Large-scale simulations with chiral symmetry

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1. introduction

chiral fermions

- theoretically clean : straightforward for various subjects

  overlap simulations w/ exact symmetry $|1 - \mathrm{sgn}[H_W]|^2 \lesssim 10^{-8}$

  - QCD vacuum ($\langle \bar{q}q \rangle$, χ_t, $\Pi_{\{VV,AA\}}$, ...)
  - light hadron physics ($F_{\{K,\pi\}}$, $F_V^{\{\pi,K,K\pi\}}$, $\pi \to \gamma\gamma$, $\langle N|\bar{q}q|N \rangle$, ...)

    $\Rightarrow$ *talks and poster by X. Feng and T. Iritani*

- computationally demanding

  overlap : $\times 100$; standard DWF : $m_{\mathrm{res}} \approx$ a few MeV @ $a^{-1} \approx 2$ GeV

- not unique

$$D_{\mathrm{eff}} = \frac{1}{2}(1 + \gamma_5\, \mathrm{sgn}[\, H_X \,])$$

this talk

- a comparative study of 5D domain-wall-type formulations

  computationally cheap w/ negligibly small $m_{\mathrm{res}} \ll m_{ud,\mathrm{phys}}$

- status of production runs with our choice of action

comparative study

2.1 setup

DWF formulations

Kaplan, 1992; Shamir, 1993; Furman-Shamir, 1995; Edwards-Heller 2001; Boriçi, 1999; Chiu, 2003; Brower-Neff-Orginos, 2005, ...

$$D_{DW} = D_{+,s}\delta_{s,s'} + D_{-,s}P_+\delta_{s-1,s'} + D_{s,-}P_-\delta_{s+1,s'} \quad \text{w/} \quad D_{\pm,s} = c_{\pm,s}D_W \pm 1$$

$$\Rightarrow \quad D_{\rm eff} = \frac{1}{2}\left(1 + \gamma_5 {\rm sgn}[H_M]\right)$$

- popular choices

$$H_M = \gamma_5 \frac{(c_+ + c_-)D_W}{2 + (c_+ - c_-)D_W} \quad \rightarrow \quad H_W, \quad H_T = \gamma_5 \frac{D_W}{2 + D_W}, \quad 2H_T$$

$${\rm sgn}[H_M] \quad \rightarrow \quad \text{Zolotarev}, \quad \text{polar} = \frac{(1+H_M)^{N_5} - (1-H_M)^{N_5}}{(1+H_M)^{N_5} + (1-H_M)^{N_5}}$$

- test 8 choices w/o and w/ (stout) smearing

thin-link : H_W + Zolo(tarev), H_T + Zolo, H_T + polar, $2H_T$ + polar

$N_{\rm smr} = 3$: H_W + Zolo, H_T + polar, $2H_T$ + polar

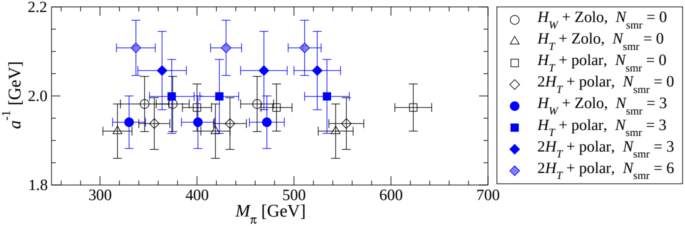
$N_{\rm smr} = 6$: $2H_T$ + polar

$\Rightarrow$ MD efficiency, $m_{\rm res}$, topological tunneling

2.1 setup

setup

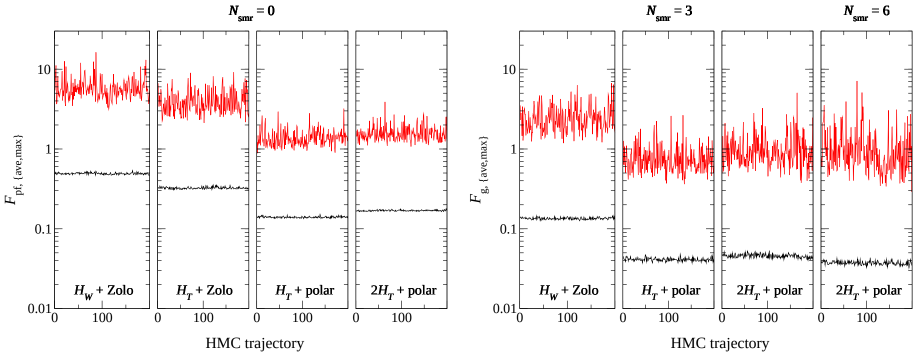
- $N_f = 2$
- tree-level Symanzik gauge
  - compatible w/ $O(a^2)$ improvements for heavy quarks $\Rightarrow$ *talk by Y-G.Cho*
- single small volume : $16^3 \times 32 \times 12$
- (roughly) constant physics : $a^{-1} \sim 2$ GeV, $M_\pi \sim 300-600$ MeV
- leap-frog / multi-time-scale MD : $N_{\rm MD,gauge} = 10 N_{\rm MD}$
- $\tau = 1$, $N_{\rm MD} \Rightarrow P_{\rm HMC} \approx 0.7-0.9$
- 1000 traj at each (β, m_{ud})



2.2 MD efficiency

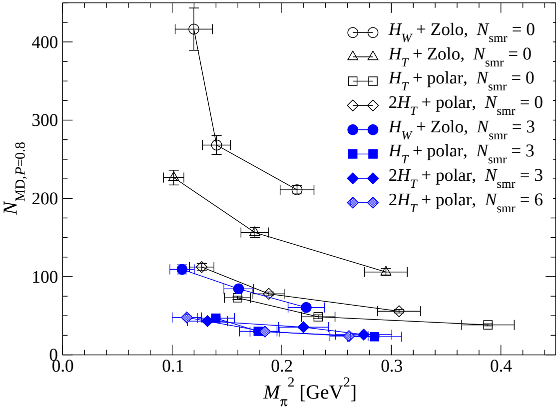
MD forces

- no big difference in gauge force
- fermionic force (strongly) depends on choice of quark action



2.2 MD efficiency

#MD steps to achieve $P_{\rm HMC} = 0.80$: $N_{{\rm MD},P=0.80}$



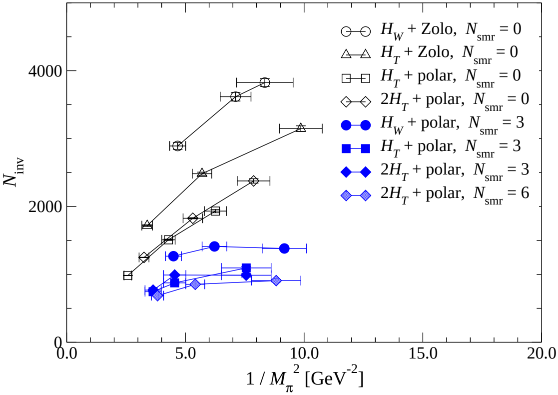
- $P_{\rm HMC} = {\rm erfc}(\sqrt{\langle \Delta H \rangle}/2)$
- $\langle \Delta H \rangle \propto 1/N_{\rm MD}^4$

  $\Rightarrow \quad N_{{\rm MD},{\rm P}_{\rm HMC}=0.8}$

- $H_W \to (2)H_T$, Zolo $\to$ polar $\Rightarrow$ $\times 1.5-2.0$ speed-up
- no big difference between H_T and $2H_T$
- smearing $\times\ 3$ $\Rightarrow$ $\times 2$ speed-up; no significant acceleration w/ larger $N_{\rm smr}$

2.2 MD efficiency

iteration count for CGNE : $N_{\rm inv}$



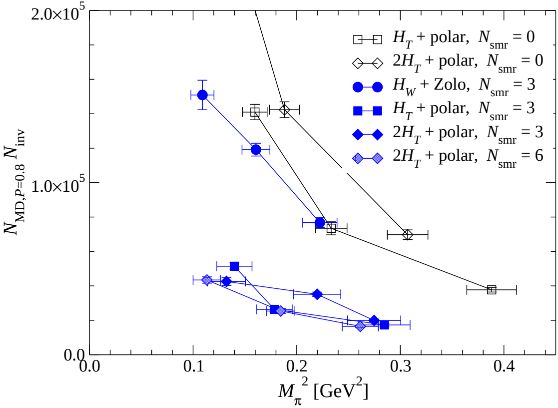
finite V effects at $M_\pi \lesssim 300$ MeV?

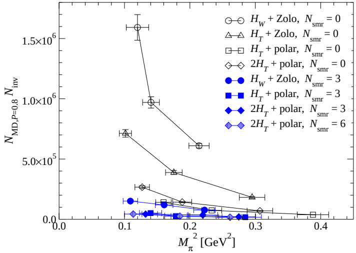
($M_\pi L \approx 2.4$)

- decreases by $H_W \to (2)H_T$, Zolo $\to$ polar, $N_{\rm smr} = 0 \to 3$
- no big difference between H_T and $2H_T$ / $N_{\rm smr} = 3$ and 6

2.2 MD efficiency

a measure of cost / traj : $N_{\mathrm{MD},P=0.8} N_{\mathrm{inv}}$



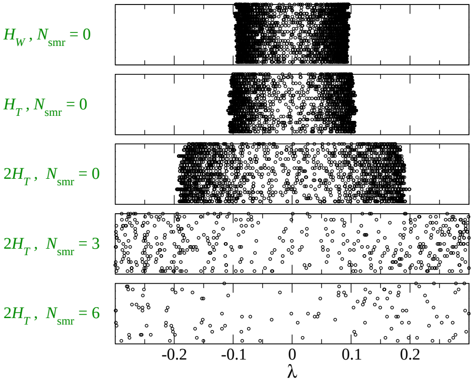


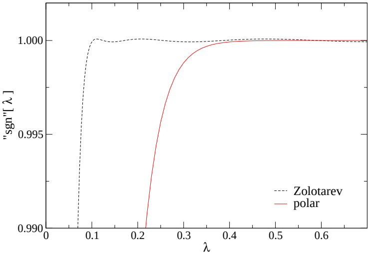
- H_W + Zolo is very costly
- H_W + Zolo $\to$ $(2)H_T$ + polar $\Rightarrow$ $\times$ 6 speed-up
- smearing $\Rightarrow$ $\times$ 3 – 4 speed-up

2.3 residual quark mass

low-lying mode distribution for kernels

lowest 100 – 150 eigenmodes

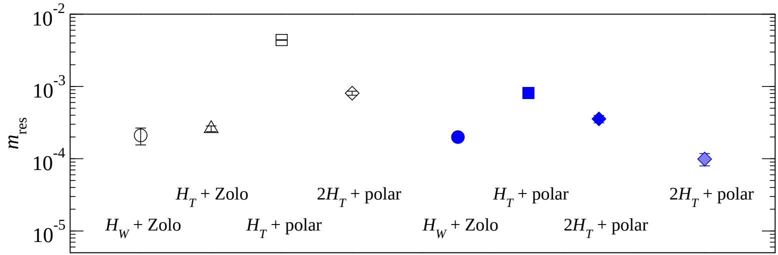




- $|1-\text{polar}^2| \gg |1-\text{Zolo}^2|$ @ $|\lambda| \lesssim 0.3$
- less low-modes in this region by $H_T \to 2H_T$ and larger $N_{\rm smr}$

2.3 residual quark mass

residual quark mass $m_{\rm res}$

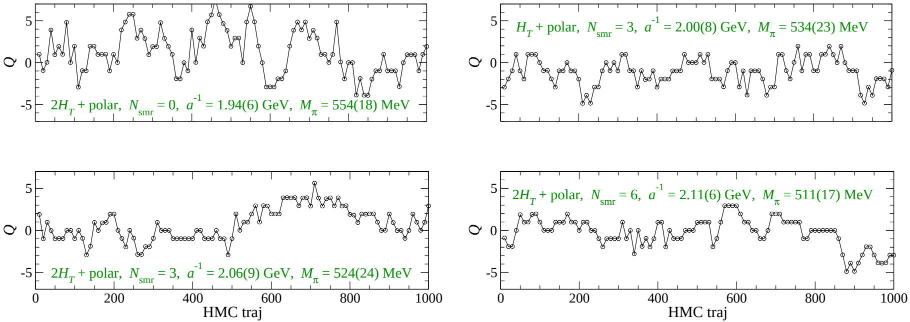


- Zolotarev $\Rightarrow$ least $m_{\rm res}$ at given N_5, $N_{\rm smr}$, but expensive...
- H_T + polar $\Rightarrow$ an order magnitude larger $m_{\rm res}$
- $m_{\rm res} < 1$ MeV with $2H_T$ + polar + $N_{\rm smr} = 3$
  - halved by $H_T \rightarrow 2H_T$ (*Brower-Neff-Orginos, 2012*)
  - $N_5 = O(10)$ is sufficient
- larger $N_{\rm smr}$ is better, if there is no side effects
- more detailed discussion (N_5 dependence, ...) $\Rightarrow$ *poster by S.Hashimoto*

2.4 topological tunneling

topological charge history

from $F\tilde{F}$ + cooling



- topology changes with any of tested formulations
- $H_T \rightarrow 2H_T$, larger $N_{\rm smr}$ $\Rightarrow$ less near-zero modes ... and less tunneling?

  $\Rightarrow$ no @ $a^{-1} \approx 2$ GeV

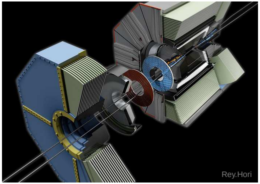
production runs

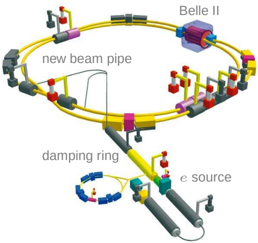
3.1 plan

project : light + heavy quark physics ... on fine lattices w/ good chiral symmetry

- $N_f = 2+1$ QCD
- tree-level Symanzik gauge + DW quarks
  - $2H_T$ + polar + $N_{\rm smr} = 3$
  - $m_{\rm res} \sim 0.1$ MeV $\ll m_{ud,\rm phys}$
- 4 lattice spacings : $a^{-1} \approx 2.4,\ 3.0,\ 3.6,\ 4.8$ GeV
  - $O((am_c)^2) \sim 10-30\%$

    $\Rightarrow$ $O((am_c)^4) \sim 1-9\%$, $O(\alpha(am_c)^2) \sim 3-9\%$
- $M_\pi L \gtrsim 4$, $32^3 \times 64$ – $64^3 \times 128$
- $M_\pi = 500,\ 400,\ 300$ MeV and smaller ($\lesssim 220$ MeV)
- 3000 HMC trajectories or more





SuperKEKB/Belle-II @ KEK

runs @ $a^{-1} \simeq 2.4$ and 3.6 GeV are in progress

3.2 algorithm

- RHMC for strange flavor (*Horváth-Kennedy-Sint, 1998; Clark-Kennedy-Sroczynski, 2004*)

- Hasenbusch preconditioning for light two flavors

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

$$\det\left[D(m_{ud})\right]^2 \det\left[D(m_s)\right] = \det\left[\frac{D(m_{ud})}{D(m')}\right]^2 \det\left[D(m_s)\right] \det\left[D(m')\right]^2$$

$$= \det\left[D[\phi_1]\right]^2 \det\left[D[\phi_2]\right] \det\left[D[\phi_3]\right]^2$$

- leap-frog (2LF) $\Rightarrow$ Omelyan (2MN) (*Omelyan,2003; Takaishi-de Forcrand, 2005*)

- 4 MD step sizes for $\phi_{1,2,3}$ and gauge

- we are still tuning algorithm / code...
  - less accurate $(D^\dagger D)^{-1}$, D^{-1} during MD, ...

- machine : IBM BlueGene/Q @ KEK
  - 1.2 PFLOPS / 6 racks
  - ≈ 8 % sustained speed for HMC (being improved)

more details $\Rightarrow$ *poster by G.Cossu*

BlueGene/Q @ KEK

3.3 status

$32^3 \times 64 \times 12$ @ $a^{-1} = 2.4$ GeV

m_{ud}	m_s	MD	N_{MD}	traj	P_{HMC}	$\langle \Delta H \rangle$	$\langle e^{-\Delta H} \rangle$	min/traj
0.019	0.040	2LF	10	3000	0.78(1)	0.19(1)	0.99(1)	2.7
0.012	0.040	2LF	13	2000	0.78(1)	0.17(1)	1.00(1)	3.5
0.012	0.040	2MN	3	1000	0.89(1)	0.07(2)	1.01(1)	2.0
0.007	0.040	2LF	16	1000	0.74(1)	0.23(2)	1.04(3)	4.4
0.007	0.040	2MN	4	2000	0.90(1)	0.06(1)	1.00(1)	2.6
0.019	0.030	2LF	10	3000	0.79(1)	0.17(1)	1.00(1)	2.8
0.012	0.030	2LF	16	2000	0.79(1)	0.14(1)	1.02(2)	3.6
0.012	0.030	2MN	3	1000	0.88(1)	0.10(3)	1.00(2)	2.0
0.007	0.030	2LF	16	2000	0.72(1)	0.27(2)	1.00(2)	4.5
0.007	0.030	2MN	4	1000	0.89(1)	0.08(2)	0.99(1)	2.6

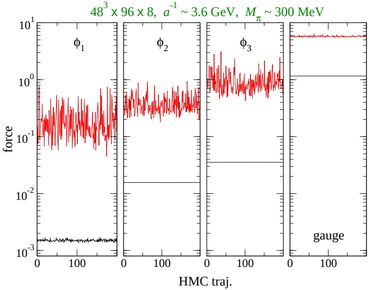
- leap-frog (2LF) $\rightarrow$ Omelyan (2MN) $\Rightarrow$ $\times 2$ speed-up
- we have accumulated 3000 traj. @ $M_\pi \simeq 300, 400, 500$ MeV
  - our choice of action $\Rightarrow$ 1 month job on BG/Q @ KEK
  - now, pushed down to $M_\pi = 220$ MeV on $48^3 \times 96 \times 12$

3.3 status

$48^3 \times 96 \times 8$ @ $a^{-1}=3.6$ GeV

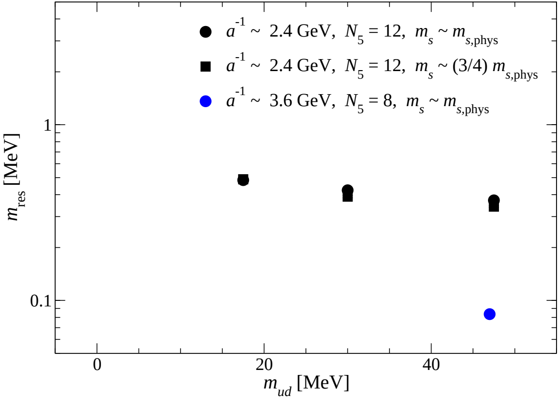
m_{ud}	m_s	m'	$N_{\rm MD}$	traj	$P_{\rm HMC}$	$\langle\Delta H\rangle$	min/traj
0.0120	0.0250	0.10	4	430	0.84(2)	0.10(2)	3.6
0.0080	0.0250	0.08	4	330	0.85(2)	0.06(2)	4.2
0.0042	0.0250	0.04	4	235	0.92(3)	0.04(2)	5.9
0.0120	0.0180	0.10	4	–	–	–	–
0.0080	0.0180	0.08	4	260	0.86(1)	0.05(1)	4.3
0.0042	0.0180	0.04	4	280	0.86(3)	0.02(2)	6.0

- preliminary runs w/ $\tau = 1$
  - $\Rightarrow$ $\tau = 2$ to reduce auto-correlation
- tune m' at each m_{ud}
  - $\Rightarrow$ small m_{ud}-dep. of $N_{\rm MD}$ w/ $P_{\rm HMC} \gtrsim 0.8$
- will be a two-month job @ KEK
- observables from these runs $\Rightarrow$ *talk by J.Noaki*



3.4 chiral symmetry violation

residual mass



$$m_{\rm res} = \frac{\langle D_{\rm eff}^{\dagger,-1} \Delta D_{\rm eff}^{-1} \rangle}{\langle D_{\rm eff}^{\dagger,-1} D_{\rm eff}^{-1} \rangle}$$

$$2\gamma_5 \Delta = \{\gamma_5, D_{\rm eff}\} - 2 D_{\rm eff} \gamma_5 D_{\rm eff}$$

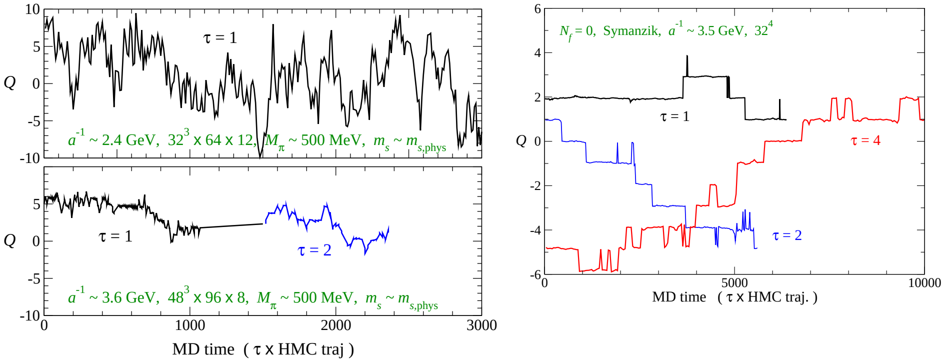
- a crude estimate of Z_m

  $\Leftarrow$ $m_{s,\rm phys} = 94$ MeV (*FLAG*)

- $m_{\rm res} \lesssim 0.5$ MeV at $a^{-1} \simeq 2.4$ GeV $< m_{ud,\rm phys} < m_{ud,\rm sim}$
- $m_{\rm res} \lesssim 0.1$ MeV at 3.6 GeV $\ll m_{ud,\rm phys} < m_{ud,\rm sim}$
- reweight to overlap ($\rm sgn$ = Zolo) w/ exact symmetry $\Rightarrow$ *talk by H.Fukaya*

3.5 auto-correlation

topological charge history



- (much) larger autocorrelation time at smaller a (Q, $t^2 E$ @ large t)
- pure gauge test : more tunneling w/ larger τ

  (⇔ *Meyer et al., 2006; Schäfer-Sommer-Virotta, 2010; Lüscher-Schäfer, 2011*)
- τ has been doubled ($\tau = 1 \rightarrow 2$) and accumulating statistics...

4. summary

JLQCD's new project of large-scale simulations with good chiral symmetry

- systematic study on MD efficiency, $m_{\rm res}$, ... $\Rightarrow$ $2H_T$ + polar + $N_{\rm smr}=3$
  - computationally cheap chiral fermions : 3000 traj on $48^3\times96\times8$ / 2 months
  - small chiral symmetry violation : $m_{\rm res}\lesssim0.1$ MeV @ $a^{-1}\gtrsim3$ GeV
    $\Rightarrow$ *poster by S.Hashimoto* (*Tuesday*)
- production runs at $a^{-1}=2.4-4.8$ GeV and $M_\pi=500$, 400, 300 and smaller
  - study QCD vacuum, light and heavy quark physics, ...
  - spectrum and Wilson flow $\Rightarrow$ *talk by J.Noaki* (*Monday, 2G*)
- still improving simulation method and code
  - improving/testing heavy quark formulations $\Rightarrow$ *talk by Y-G.Cho* (*Thursday, 8G*)
    in collaboration with UKQCD
  - reweighting to overlap $\Rightarrow$ *talk by H.Fukaya* (*Friday, 9D*)
  - optimization of code $\Rightarrow$ *poster by G.Cossu* (*Tuesday*)