

PACS-CSの取り組み

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for PACS-CS Collaboration

「ストレンジを含むクォーク多体系分野の理論的将来を考える」研究会

2009年2月27 - 28日 @ KKRホテル熱海 (熱海市)

PACS-CS Collaboration Member

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PACS-CS Project:

$N_f = 2 + 1$ Simulations at the Physical Point on large enough lattices

- $O(a)$ improved Wilson quark action with nonperturbative c_{SW}
(CP-PACS and JLQCD Collaborations, 2006)
- Iwasaki gauge action (Iwasaki, 1983)
- $\beta = 1.90$ ($a = 0.0907(13)\text{fm}$)
- $32^3 \times 64$ lattice ($V \approx (2.9\text{fm})^3$)
- $m_\pi = 156 \sim 702 \text{ MeV}$
- $m_\pi L \gtrsim 2.3$

u-d quarks : Domain-Decomposed HMC (DDHMC) algorithm (Lüscher, 2003)
+ Hasenbusch trick (Hasenbusch, 2001; Hasenbusch, Jansen, 2003) + . . .

s quark : UV-filtered Polynomial HMC (UVPHMC) algorithm (JLQCD Collaborations, 2002)

on the PACS-CS (2560nodes, 14.3TFLOPS) and the T2K (95+140+61TFLOPS).

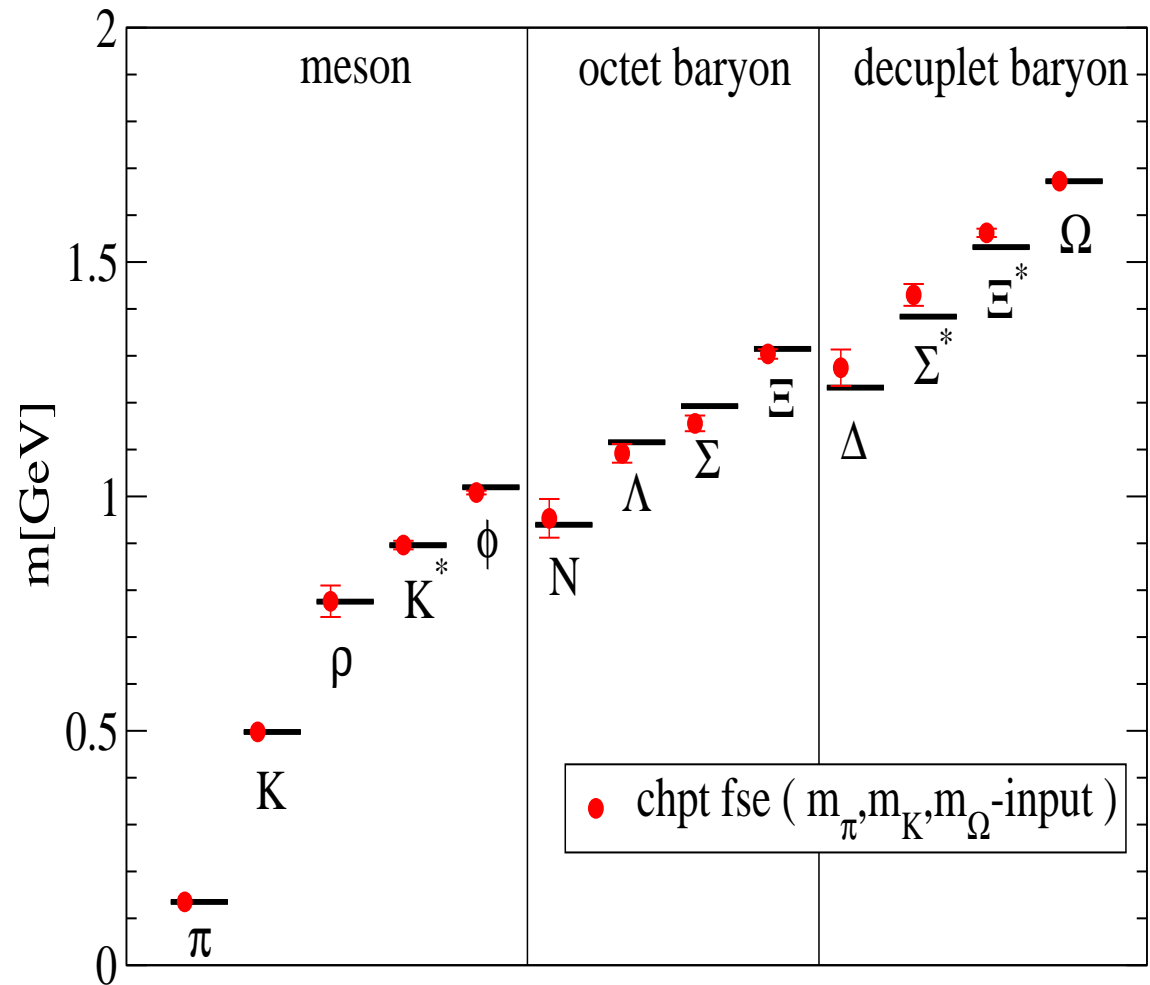
Introduction

Comparison with other groups for $N_f = 2 + 1$ simulations:

Collaboration	Dirac op.	m_π (MeV)	$m_\pi^{\min} L$	a (fm)
PACS-CS	clover	$\gtrsim 156$	2.3	0.09 [M_Ω]
BMW('08)	stout clover	$\gtrsim 190$	4	0.065-0.125 [M_Ξ]
MILC('04,'07)	staggered	$\gtrsim 240$	4	0.06-0.18 [F_π]
NPLQCD('07)	staggered+DW	$\gtrsim 290$	3.7	0.13 [r_0]
RBC/UKQCD('08)	DW	$\gtrsim 330$	4.6	0.1 [M_Ω]
JLQCD/TWQCD('08)	Overlap	$\gtrsim 310$	2.8	0.108 [r_0]

Introduction

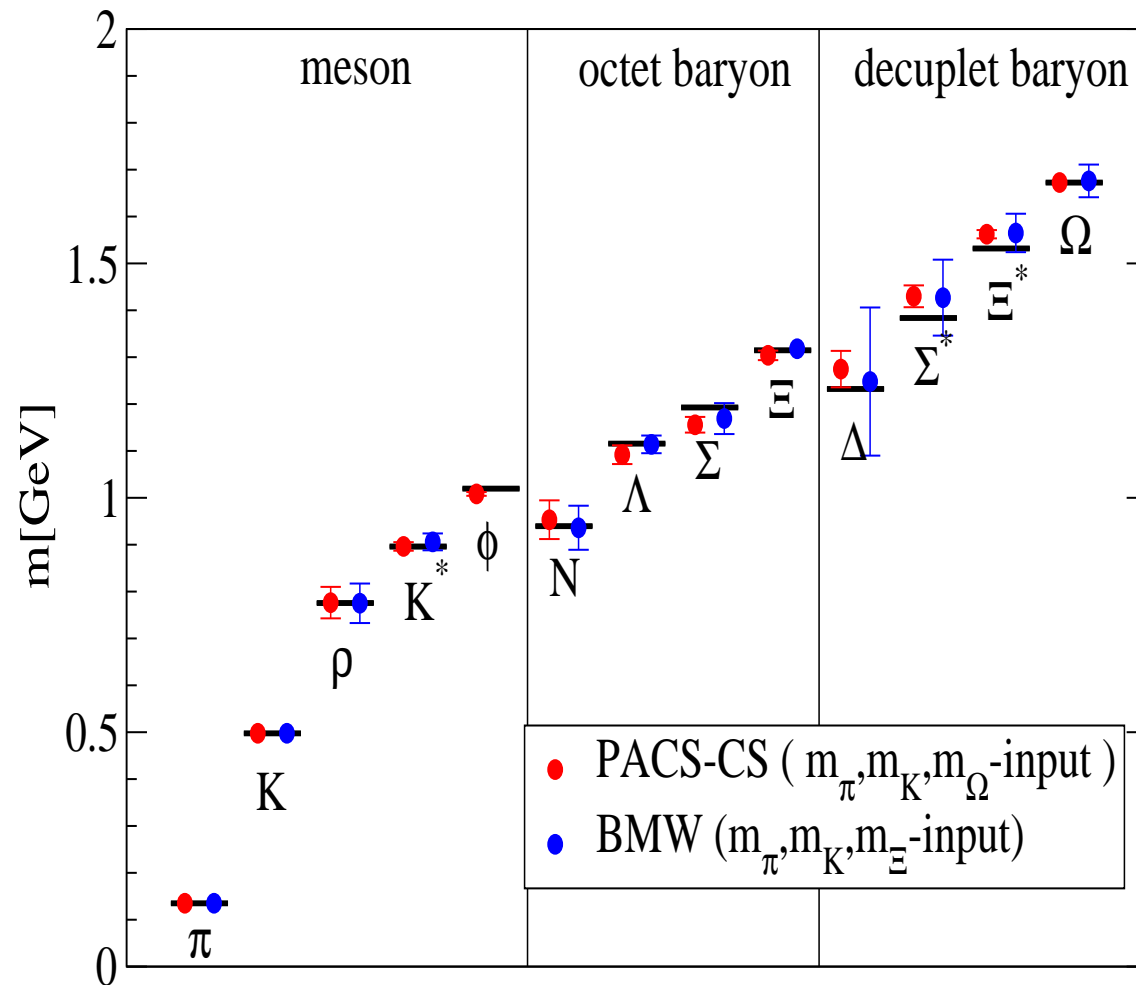
The light hadron spectrum of QCD at $a = 0.09\text{fm}$



Introduction

The light hadron spectrum of QCD :

PACS-CS ($a=0.09\text{fm}$) and BMW ($a \rightarrow 0$)



Plan to this talk :

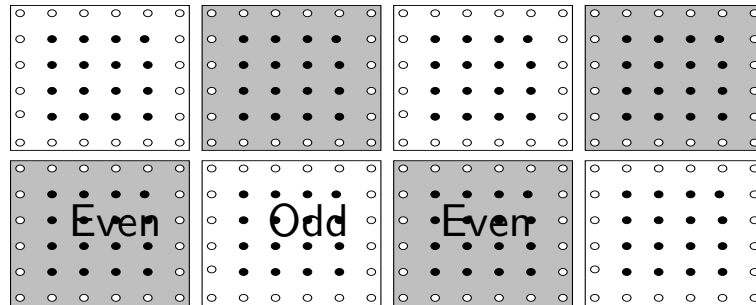
- Introduction
- Algorithm for $N_f = 2$ part : DDHMC, Hasenbusch trick, Solver
- Simulation Parameters and Data Set
- Run Status
- ChPT Analysis : SU(2) and SU(3) ChPT up to NLO
- The Physical Point Simulation
- Conclusion

Algorithm for $N_f = 2 + 1$ part
DDHMC, Hasenbusch trick, Solver

DDHMC Algorithm (Lüscher, 2003)

Key to reduce the cost : Domain Decomposition & Multi Time Step Integrator

- Domain Decomposition splitting lattice sites into even & odd domains as a preconditionor for $N_f = 2$ $O(a)$ -improved Wilson-Dirac op.



domain size we use is 8^4

$$D = \begin{pmatrix} D_{EE} & D_{EO} \\ D_{OE} & D_{OO} \end{pmatrix} = \begin{pmatrix} D_{EE} & 0 \\ 0 & D_{OO} \end{pmatrix} \begin{pmatrix} 1 & D_{EE}^{-1} D_{EO} \\ D_{OO}^{-1} D_{OE} & 1 \end{pmatrix}$$

$$|\det D|^2 = \underbrace{|\det D_{EE}|^2 |\det D_{OO}|^2}_{\text{UV part}} \underbrace{|\det(1 - D_{EE}^{-1} D_{EO} D_{OO}^{-1} D_{OE})|^2}_{\equiv D_{IR} : \text{IR part}}$$

After this preconditioning, we have a partition function,

$$\begin{aligned}
 Z &= \int_U \underbrace{e^{-S_G} |\det(1 + T)|^2}_{\text{Gauge part}} \underbrace{|\det \bar{D}_{EE}|^2 |\det \bar{D}_{OO}|^2}_{\text{UV part}} \underbrace{|\det D_{IR}|^2}_{\text{IR part}} \\
 &= \int_{P,U,\phi,\chi} \exp \left\{ -\frac{1}{2} \text{Tr}(P^2) - S'_G[U] - S_{UV}[U, \phi] - S_{IR}[U, \chi] \right\}.
 \end{aligned}$$

Molecular dynamics equation : set random ϕ, χ

$$\begin{aligned}
 \dot{U} &= P, \\
 \dot{P} &= F_G[U] + F_{UV}[U, \phi] + F_{IR}[U, \chi]
 \end{aligned}$$

- Multi time step integrator for Gauge, UV and IR parts (Sexton and Weingarten, 1992)

Relative magnitudes of force terms, F_G, F_{IR}, F_{UV} :

$$\|F_G\| : \|F_{UV}\| : \|F_{IR}\| \approx 16 : 4 : 1.$$

We choose the associated step sizes, $\delta\tau_G, \delta\tau_{UV}, \delta\tau_{IR}$ such that

$$\delta\tau_G \|F_G\| \approx \delta\tau_{UV} \|F_{UV}\| \approx \delta\tau_{IR} \|F_{IR}\|,$$

$$\delta\tau_G = \tau/N_0 N_1 N_2, \quad \delta\tau_{UV} = \tau/N_1 N_2, \quad \delta\tau_{IR} = \tau/N_2, \quad N_0 = N_1 = 4.$$

For strange quark, we employ UVPHMC algorithm (CP-PACS and JLQCD Collaborations, 2006) where the domain decomposition is not used.

$$\|F_s\| \approx \|F_{IR}\| \Rightarrow \delta\tau_s = \delta\tau_{IR}.$$

⇓

○ $m_\pi \gtrsim 296\text{MeV}$: DDHMC + UVPHMC algorithm works stable.

× $m_\pi = 156\text{MeV}$: large fluctuation of $\|F_{IR}\|$, slow to keep simulation stable.

- **Hasenbusch trick** (Hasenbusch, 2001; Hasenbusch, Jansen, 2003)

$D'_{IR} = D_{IR}(\kappa \rightarrow \kappa' = \rho\kappa)$, eg. $\rho = 0.9995$ to shift to the heavier mass

$$|\det D_{IR}|^2 = |\det D'_{IR}| \left| \det \left(\frac{D_{IR}}{D'_{IR}} \right) \right|^2 \Rightarrow F_{IR'}, F_{IR/IR'}$$

Step sizes, $\delta\tau_G$, $\delta\tau_{UV}$, $\delta\tau_{IR'}$, $\delta_{IR/IR'}$, are controlled by (N_0, N_1, N_2, N_3) .

$N_0 = N_1 = 4$, N_2 and N_3 are chosen to reduce the fluctuation of $\|F_{IR'}\|$, $\|F_{IR/IR'}\|$.

Solver for $m_\pi \gtrsim 296\text{MeV}$: $Dx = b$

For DDHMC algorithm ($m_\pi \gtrsim 296\text{MeV}$),

- IR solver : SAP(single prec.) preconditioned GCR(double prec.) (Lüscher, 2004)
- UV solver : SSOR(single prec.) preconditioned GCR(double prec.)
- Stopping condition : $\|Dx - b\|/\|b\| \leq 10^{-14}$ for H, 10^{-9} for F

Solver for $m_\pi = 156\text{MeV} : Dx = b$

For MPDDHMC algorithm ($m_\pi = 156\text{MeV}$),

★ Chronological guess for IR part (Brower, Ivanenko, Levi, Orginos, 1997)

★ nested BiCGStab solver for IR and UV part :

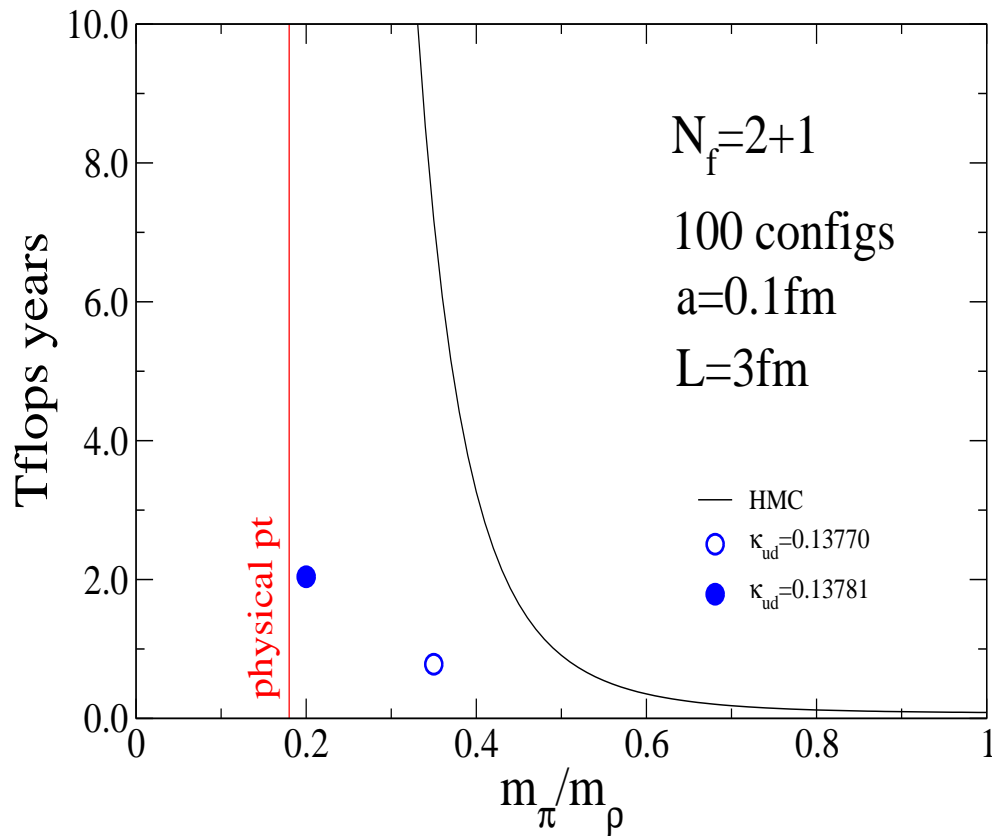
- Outer solver(double prec.) : Solve $Dx = b$ with preconditioner $M \approx D^{-1}$ with strict stopping condition 10^{-14} for F

- Inner solver(single prec.) : Solve $M \approx D^{-1}$ with appropriate preconditioner with automatic tolerance control $tol_{inner} = \min \left(\max \left(\frac{err_{outer}}{tol_{outer}}, 10^{-6} \right), 10^{-3} \right)$

★ Deflation technique (Morgan, Wilcox, 2002; Lüscher, 2007)

- inner BiCGStab stagnant \rightarrow GCRO-DR (Parks et al, 2006)

(Generalized Conjugate Residual with implicit inner Orthogonalization and Deflated Restarting)



$$\text{Cost} \propto (m_\pi/m_\rho)^{-3} \text{ for HMC,}$$

$$\propto (m_\pi/m_\rho)^{-2} \text{ for MPDDHMC.}$$

(Ukawa, 2002; PACS-CS Collaboration, 2007)

Physical Point simulations require

HMC : $O(100)$ Tflops computer ,

MPDDHMC : $O(10)$ Tflops computer.

Simulation Parameters and Data Set

Simulation Parameters and Data Set

κ_{ud}	0.13700	0.13727	0.13754	0.13754	0.13770	0.13781	0.137785
κ_s	0.13640	0.13640	0.13640	0.13660	0.13640	0.13640	0.13660
Algorithm	DDHMC	DDHMC	DDHMC	DDHMC	DDHMC	MPDDHMC	MPDDHMC
τ	0.5	0.5	0.5	0.5	0.25	0.25	0.25
$(N_0, N_1, N_2, N_3, N_4)$	(4,4,10)	(4,4,14)	(4,4,20)	(4,4,28)	(4,4,16)	(4,4,4,6) (4,4,6,6)	(4,4,2,4,4)
ρ_1	—	—	—	—	—	0.9995	0.9995
ρ_2	—	—	—	—	—	—	0.9990
N_{poly}	180	180	180	220	180	200	220
Replay	on	on	on	on	on	off	off
MD time	2000	2000	2250	2000	2000	1400	1000
$m_{ud}[MeV]$	67	45	24	21	12	3.5	3.6
$m_\pi[MeV]$	702	570	411	385	296	156	162
m_π/m_ρ	0.64	0.57	0.46	0.45	0.35	0.20	0.23
CPU time [h]/ τ	0.29	0.44	1.3	1.1	2.7	7.1	6.0

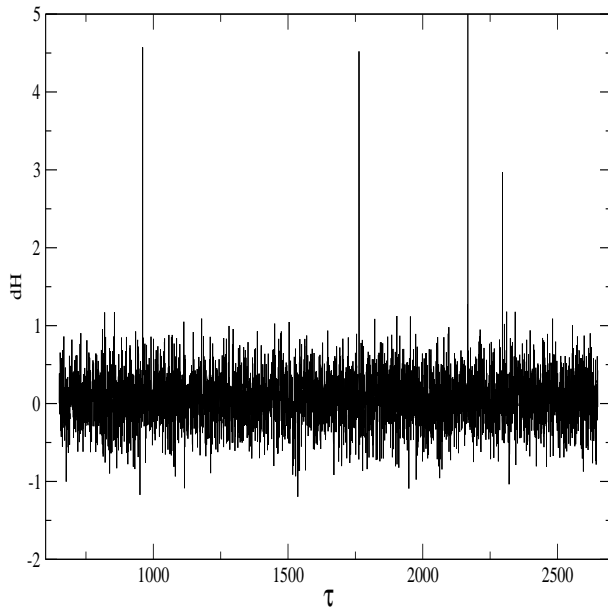
shifted hopping parameter $\kappa'_{ud} = \rho_1 \kappa_{ud} \sim 0.1377$

Run Status

dH and Force histories, Effective masses

dH History

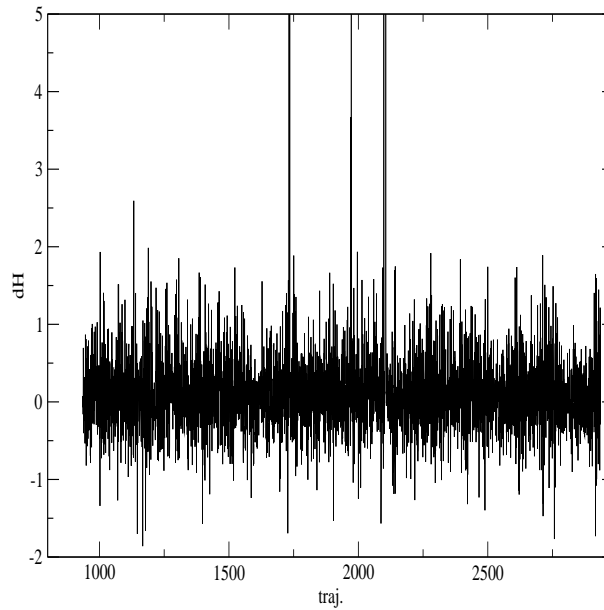
$m_\pi = 570\text{MeV}$



acc(HMC)=0.87

replay trick $\sim 0.1\%$

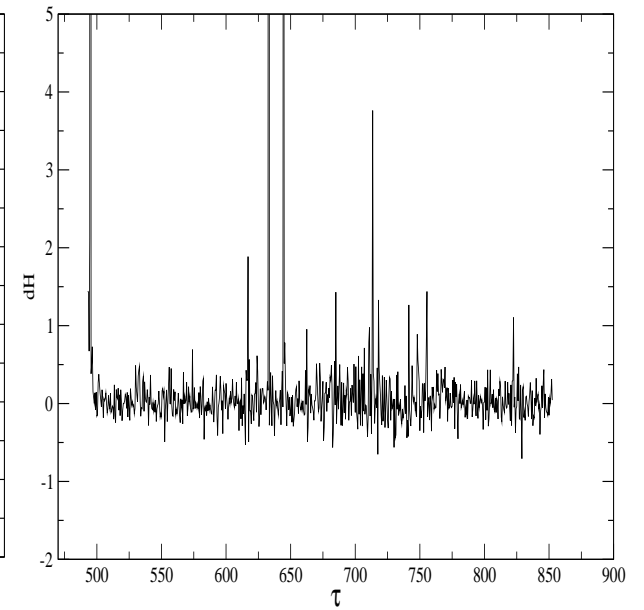
$m_\pi = 296\text{MeV}$



acc(HMC)=0.84

replay trick $\sim 3\%$

$m_\pi = 156\text{MeV}$



acc(HMC)=0.88

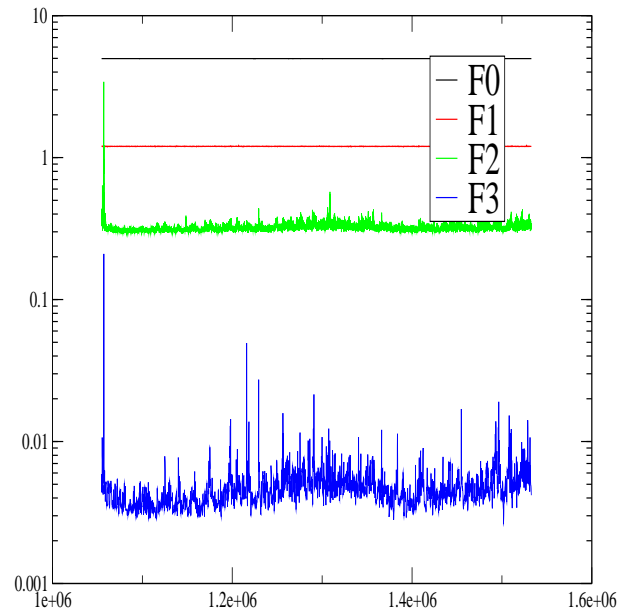
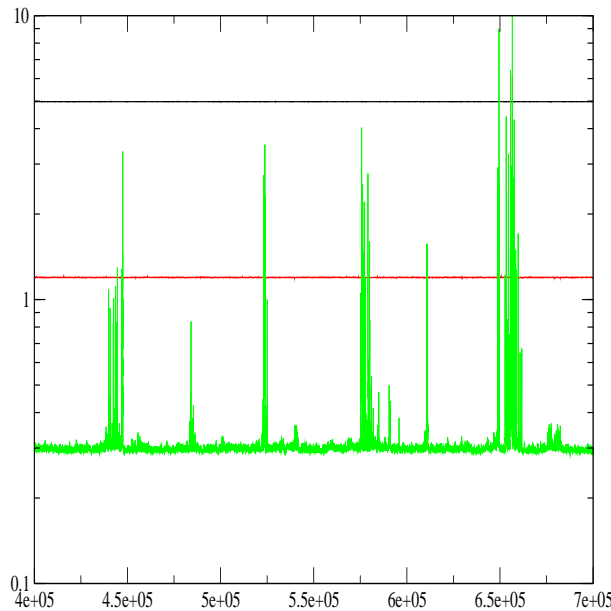
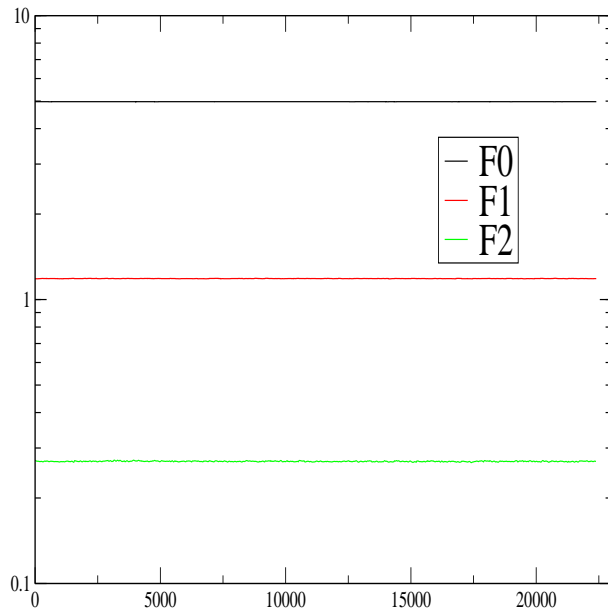
rate($|dH| > 2$) $\sim 3\%$

Force History

$m_\pi = 570\text{MeV}$

$m_\pi = 296\text{MeV}$

$m_\pi = 156\text{MeV}$



F_0 : Gauge + clv
 F_1 : UV
 F_2 : IR

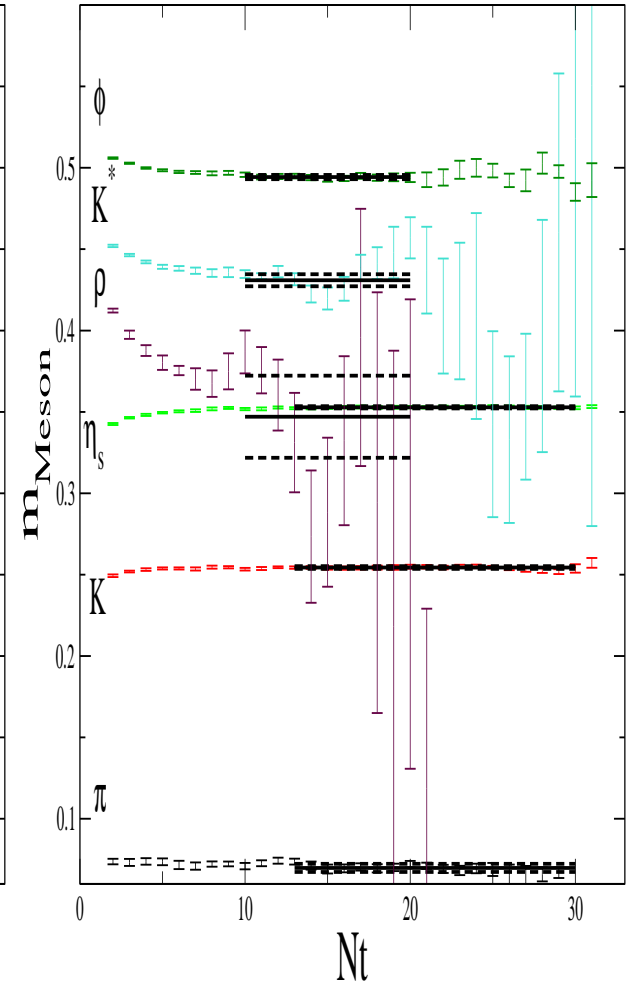
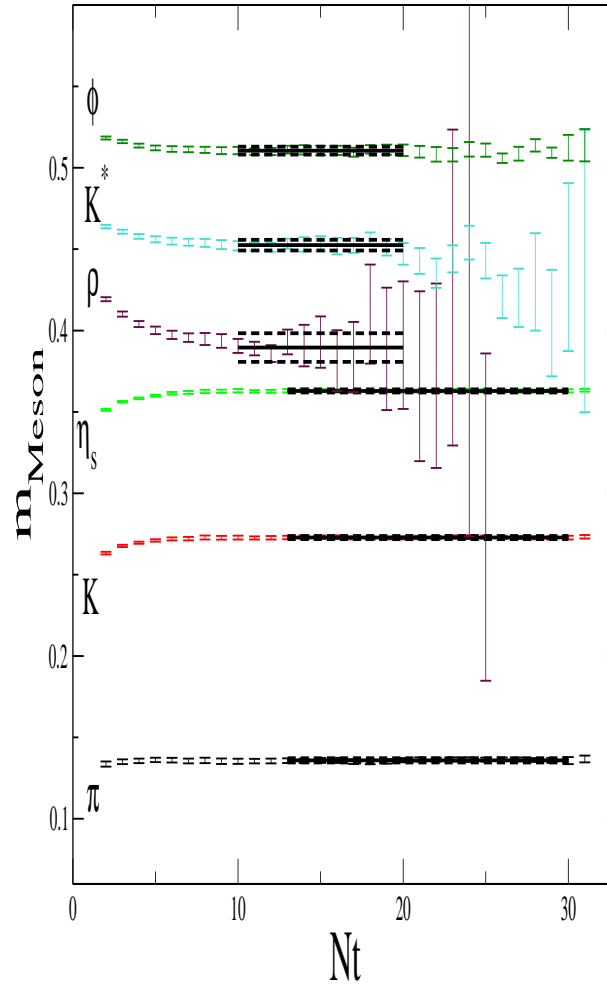
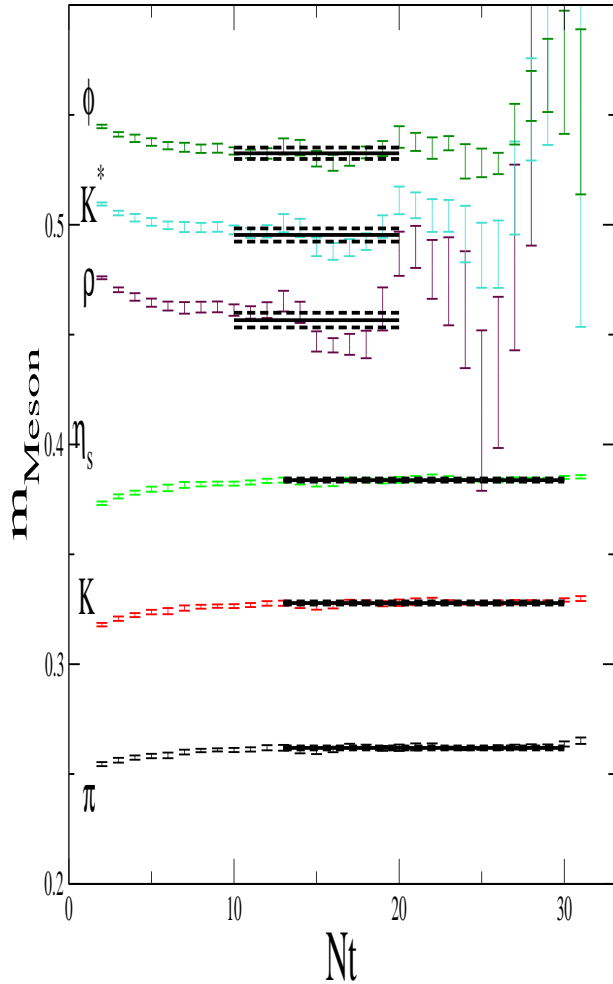
F_0 : Gauge + clv
 F_1 : UV
 F_2 : IR'
 F_3 : IR/IR'

Effective mass : Meson

$$k_{ud} = 0.13727$$
$$m_{\pi} = 570\text{MeV}$$

$$k_{ud} = 0.13770$$
$$m_{\pi} = 296\text{MeV}$$

$$k_{ud} = 0.13781$$
$$m_{\pi} = 156\text{MeV}$$



Fit Range $[t_{\min}, t_{\max}]$: Pseudoscalar $[13 - 30]$, Vector $[10 - 20]$

Effective mass : Baryon

$$k_{ud} = 0.13727$$

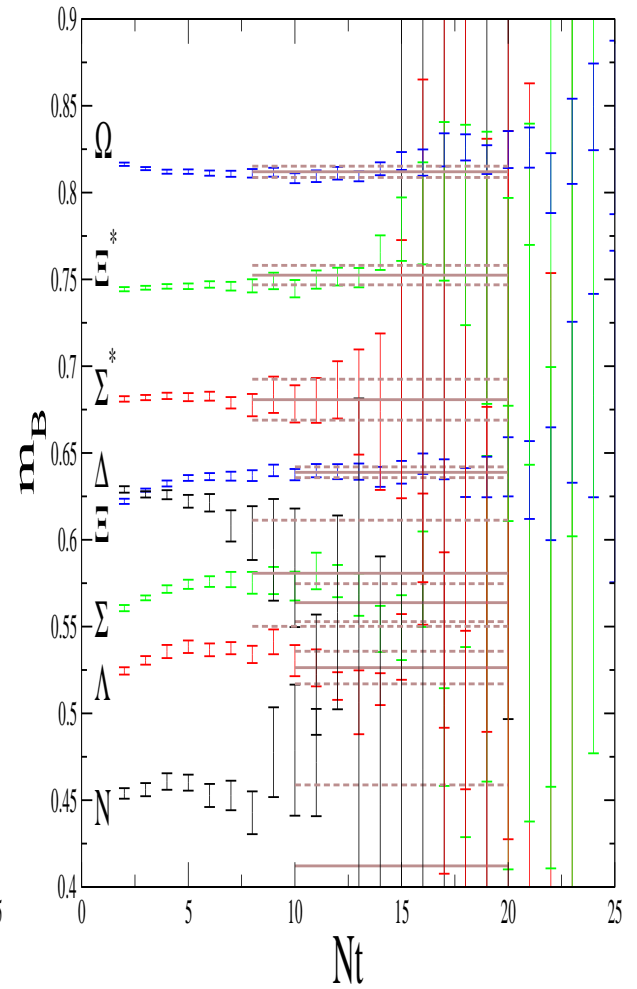
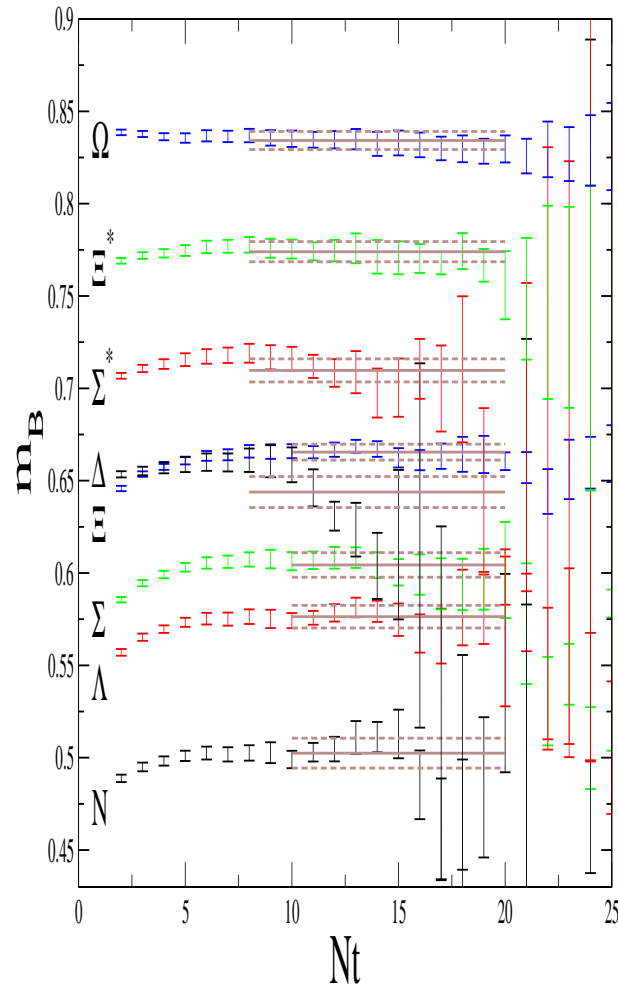
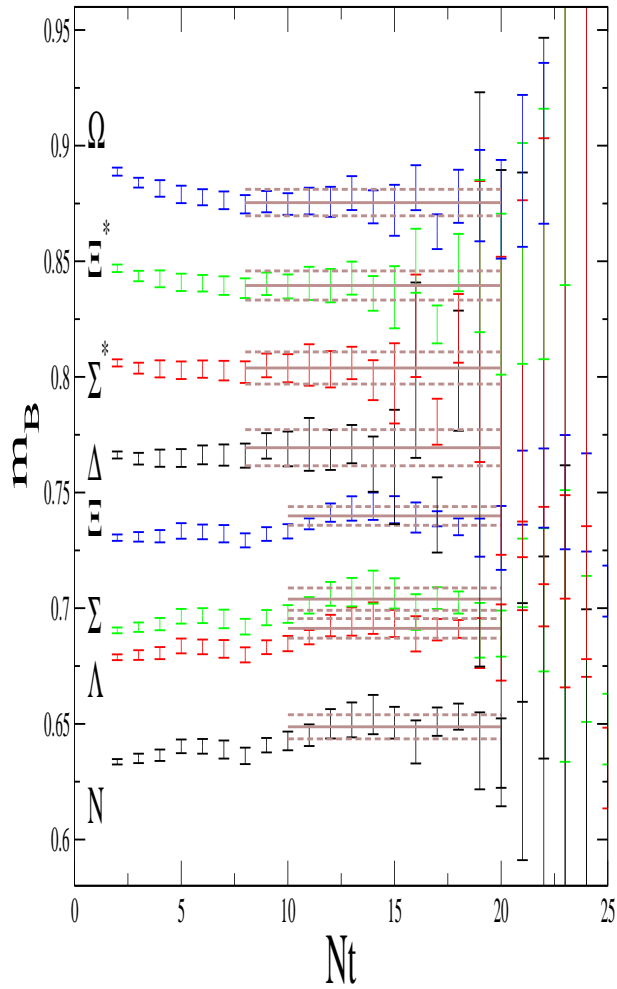
$$m_\pi = 570\text{MeV}$$

$$k_{ud} = 0.13770$$

$$m_\pi = 296\text{MeV}$$

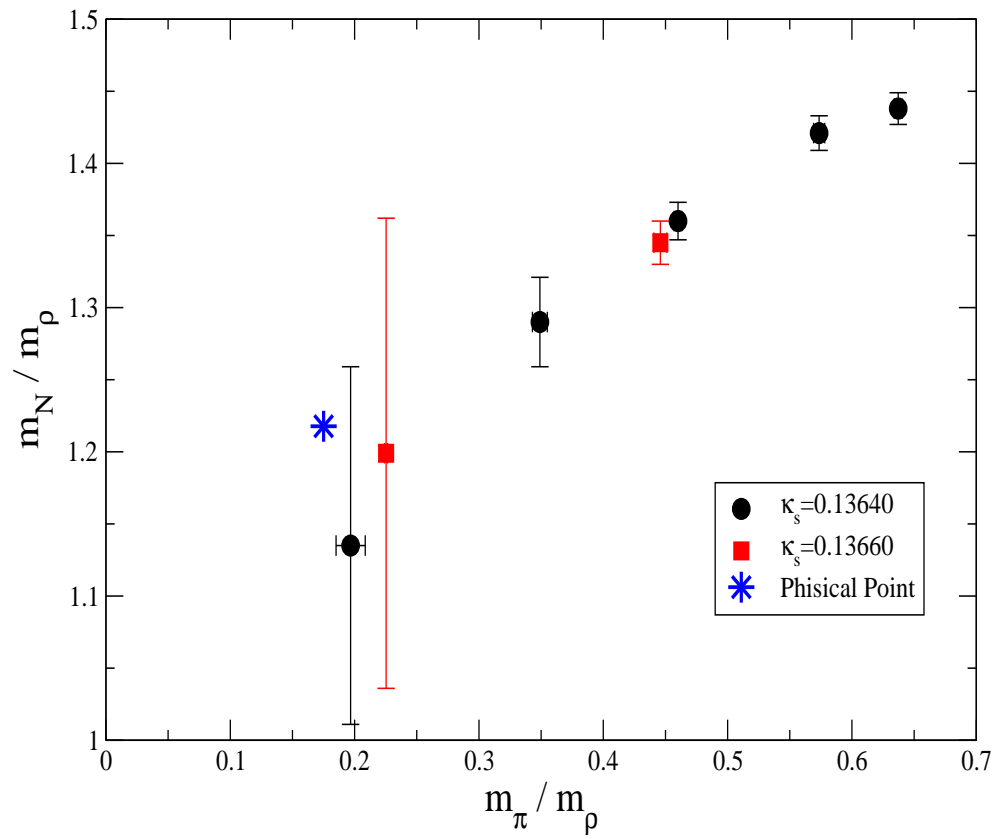
$$k_{ud} = 0.13781$$

$$m_\pi = 156\text{MeV}$$

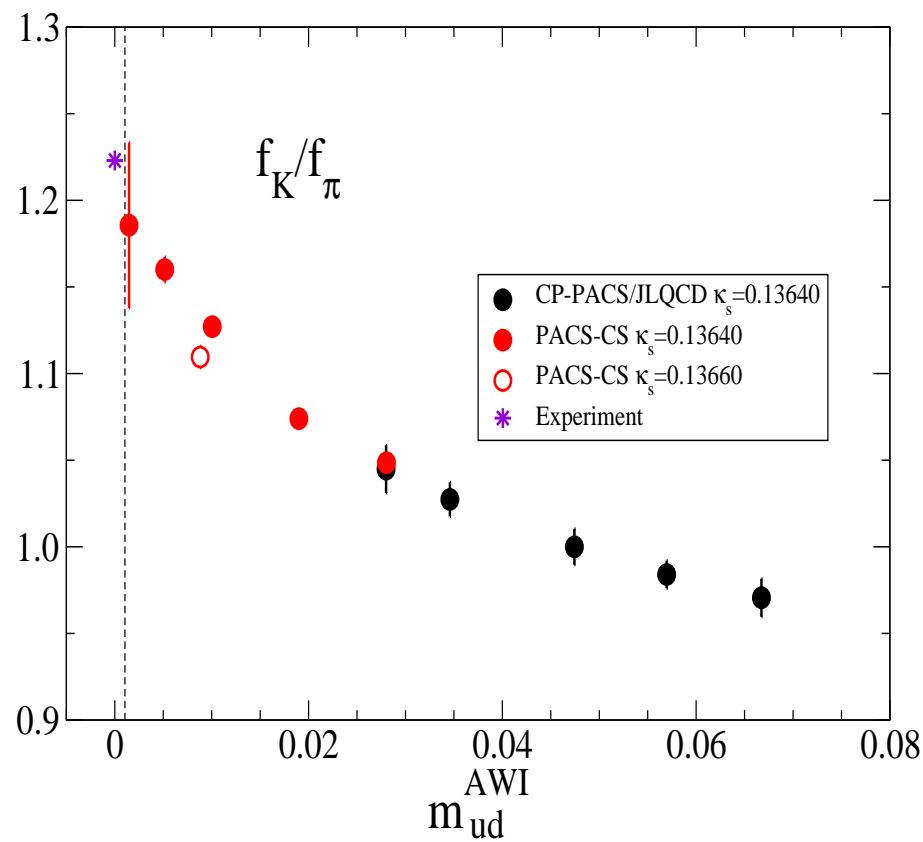
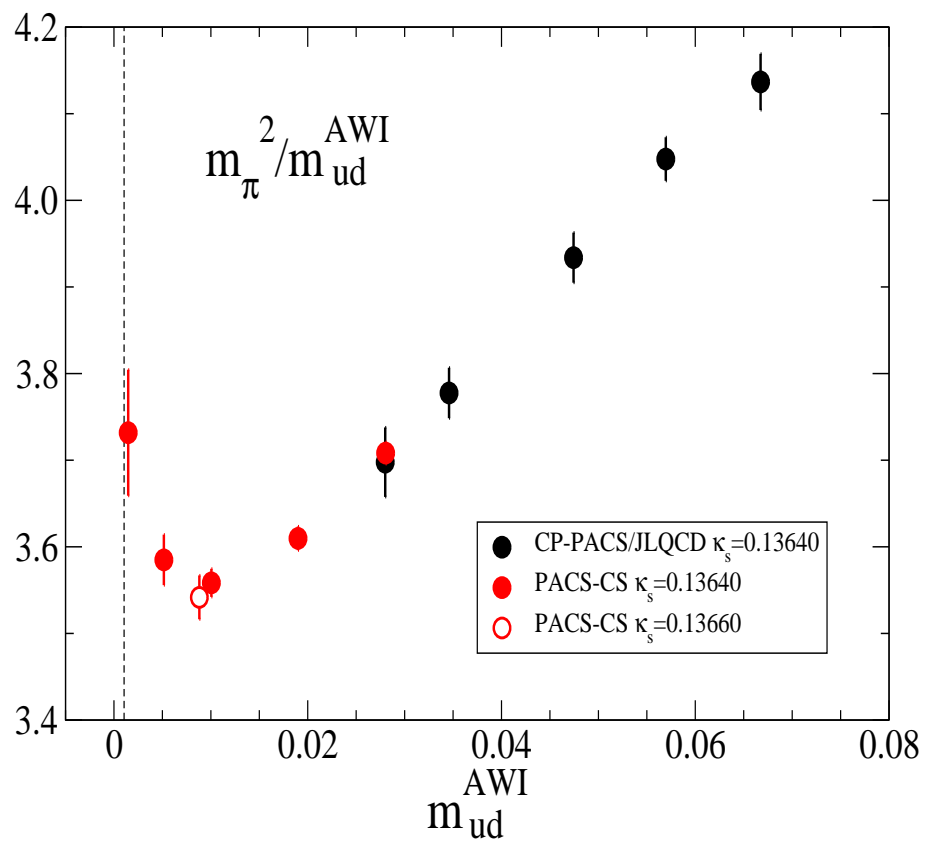


Fit Range $[t_{\min}, t_{\max}]$: Decuplet $[13 - 30]$, Octet $[10 - 20]$

Edinburgh Plot



$m_\pi^2/m_{ud}, f_K/f_\pi$ vs m_{ud}



SU(3) ChPT analysis

Continuum SU(3) ChPT up to NLO = WChPT up to NLO :

$$\begin{aligned} \frac{m_\pi^2}{2m_{\text{ud}}} &= B_0 \left\{ 1 + \mu_\pi - \frac{1}{3}\mu_\eta + \frac{2B_0}{f_0^2} (16m_{\text{ud}}L_{85} + 16(2m_{\text{ud}} + m_s)L_{64}) \right\}, \\ \frac{m_K^2}{(m_{\text{ud}} + m_s)} &= B_0 \left\{ 1 + \frac{2}{3}\mu_\eta + \frac{2B_0}{f_0^2} (8(m_{\text{ud}} + m_s)L_{85} + 16(2m_{\text{ud}} + m_s)L_{64}) \right\}, \\ f_\pi &= f_0 \left\{ 1 - 2\mu_\pi - \mu_K + \frac{2B_0}{f_0^2} (8m_{\text{ud}}L_5 + 8(2m_{\text{ud}} + m_s)L_4) \right\}, \\ f_K &= f_0 \left\{ 1 - \frac{3}{4}\mu_\pi - \frac{3}{2}\mu_K - \frac{3}{4}\mu_\eta + \frac{2B_0}{f_0^2} (4(m_{\text{ud}} + m_s)L_5 + 8(2m_{\text{ud}} + m_s)L_4) \right\}, \end{aligned}$$

where we have six unknown LECs $B_0, f_0, L_{4,5,6,8}$. μ_{PS} denotes the chiral logarithm defined by

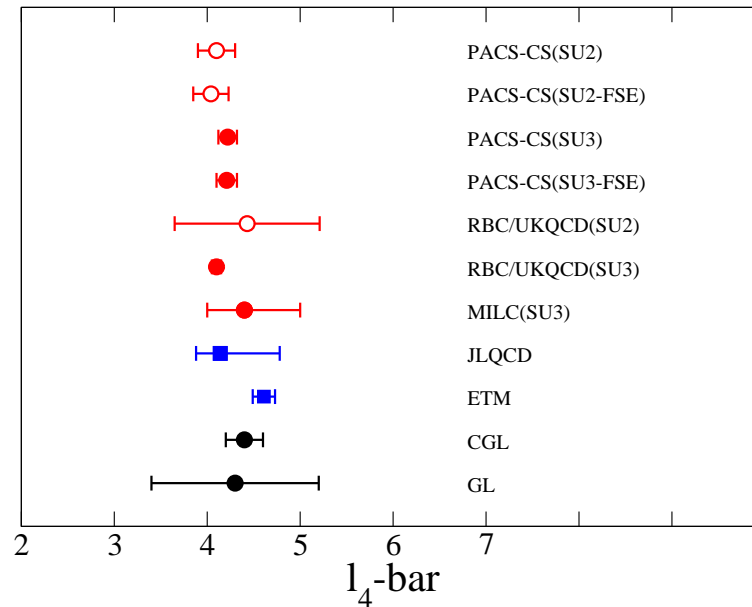
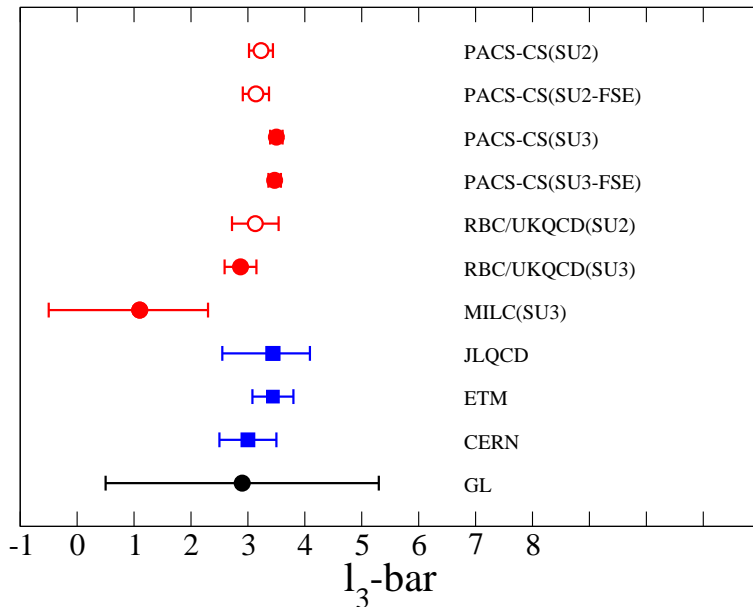
$$\mu_{\text{PS}} = \frac{1}{16\pi^2} \frac{\tilde{m}_{\text{PS}}^2}{f_0^2} \ln \left(\frac{\tilde{m}_{\text{PS}}^2}{\mu^2} \right),$$

where

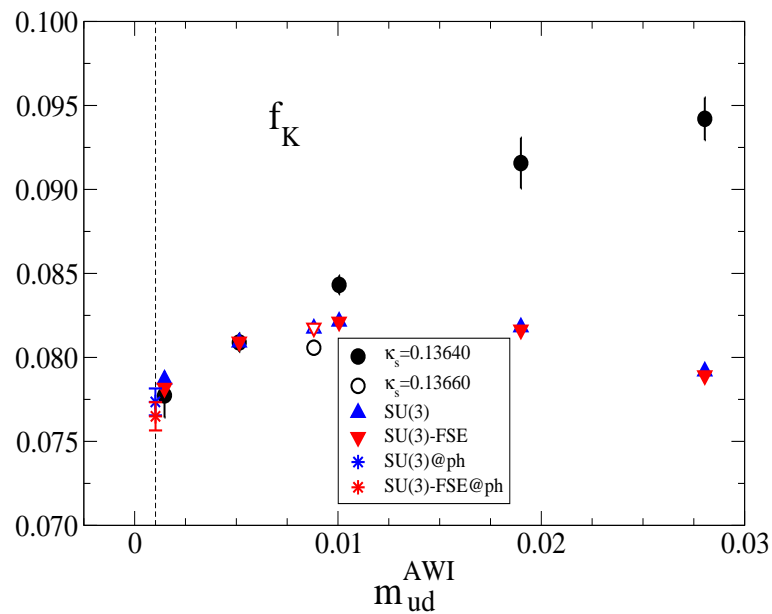
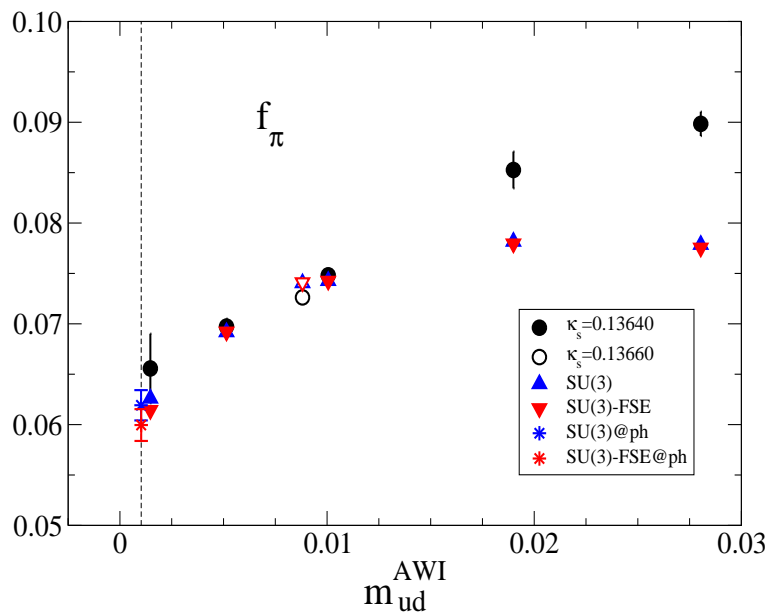
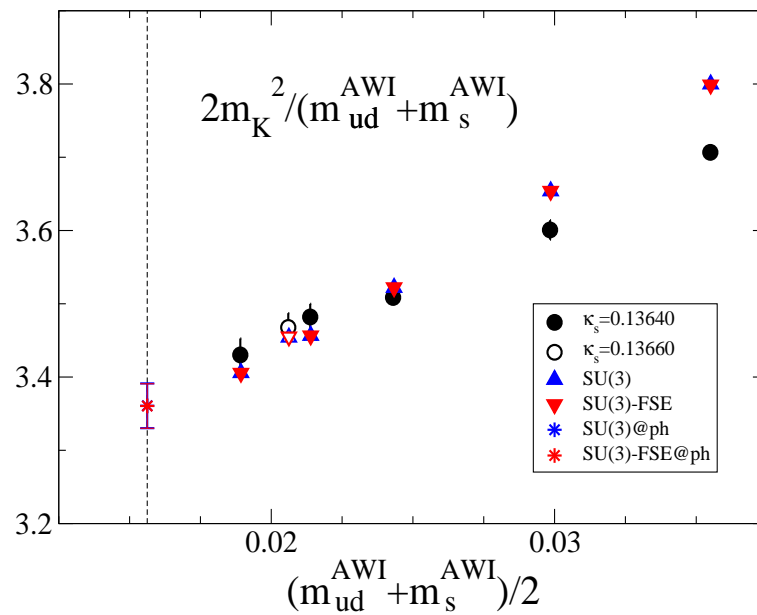
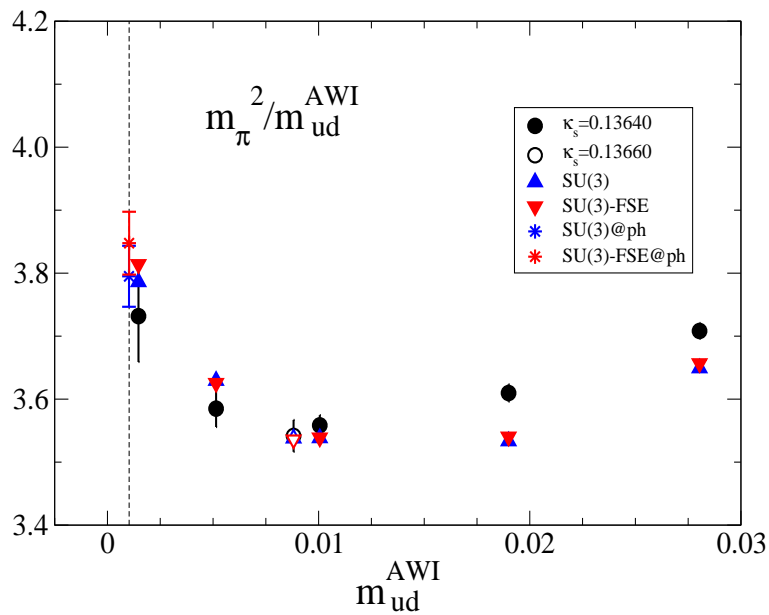
$$\tilde{m}_\pi^2 = 2m_{\text{ud}}B_0, \quad \tilde{m}_K^2 = (m_{\text{ud}} + m_s)B_0, \quad \tilde{m}_\eta^2 = \frac{2}{3}(m_{\text{ud}} + 2m_s)B_0$$

Result for the LEC's in the SU(3) ChPT

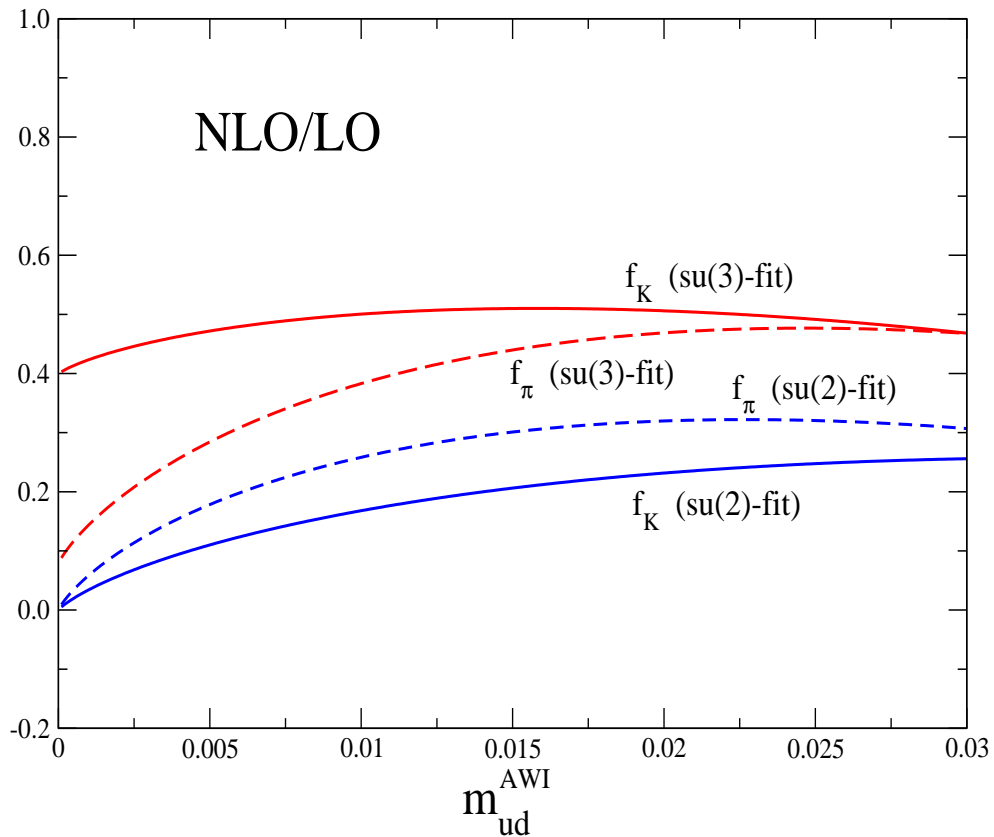
	PACS-CS		phenomenology	RBC/UKQCD	MILC
	w/o FSE	w/ FSE			
$f_0[\text{GeV}]$	0.1160(88)	0.1185(90)	0.115	0.0935(73)	—
f_π/f_0	1.159(57)	1.145(56)	1.139	1.33(7)	1.21(5) $\left(\begin{smallmatrix} +13 \\ -3 \end{smallmatrix}\right)$
L_4	-0.04(10)	-0.06(10)	0.00(80)	0.139(80)	0.1(3) $\left(\begin{smallmatrix} +3 \\ -1 \end{smallmatrix}\right)$
L_5	1.43(7)	1.45(7)	1.46(10)	0.872(99)	1.4(2) $\left(\begin{smallmatrix} +2 \\ -1 \end{smallmatrix}\right)$
$2L_6 - L_4$	0.10(2)	0.10(2)	0.0(1.0)	-0.001(42)	0.3(1) $\left(\begin{smallmatrix} +2 \\ -3 \end{smallmatrix}\right)$
$2L_8 - L_5$	-0.21(3)	-0.21(3)	0.54(43)	0.243(45)	0.3(1)(1)
χ^2/dof	4.2(2.7)	4.4(2.8)	—	0.7	—



SU(3) ChPT Fit up to NLO



Ratio of NLO contribution to LO one



m_s is not small enough to be treated in the SU(3) ChPT up to NLO.



The SU(2) ChPT with the analytical expansion of m_s about the physical value.

SU(2) ChPT analysis

Continuum SU(2) ChPT up to NLO :

$$\frac{m_\pi^2}{2m_{\text{ud}}} = B \left\{ 1 + \frac{1}{16\pi^2} \frac{\bar{m}_\pi^2}{f^2} \ln \left(\frac{\bar{m}_\pi^2}{\mu^2} \right) + 4 \frac{\bar{m}_\pi^2}{f^2} l_3 \right\},$$

$$f_\pi = f \left\{ 1 - \frac{1}{8\pi^2} \frac{\bar{m}_\pi^2}{f^2} \ln \left(\frac{\bar{m}_\pi^2}{\mu^2} \right) + 2 \frac{\bar{m}_\pi^2}{f^2} l_4 \right\}.$$

B and f are linearly expanded in terms of m_s :

$$B = B_s^{(0)} + m_s B_s^{(1)}, \quad f = f_s^{(0)} + m_s f_s^{(1)}.$$

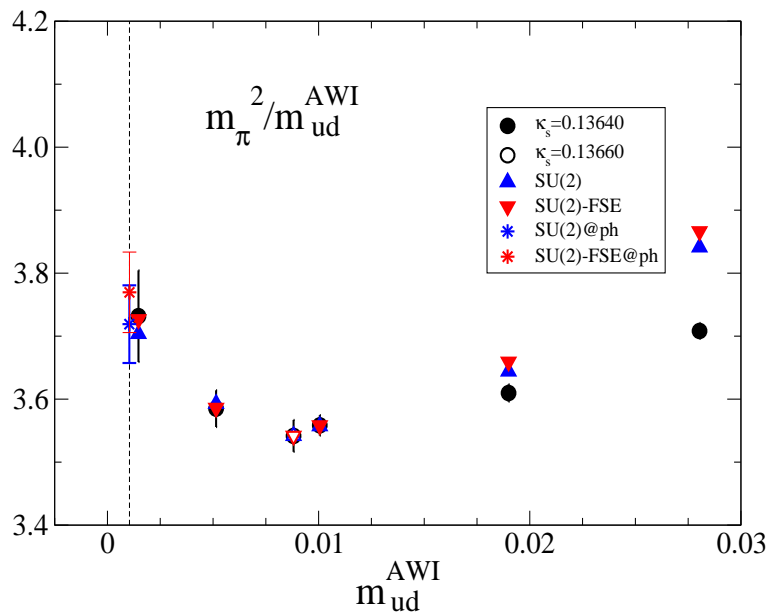
For m_K and f_K we employ the following fit formulae:

$$m_K^2 = \alpha_m + \gamma_m m_s + \beta_m m_{\text{ud}},$$

$$f_K = \bar{f} \left\{ 1 + \beta_f m_{\text{ud}} - \frac{3}{4} \frac{2B m_{\text{ud}}}{16\pi^2 f} \ln \left(\frac{2B m_{\text{ud}}}{\mu^2} \right) \right\},$$

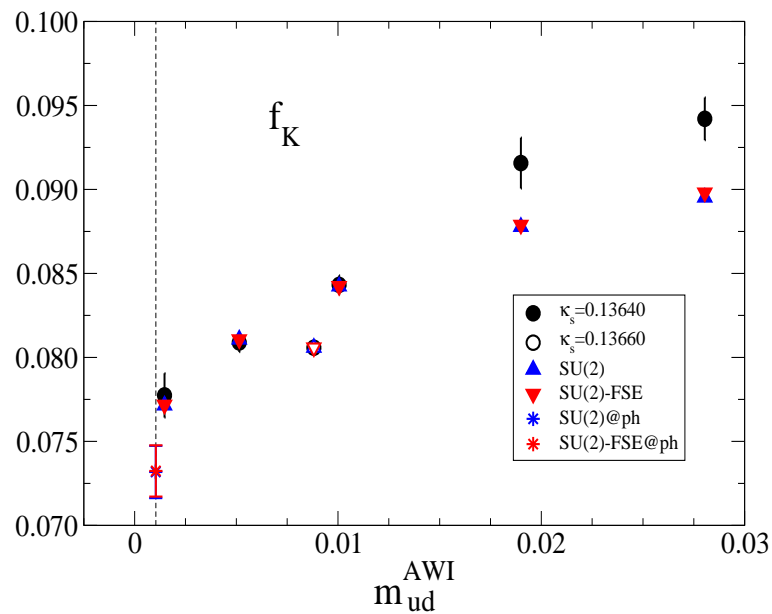
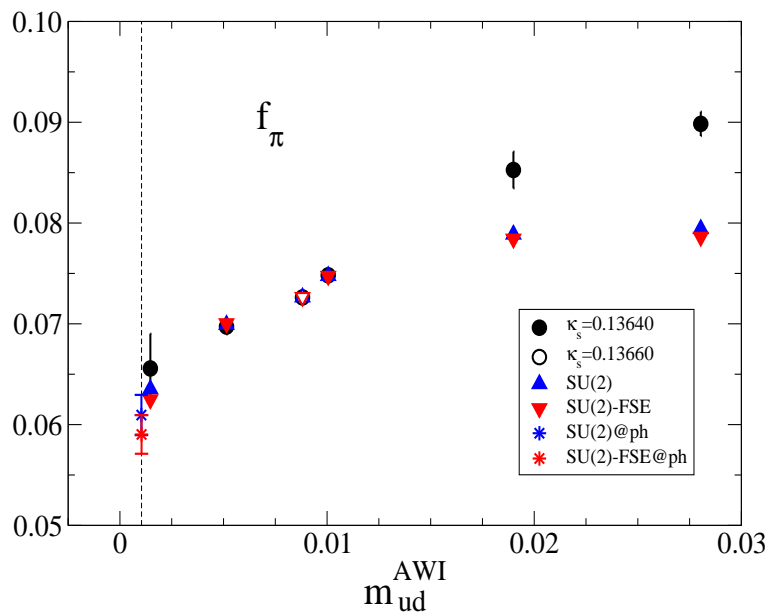
where $\bar{f} = \bar{f}_s^{(0)} + m_s \bar{f}_s^{(1)}$.

SU(2) ChPT Fit up to NLO

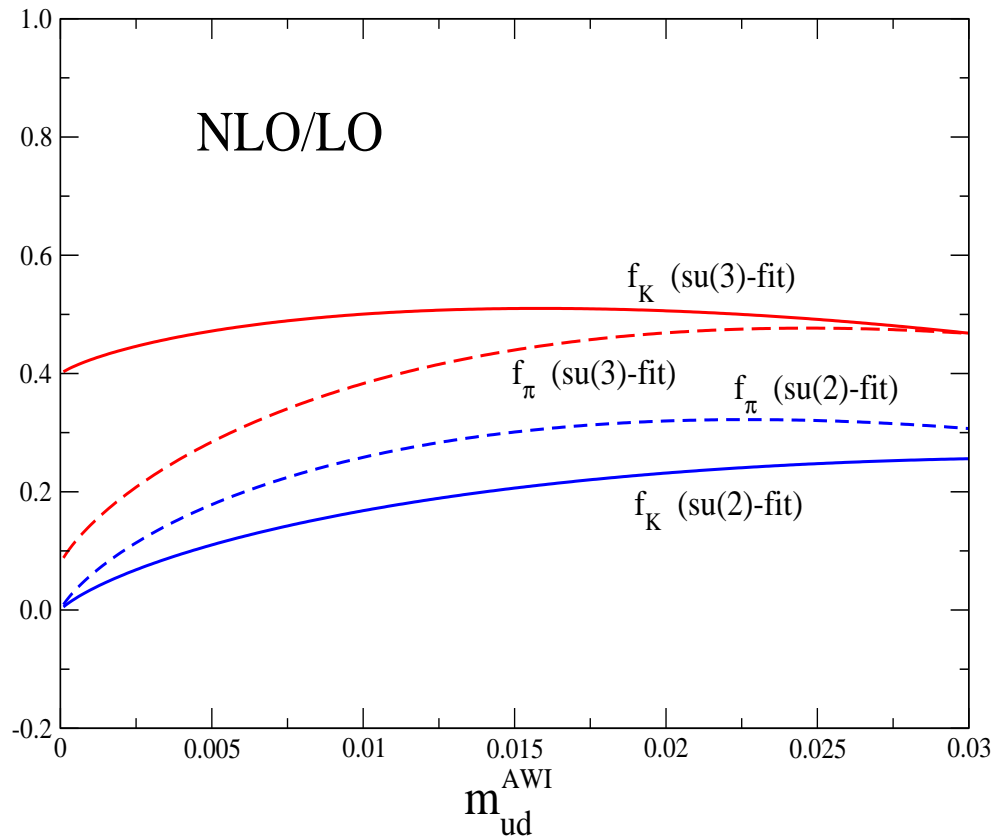


$$\chi^2 / \text{dof} = 0.43(77) \text{ with FSE,}$$

$$= 0.33(68) \text{ without FSE,}$$

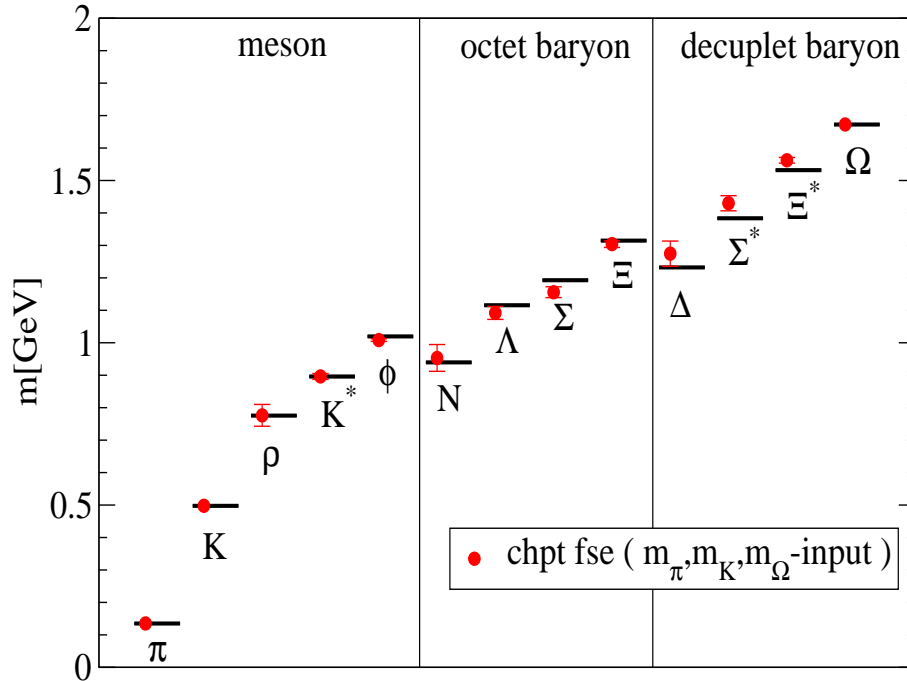


Ratio of NLO contribution to LO one



The ratio NLO/LO in the SU(2) ChPT is reduced from the SU(3) ChPT case.

Result in the SU(2) ChPT

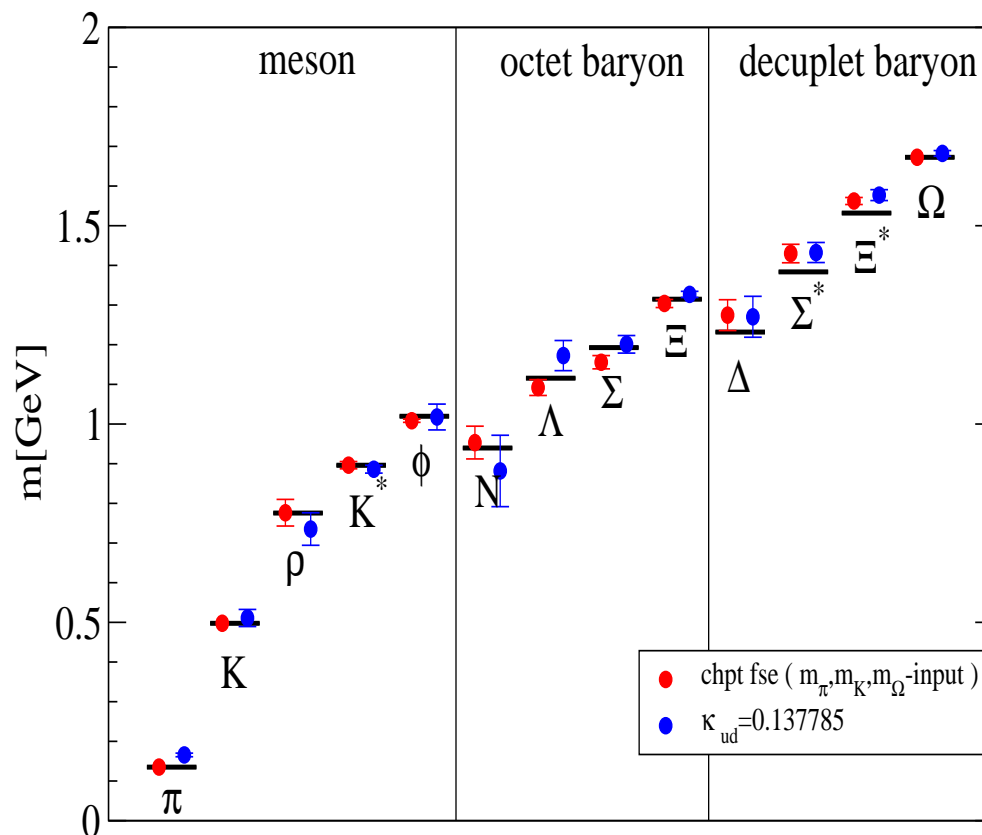


	PACS-CS	experiment	RBC/UKQCD	MILC
a^{-1} [GeV]	2.176(31)	—	1.729(28)	continuum
$m_{ud}^{\overline{MS}}$ [MeV]	2.527(47)	—	3.72(16)(33)(18)	3.2(0)(1)(2)(0)
$m_s^{\overline{MS}}$ [MeV]	72.72(78)	—	107.3(4.4)(9.7)(4.9)	88(0)(3)(4)(0)
m_s/m_{ud}	28.8(4)	—	28.8(0.4)(1.6)	27.2(1)(3)(0)(0)
f_π [MeV]	134.0(4.2)	$130.7 \pm 0.1 \pm 0.36$	124.1(3.6)(6.9)	input
f_K [MeV]	159.4(3.1)	$159.8 \pm 1.4 \pm 0.44$	149.6(3.6)(6.3)	$156.5(0.4)_{(-2.7)}^{(+1.0)}$
f_K/f_π	1.189(20)	1.223(12)	1.205(18)(62)	$1.197(3)_{(-13)}^{(+6)}$

$$\kappa_{\text{ud}} = 0.137785, \kappa_{\text{s}} = 0.13660$$

is estimated as the physical point from our ChPT analysis.

$$\kappa_{ud} = 0.137785, \kappa_s = 0.13660$$



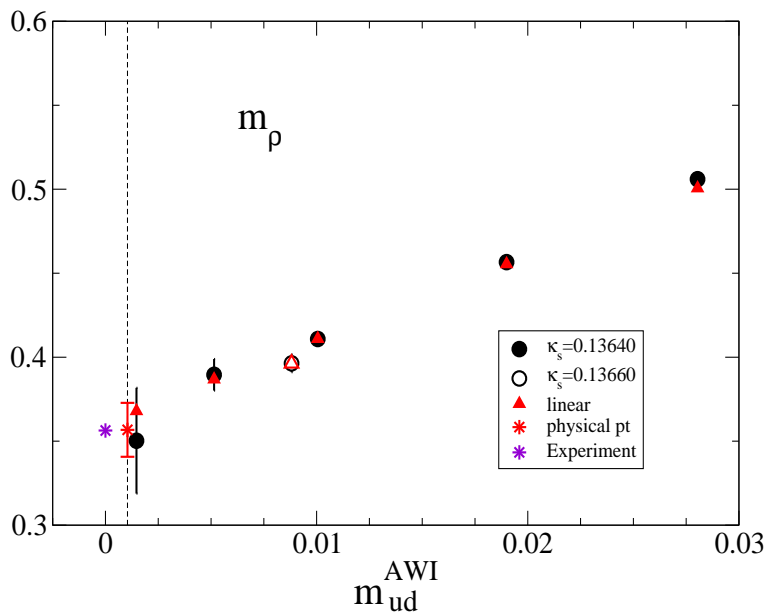
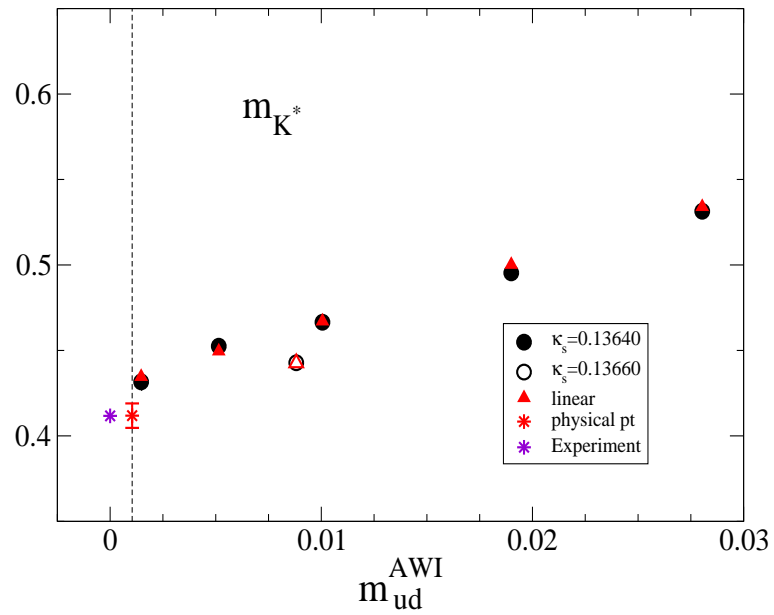
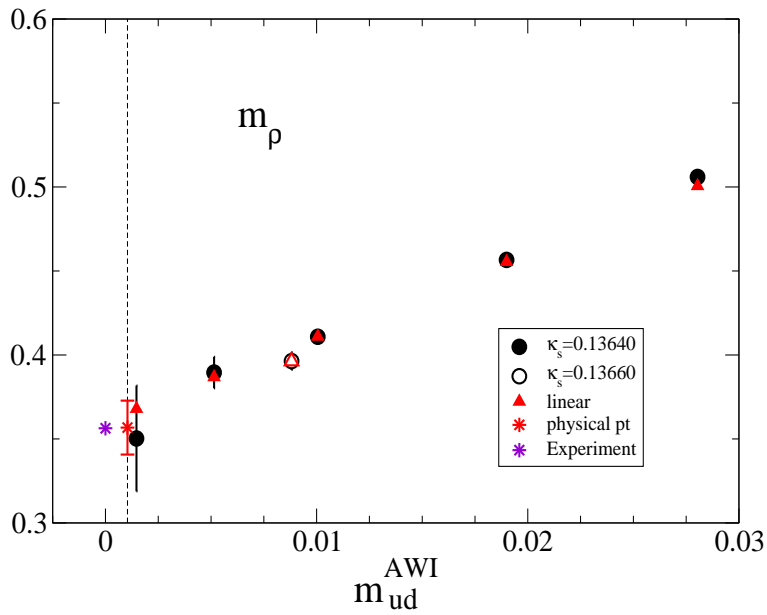
	ChPT	experiment	$\kappa_{ud} = 0.137785$
$m_{ud}^{\overline{MS}}$ [MeV]	2.53(5)	—	3.5(3)
$m_s^{\overline{MS}}$ [MeV]	72.7(8)	—	73.4(2)
f_π [MeV]	134.0(4.2)	$130.7 \pm 0.1 \pm 0.36$	129.0(5.4)
f_K [MeV]	159.4(3.1)	$159.8 \pm 1.4 \pm 0.44$	160.6(1.4)

- $N_f = 2 + 1$ full QCD with $O(a)$ improved Wilson quarks on $(2.9\text{fm})^3$
- domain-decomposed HMC + Hasenbusch trick
- $m_\pi = 156 \sim 702[\text{MeV}]$
- $m_\pi/m_\rho = 0.20 \sim 0.64$
- $a = 0.0907(13) \text{ fm}$
- $m_\pi L \gtrsim 2.3$

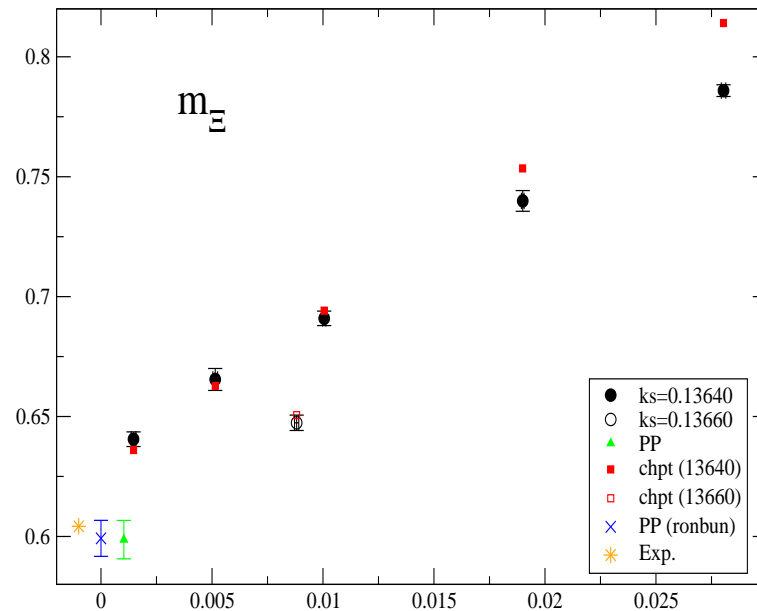
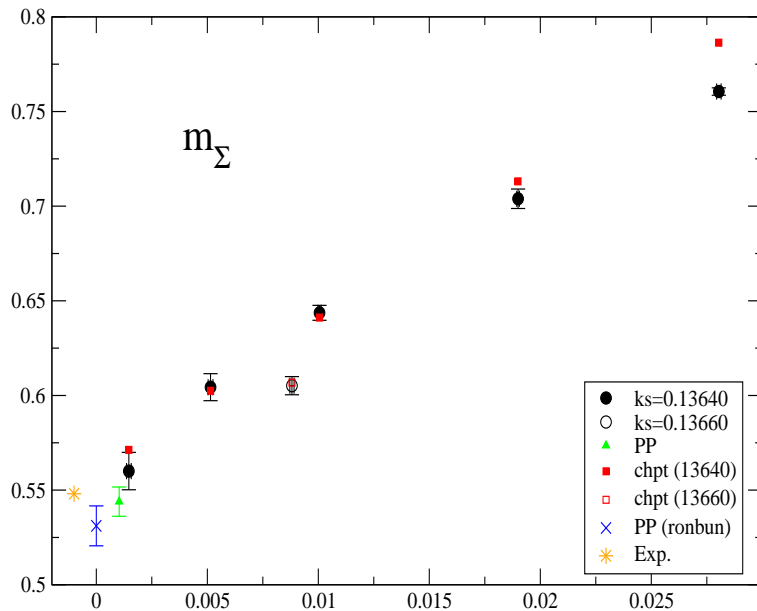
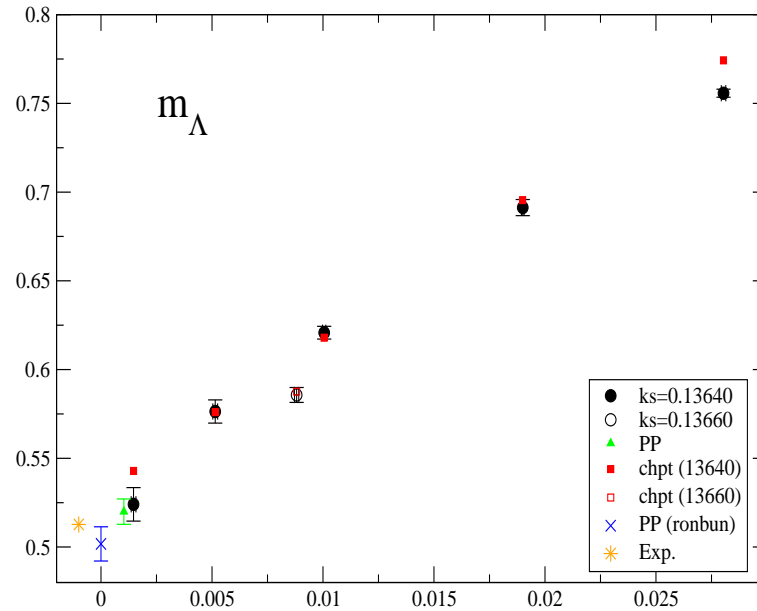
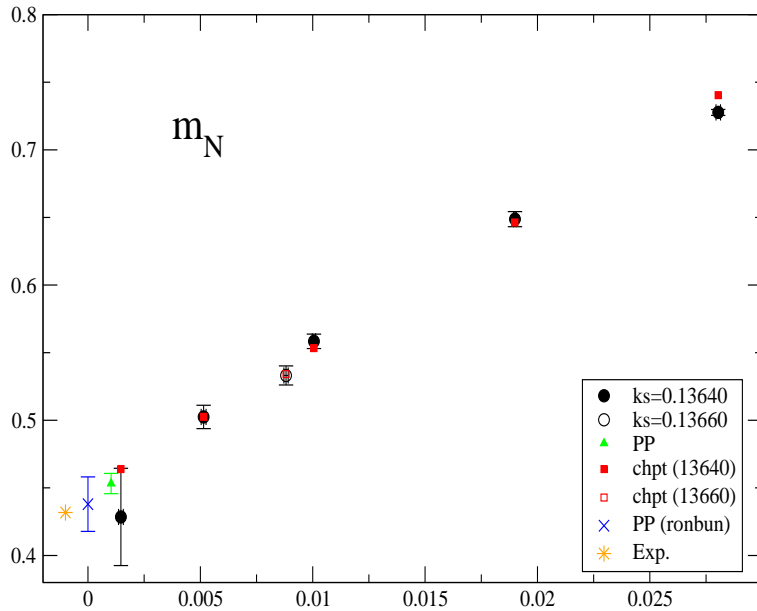
We need

- ★ Nonperturbative renormalization factors to remove perturbative uncertainties,
- ★ To investigate the finite size effects and the discretization errors.

Linear fit for the vector meson masses



Linear fit for the octet baryon masses



Linear fit for the decuplet baryon masses

