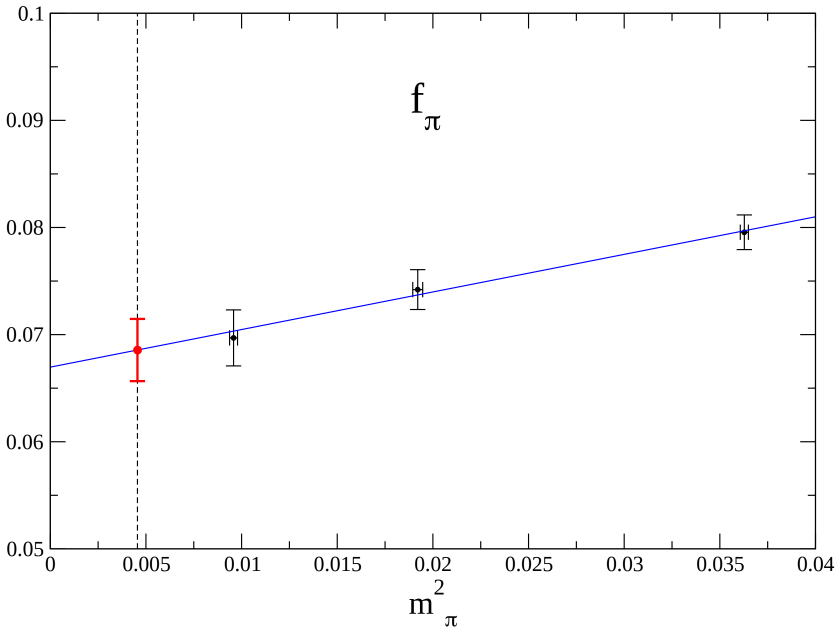


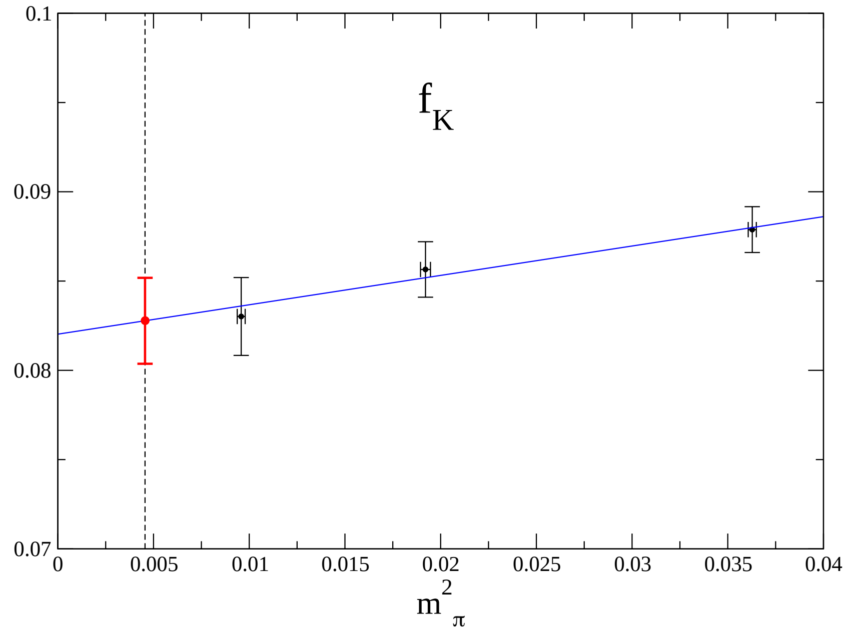




more than encouraging albeit possible $O((a\Lambda_{\mathrm{QCD}})^2)$ errors

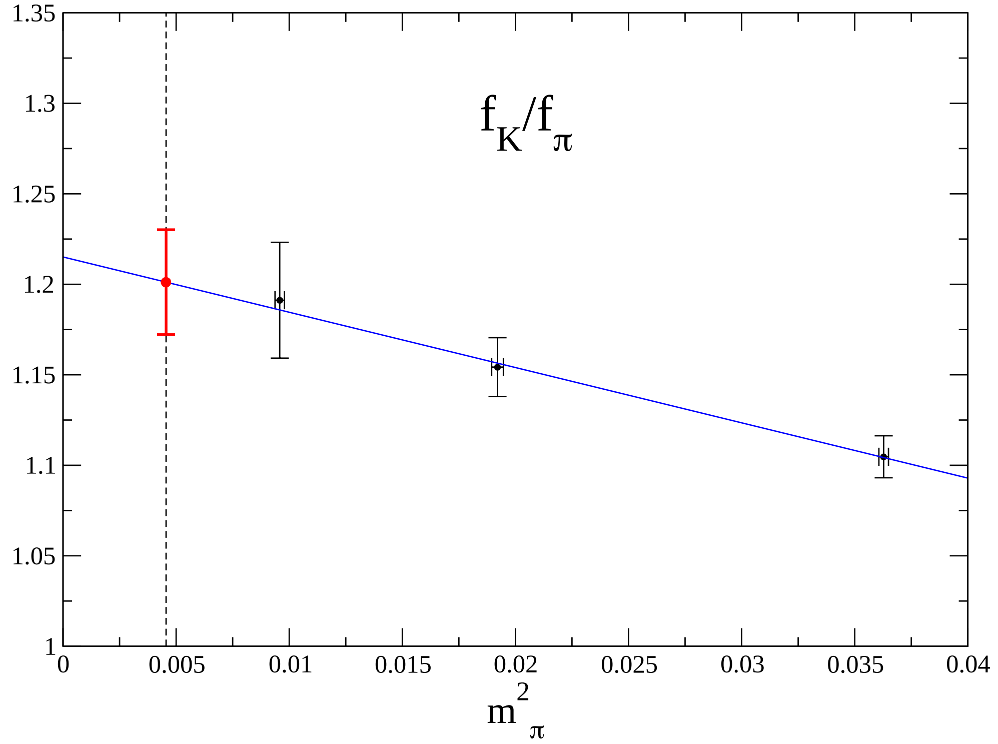
f_{PS} with perturbative Z_A





$$f_\pi = 137.1(5.8)\text{MeV}$$
$$130.7(4)\text{MeV (exp.)}$$

$$f_K = 165.5(4.8)\text{MeV}$$
$$159.8(1.5)\text{MeV (exp.)}$$



$$f_K/f_\pi \;=\; 1.201(29)$$
$$1.207(12)\ \text{(exp.)}$$

consistent with the experimental value

§7. Summary

target of the PACS-CS project

– three β values, two κ_s, (3.0fm)^3

– aim at the physical point

next step

– examine chiral logs

– investigate phase structure

– simulations at another κ_s

– nonperturbative Z_A, Z_m with the SF method

– calculation of η' meson mass