Approaching the Chiral Limit with Dynamical Overlap Fermions

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1.1 introduction: JLQCD collaboration

- JLQCD: studying lattice QCD using computers at KEK
- members:

KEK:	S.Hashimoto, TK, M.Matsufuru, M.Okamoto, N.Yamada
RIKEN:	H.Fukaya
YITP:	T.Onogi
Tsukuba:	S.Aoki, K.Kanaya, A.Ukawa, T.Yoshie
Hiroshima:	K-I.Ishikawa, M.Okawa

- – 2005: w/ Hitachi SR8000/F1 (1.2TFLOPS)

  $N_f = 2$, $a^{-1} \simeq 2$ GeV, plaq. + NP clover

  $N_f = 2+1$, $a \to 0$, Iwasaki + NP clover (w/ CP-PACS Collab.)

  - heavy sea quark masses $m_{\rm ud} \gtrsim m_{s,\rm phys}/2$
  - chiral symmetry breaking $\Rightarrow$ haven't calculated B_K, ...

1.2 new supercomputer system @ KEK

- new machines were installed at KEK this year

Hitachi SR11000

- 16 nodes
- 2.15 TFLOPS
- 512 GB memory

IBM Blue Gene/L

- 10,240 nodes
- 57.3 TFLOPS
- 5 TB memory

1.3 JLQCD's new project

large-scale simulations with dynamical overlap fermions

- target simulation parameters:
  - $a \lesssim 0.125$ fm, $L \gtrsim 2$ fm
  - lightest $m_{ud} \lesssim m_{s,\mathrm{phys}}/4$
  - $O(10,000)$ HMC trajectories
  - $N_f = 2,\ 2+1$ QCD
- this talk: overview of first production run in two-flavor QCD

  $a \sim 0.125$ fm, $L \sim 2$ fm, $m_{ud} \gtrsim m_{s,\mathrm{phys}}/6$

  for details, see proceedings for Lattice 2006:

  S.Hashimoto, N.Yamada, H.Matsufuru, H.Fukaya, TK
- talk by Matsufuru: extension to $N_f = 2+1$ QCD

1. introduction

– confi guration generation –

2. lattice action
3. simulation algorithm
4. production run

5. static potential
6. meson masses / decay constant

7. summary

2.1 lattice action: quarks

- quark action = overlap w/ std. Wilson kernel

$$S_q = \bar{q}\, D_{\rm ov}\, q,$$
$$D_{\rm ov} = \left(m_0 + \frac{m}{2}\right) + \left(m_0 - \frac{m}{2}\right) \gamma_5\, {\rm sgn}[H_{\rm w}(-m_0)], \quad m_0 = 1.6$$

- w/ std. Wilson kernel $H_{\rm W}$ $\Rightarrow$ (near-)zero modes of $H_{\rm W}$
  - zero modes $\Rightarrow$ discontinuity in S_q
    $\Rightarrow$ reflection/refraction *(Fodor-Katz-Szabo, 2003)*
  - extended modes w/ small mobility edge λ_c
    $\Rightarrow$ spoil locality of $D_{\rm ov}$
  - near-zero modes $\Rightarrow$ expensive approx. for ${\rm sgn}[H_{\rm W}]$

2.2 gauge action

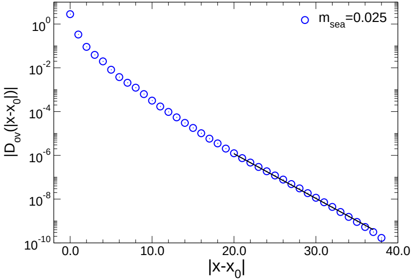
- preparatory study for $N_f = 0$
  - plaquette / admissibility / Iwasaki gauge actions
  - no extended zero modes at $a \sim 0.125$ fm
  - Iwasaki gauge:
    local: reduced density $\rho(\lambda)$
    extended: $\lambda_c \approx 600$ MeV
  - exp.locality of $D_{\rm ov}$

$\Downarrow$

employ Iwasaki gauge

- exp. locality for $N_f = 2$

$|D_{\rm ov}(x,y)\,\delta(y-x_0)|$ vs $|x-x_0|$



local.range $\approx (800 \text{ MeV})^{-1}$

2.3 extra-Wilson fi elds

- even w/ impr.gauge action

  $\Rightarrow$ $\lambda[H_W]$ can cross zero

  $\Rightarrow$ time consuming reflection/refraction

- suppress (near)zero modes by extra fields

  Vranas, 2000; RBC, 2002 (DWF); JLQCD, 2006 (ovr)

  - two flavors Wilson fermion $\Rightarrow$ suppress zero modes
  - two flavors of twisted mass ghost ($\mu = 0.2$)

    $\Rightarrow$ suppress effects of higher modes

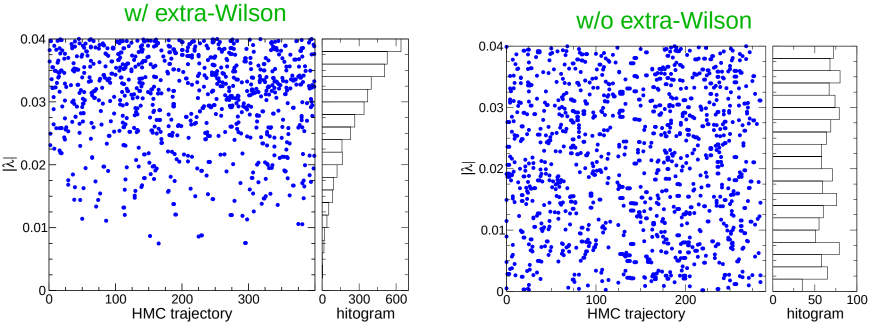
$$\text{Boltzmann weight} \propto \frac{\det[H_W(-m_0)^2]}{\det[H_W(-m_0)^2 + \mu^2]}$$

  - extra-fi elds : mass $\propto a^{-1}$

    $\Rightarrow$ do not change the continuum limit

2.3 extra-Wilson fi elds

- example of $\lambda[H_W]$ $(N_f = 2,\ a \sim 0.1\,\text{fm},\ m_{\text{sea}} \sim m_{\text{s,phys}})$



- extra-fields: fix global topology during HMC
  - do NOT forbid local topological fluctuations
  - effects have to be studied *(Brower et al., 2003)*

3.1 algorithm: multiplication of $D_{\rm ov}$ / solver

- multiplication of $D_{\rm ov} \Rightarrow {\rm sgn}[H_{\rm W}]$
  - $\sigma[H_W] \Rightarrow [\lambda_{\rm min}, \lambda_{\rm thrs}] \cup [\lambda_{\rm thrs}, \lambda_{\rm max}]$
  - low mode preconditioning
    eigenmodes w/ $\lambda \in [\lambda_{\rm min}, \lambda_{\rm thrs}] \Rightarrow$ projected out
  - Zolotarev approx. of ${\rm sgn}[H_W]$ for $\lambda \in [\lambda_{\rm thrs}, \lambda_{\rm max}]$
    $N = 10 \Rightarrow$ accuracy of $|1 - {\rm sgn} H_W{}^2| \lesssim 10^{-7}$
- $D_{\rm ov}$ solver
  - 4D nested solver
    - inner: partial fraction + multi-shift CG *(Frommer et al., 1995)*
    - outer: relaxed CG *(Cundy et al., 2004)*
      factor ∼2 faster than unrelaxed CG
    - haven't tried recursive preconditioning *(Cundy et al., 2004)*

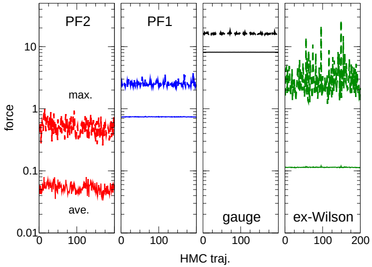
3.2 HMC w/ 4D solver

- Hasenbusch preconditioning *(Hasenbusch, 2001)*

$$\det[D_{\rm ov}(m)^2] \quad = \quad \det[D_{\rm ov}(m')^2] \det\left[\frac{D_{\rm ov}(m)^2}{D_{\rm ov}(m')^2}\right] = \text{“PF1”} \cdot \text{“PF2”}$$

- multiple time scale in MD *(Sexton-Weingargen, 1992)*
- switch off reflection/refraction step $\Rightarrow$ about factor 3 faster

force (ave,max) at $m_{\rm sea} = 0.015$



- hierarchy in force
  PF2 $\ll$ PF1 $\ll$ gauge $\approx$ ex-Wilson
- 3 nested loops for MD
  - PF2: outer-most loop
  - PF1: intermediate
  - gauge, ex-Wilson: inner-most

3.3 HMC w/ 5D $D_{\rm ov}$ solver

- 5D solver *(Boriçi, 2004; Edwards et al.,2005)*
  - 5D representation of overlap *(Boriçi, 1999)*
  - even-odd preconditioning: implemented
  - low mode preconditioning: not yet
- HMC w/ 5D solver

$$\det[D_{\rm ov}(m)^2] = \det[D_{\rm ov,5D}(m')^2] \det\left[\frac{D_{\rm ov,5D}(m)^2}{D_{\rm ov,5D}(m')^2}\right] \det\left[\frac{D_{\rm ov}(m)^2}{D_{\rm ov,5D}(m)^2}\right]$$

$$= \text{“PF1”} \cdot \text{“PF2”} \cdot \text{“noisy Metropolis test”}$$

  - suffi ciently high “N_s” to achieve reasonable $P_{\rm HMC}$
  - factor 2 faster than HMC w/ 4D solver

4.1 production run: parameters

- $N_f = 2$ QCD
- Iwasaki-gauge + overlap + extra-Wilson ($\mu = 0.2$)
- $\beta = 2.30 \Rightarrow a \approx 0.125$ fm

  preparatory studies at $\beta = 2.35, 2.50$

  - 1000 traj., $a \simeq 0.10 - 0.11$ fm
- $16^3 \times 32$ lattice $\Rightarrow L \simeq 2$ fm
- 6 sea quark masses $\in [m_{s,\mathrm{phys}}/6, m_{s,\mathrm{phys}}]$

  $m_{\mathrm{sea}} = 0.015, 0.025, 0.035, 0.050, 0.070.0.100$
- $\tau = 0.5$: 1 HMC trajectory

  larger τ is better? (*RBC, 2006; ALPHA, 2006*)
- $Q = 0$ (runs w/ $Q \neq 0$ are on-going)

4.2 runs w/ 4D solver HMC

- Hasenbusch preconditioning + multiple time scale

$$\det[D_{\rm ov}(m)^2] \; = \; \det[D_{\rm ov}(m')^2] \, \det\left[\frac{D_{\rm ov}(m)^2}{D_{\rm ov}(m')^2}\right] \; = \text{“PF1”} \cdot \text{“PF2”}$$

PF2 : $N_{\rm MD}$ times / traj. PF1 : $(N_{\rm MD} \cdot R_{\rm PF})$ / traj.

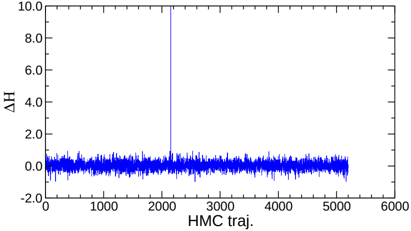
gauge, extra-Wilson : $(N_{\rm MD} \cdot R_{\rm PF} \cdot R_{\rm G})$ / traj.

$m_{\rm sea}$	$N_{\rm MD}$	$R_{\rm PF}$	$R_{\rm G}$	m'	traj.	$P_{\rm HMC}$	$M_{\rm PS}/M_{\rm V}$	time[min]
0.015	9	4	5	0.2	2800	0.89	0.34	6.1
0.025	8	4	5	0.2	5200	0.90	0.40	4.7
0.035	6	5	6	0.4	4600	0.74	0.46	3.0
0.050	6	5	6	0.4	4800	0.79	0.54	2.6
0.070	5	5	6	0.4	4500	0.81	0.60	2.1
0.100	5	5	6	0.4	4600	0.85	0.67	2.0

4.3 basic properties of HMC

area preserving

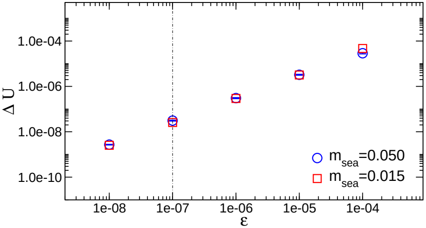
ΔH at $m_{\rm sea}=0.025$



- a few spikes per $O(5,000)$ trajectories: $P_{\rm spike} < 0.1$ %
- $\langle\exp[-\Delta H]\rangle = 1$ in all runs
- does not need "replay" trick

reversibility

ΔU vs ϵ



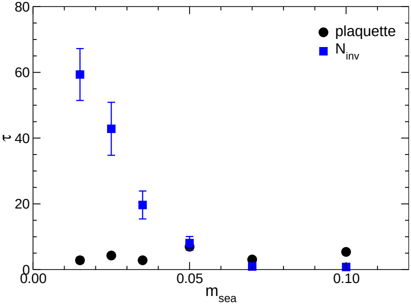
$$\Delta U = \sqrt{\sum |U(\tau+1-1) - U(\tau)|^2 / N_{\rm dof}}$$

ϵ : stop. cond. for MS/overlap solver

- $\Delta U \lesssim 10^{-8}$: comparable to previous simulations

4.4 autocorrelation

$\tau_{\rm int}$ vs $m_{\rm sea}$



- plaquette: local

  $\Rightarrow$ small m_q dependence

- $N_{\rm inv,H}$: long range

  $\Rightarrow$ rapid increase as $m_q \to 0$

- accumulate 10,000 trajectories $\simeq 100$ conf

  $\Rightarrow$ precise determination of matrix elements:

4.5 runs w/ 5D solver HMC

m_{sea}	N_{MD}	R_{PF}	R_G	m'	traj	P_{HMC}	time[min]	traj_{total}
0.015	13	6	8	0.2	6480	0.68	2.6	9280
0.025	10	6	8	0.2	4800	0.82	2.2	10000
0.035	10	6	8	0.4	4810	0.87	1.5	9410
0.050	9	6	8	0.4	4730	0.87	1.3	9530
0.070	8	6	8	0.4	4390	0.90	1.1	8890
0.100	7	6	8	0.4	3260	0.91	1.0	7860

- N_{MD}: mild dependence of on m_{sea}

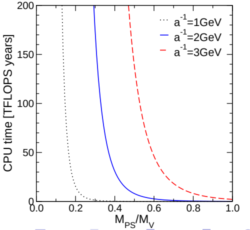
  $\Leftrightarrow$ $N_{MD} \propto 1/m_{sea}$ for "Berlin wall" in CPU time

- whole BG/L (10 racks) $\times$ 1 month

  $\Rightarrow$ 4000 traj. at all m_{sea}

- 8000 – 10000 traj.

for clover: A.Ukawa @ Lattice2001 (Berlin)



4.6 on-going calculations

simultions with $Q \neq 0$

$m_{\rm sea}$	Q	$N_{\rm MD}$	$R_{\rm PF}$	$R_{\rm G}$	m'	traj$_{\rm total}$	$P_{\rm HMC}$
0.050	-2	9	6	8	0.4	3480	0.89
0.050	-4	9	6	8	0.4	380	0.88

measurements

Q	0						-2
$m_{\rm sea}$	0.015	0.025	0.035	0.050	0.070	0.100	0.050
conf	928	1000	941	953	889	786	348
pot.	780	920	910	880	800	760	260
had.	173	410	403	310	243	319	–

- using configurations every 10 trajectories
- static potential: $\approx$ current statistics
- hadron correlators: on going

1. introduction
2. lattice action
3. simulation algorithm
4. status

– preliminary results –

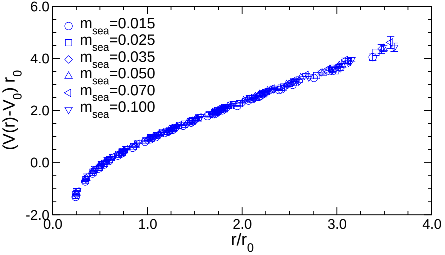
5. static potential
6. meson masses / decay constant

7. summary

5.1 static quark potential

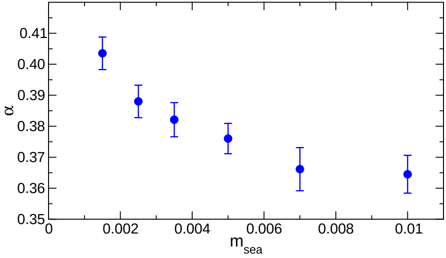
- $V(r)$: smeared Wilson loops $W(r,t) = c(r)\ \exp[-V(r)\,t]$
- r_0: $V(r) = V_0 - \alpha/r + \sigma\, r \Rightarrow r_0 = \sqrt{(1.65-\alpha)/\sigma}$

$V(r)$ vs r ($Q=0$)



- almost lie on a single curve

α vs $m_{\rm sea}$



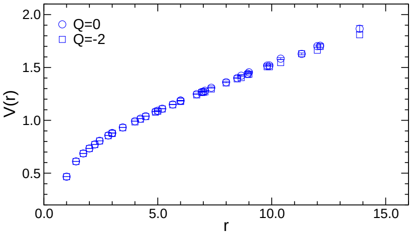
- larger α $\Leftarrow$ smaller $m_{\rm sea}$
  (*SESAM/TχL, CP-PACS, MILC, RBC*)

5.2 lattice spacing from r_0

systematic error in r_0

- choice of fi t range: small ($\lesssim 1$ %) and included
- fi xed Q: small (?)

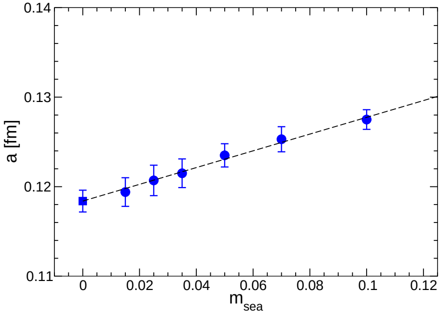
at $m_{\rm sea} = 0.050$



$$Q=0: \quad r_0 = 3.97(4)$$
$$Q=-2: \quad r_0 = 3.99(7)$$

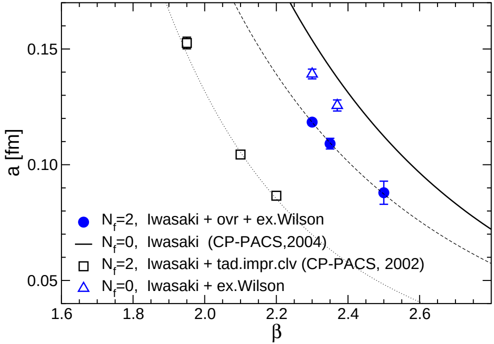
chiral extrapolation

- $a_{r_0} = A_{r_0} + B_{r_0}\, m_{\rm sea}$
- $r_0 = 0.49$ fm $\Rightarrow a = 0.1184(12)$ fm



5.3 β shift

- inclusion of dynamical fermion
  $\Rightarrow$ smaller β with a fixed $\Rightarrow$ unphysical phase trans. (?)
  (T.Blum et al., 1994; F.Farchioni et al., 2004; JLQCD, 2004)
- in our simulations : due to overlap and extra-Wilson



- due to overlap:
  $\Delta\beta \approx 0.10$
- due to extra-Wilson:
  $\Delta\beta \approx 0.05$
- significantly smaller than tad.impr. clover
  $\Delta\beta \approx 0.40$

6.1 meson masses: effective mass

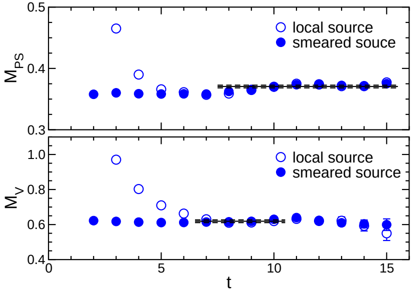
- very preliminary!!

  # independent conf.: ~ 20 conf at $m_{\rm sea} = 0.015$,

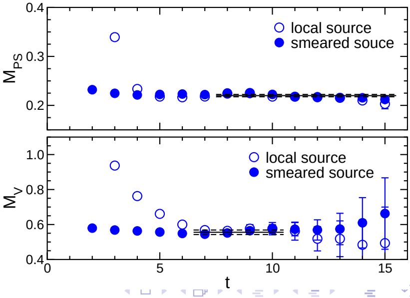
  $\gtrsim 50$ conf at $m_{\rm sea} \geq 0.025$

- local and exponential smeared source: $\phi(r) = a\, \exp[-b\, r]$

$m_{\rm sea} = 0.070$ (2nd heaviest)



$m_{\rm sea} = 0.025$ (2nd lightest)



6.1 meson masses: chiral extrapolation

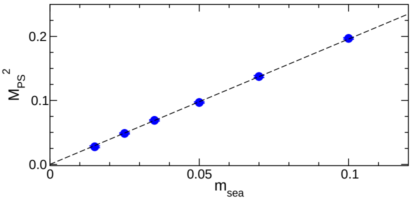
- with current statistics
  no significant deviation from simple linear fit

$$M_{\rm PS}^2 = B_{\rm ps}\, m_{\rm sea}$$
$$M_{\rm V} = A_{\rm v} + B_{\rm v}\, M_{\rm PS}^2$$
$$\Rightarrow \chi^2/{\rm dof} \lesssim 1.0$$

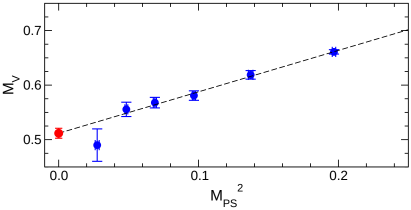
- a from M_ρ
  $a = 0.1312(23)$ fm
  $\sim a_{r_0}$ with 10 % accuracy

- FSE?
  $M_{\rm PS}\, L \gtrsim 2.6$
  $\Rightarrow$ FSE $\propto \exp[-M_{\rm PS}\, L] \approx 1-2\%$

$M_{\rm PS}^2$ vs $m_{\rm sea}$



$M_{\rm V}$ vs $M_{\rm PS}^2$

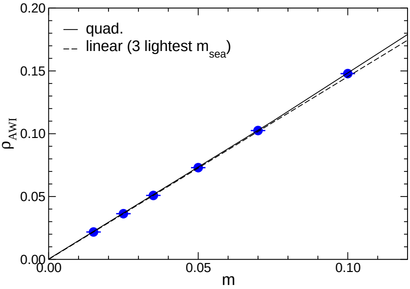


6.2 chiral symmetry breaking

- ratio from AWI

$$\rho_{\rm AWI} = \frac{\langle \nabla_4 A_4 P^\dagger \rangle}{\langle P P^\dagger \rangle} = A_{\rm AWI} + B_{\rm AWI}\, m + C_{\rm AWI}\, m^2 + \ldots$$

$\rho_{\rm AWI}$ vs m



- $A_{\rm AWI}$

  quad.: $-0.00026(11)$

  linear (3 lighter $m_{\rm sea}$): $-0.00001(12)$

  $\Rightarrow$ small symmetry breaking

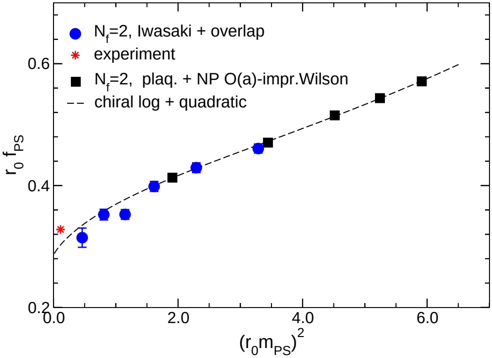
- $B_{\rm AWI}$

  $Z_A = 2/B_{\rm AWI} = 1.398(5)(23)$

6.3 decay constant

- with NP Z_A from AWI

$r_0\, f_{\rm PS}$ vs $(r_0\, m_{\rm PS})^2$



- at heavy $m_{\rm sea}$
  consistent with prev. results
  $\Rightarrow$ small scaling violation (?)

- at small $m_{\rm sea}$
  $m_{\rm sea}$-dep. is not smooth
  $\Leftarrow$ small statistics

6.4 on-going measurement

restarting measurements w/ the following method...

- 100 lowest eigenpairs (λ_k, u_k) of $D_{\rm ov}$ ($\lesssim 3$ min./1conf/BGL)

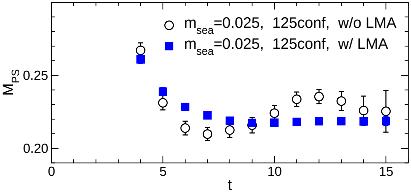
$$(D_{\rm ov}^{-1})_{\rm L} = \sum_k \frac{1}{\lambda_k} u_k u_k^\dagger$$

- low mode preconditioning for $D_{\rm ov}$ solver: 8 times faster
- low mode averaging for 2-pt. function

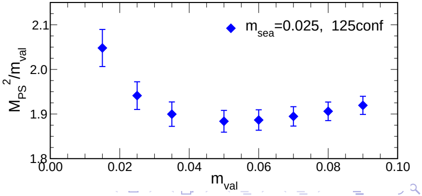
$$C^{(\rm had)}(x';x) = C_{\rm LL}^{(\rm had)}(x';x) + C_{\rm LH}^{(\rm had)}(x';x) + C_{\rm HL}^{(\rm had)}(x';x) + C_{\rm HH}^{(\rm had)}(x';x)$$

$C_{\rm LL}^{(\rm had)}(x';x)$: take average over source points

$M_{\rm PS,eff}$ (only 1250 traj)



test of PQChPT log (only 1250 traj)



7. summary

- JLQCD's dynamical overlap project
  - 4000traj/month at 6 $m_{\rm sea}$'s at $a \approx 0.125$ fm, $L \approx 2.0$
    - action: Iwasaki + overlap + extra-Wilson
    - algorithm: Hasenbusch + multiple time scale MD + $\cdots$
  - autocorrelation $\Rightarrow$ accumulate 10,000 traj. at each $m_{\rm sea}$
  - preliminary results: no clear sign of chiral log
- future prospects
  - measurements have to be completed w/ LMA
    spectrum, matrix elements ($f_{\{\pi,K\}}$, B_K, $f_{\{+,0\}}^{K\to\pi}(q^2)$,...)
  - effects due to fixed topology
    runs w/ $Q\neq 0 \Rightarrow Q$-dependence
    fixed topology $\Rightarrow \epsilon$-regime
  - extension to $N_f=3$ *(talk by Matsufuru)*, larger volumes