Towards Simulations of 1+1 Flavor QCD

Lattice 2013 - Mainz

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Outline

Presenting:

- HMC-algorithm combined with mass-reweighting: show concept, first results and compare costs
- summary of mass-reweighting methods

Using tools:

One-flavor integral:

$$\frac{1}{\det M} = \int \mathrm{D}[\eta] \exp\{-\eta^\dagger M \eta\} \to \frac{1}{N_\eta} \sum_{i=1}^{N_\eta} e^{-\eta_i^\dagger (M-1)\eta_i}$$

with $\mathrm{Re}[\lambda(M)] > 0$ [J.F., Knechtli, Leder (2013)]

Domain Decomposition (DD):

$$\det D = \det \hat{D} \prod \det D_b$$

factorization into Schur complement $\hat{D}$ (IR) and block operators D_b (UV)

[Lüscher (2005)]

Idea

Facts:

- simulation destabilized for small quark masses, force increases with $1/m_q$
- condition number of Dirac operator increases for smaller m_q
  $\rightarrow$ solver cost increases
- fluctuations of small(smallest) eigenvalues of $\sqrt{D^\dagger D}$ scales with $1/V^2(1/V)$

Idea:

Using mass-reweighting to stabilize HMC
$\longrightarrow$ like μ-reweighting (OpenQCD)

[Lüscher,Palombi (2008)],[Lüscher, Schaefer (2012)]

here we will use DD (based on DD-HMC)

- DD factorizes force of D into forces of $\hat{D}$ and D_b
- force of $\hat{D}$ destabilizes HMC (IR-modes)
- choose different mass values for $\hat{D}$ and D_b in the HMC
- correct with mass reweighting towards the right weight

setting the higher mass to $\hat{D}$

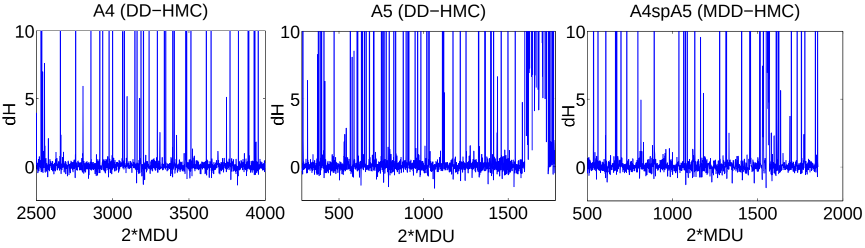
Advantage:

- stabilizes simulation
- direct access to isospin broken ensembles, by combination of reweighting methods

Disadvantage:

- mass-reweighting introduces additional fluctuations

Stabilization of Simulation - Fluctuation of δH



$N_0 = 150$ $N_{iter} = 24$ $N_0 = 175$ $N_{iter} = 27$ $N_0 = 150$ $N_{iter} = 24$

Ensembles: $\mathcal{O}(a)$-improved Wilson fermions - $V = 64 \times 32^3(8^4 blks)$

A-lattices:
$a = 0.076$ fm, $V = 64 \times 32^3(8^4 blks)$
$m_{PS}(m_1) = 380$ MeV (A4)
$m_{PS}(m_2) = 330$ MeV (A5)

E-lattices:
$a = 0.066$ fm, $V = 64 \times 32^3(8^4 blks)$
$m_{PI}(m_1) = 440$ MeV (E5)
$m_{PI}(m_2) = 310$ MeV (E6)

[Fritzsch et al. (2012)]

for scaling fits: additional ensembles with smaller volumes

Setup - Reweighting

Simulation: Boltzmann-weight

$$\det \hat{D}^2(m_1) \prod \det D_b^2(m_2) = \det \hat{D}(m_1) \prod \det D_b(m_2) \cdot \det \hat{D}(m_1) \prod \det D_b(m_2)$$

Reweighting towards: Boltzmann-weight

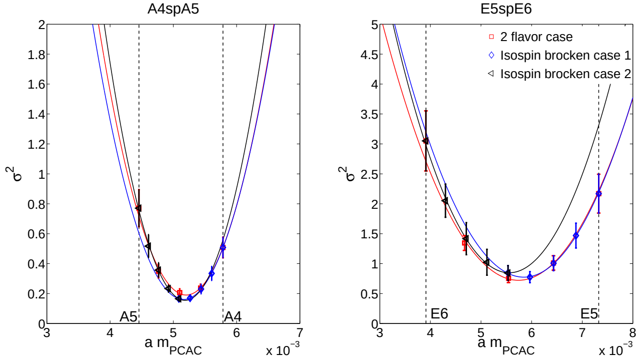
$$\det D(m_u) \quad \det D(m_d) = \det \hat{D}(m_u) \prod \det D_b(m_u) \cdot \det \hat{D}(m_d) \prod \det D_b(m_d)$$

	2 flavor-case	**Isospin broken case 1**	**Isospin broken case 2**
	$m_d = m_u = m_{ud}$	$m_d = const = m_1$	$m_u = const = m_2$
schur (m_u)	$m_{ud} \xleftarrow[\hat{W}^2]{} m_1$	$m_u \xleftarrow[\hat{W}]{} m_1$	$m_u \xleftarrow[\hat{W}]{} m_d \xleftarrow[\hat{W}^2]{} m_1$
schur (m_d)	$m_{ud} \longleftarrow m_1$		$m_d \longleftarrow m_1$
blks (m_u)	$m_2 \longrightarrow m_{ud}$	$m_2 \longrightarrow m_u$	
blks (m_d)	$m_2 \xrightarrow{W_b^2} m_{ud}$	$m_2 \xrightarrow{W_b^2} m_u \xrightarrow{W_b} m_d$	$m_2 \xrightarrow{W_b} m_d$

with $W_b(m_1 \to m_2) = \prod \frac{\det D_b(m_2)}{\det D_b(m_1)}$ and $\hat{W}(m_1 \to m_2) = \frac{\det \hat{D}(m_2)}{\det \hat{D}(m_1)}$

fluctuations e.g. 2-flavor case: $\sigma^2 = \text{var}\left(\ln[\hat{W}^2] + \ln[W_b^2]\right)$

Fluctuation of the reweighting factor - with the average $m_{PCAC}(m_u, m_d)$



– large anti–correlation between blocks and Schur-complement:

→ Fluctuation have a minimum arround ($m_1 = m_d$ and $m_2 = m_u$ (Isospin broken))

parametrization of fluctuation

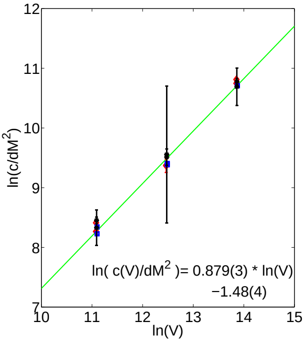
$$\sigma^2 = b(V)(m - x_0)^2 + c(\Delta M, V)$$

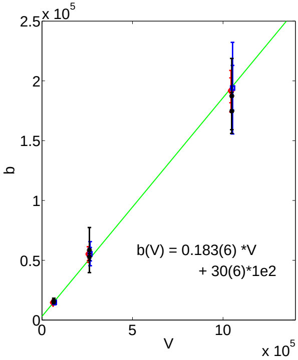
with coefficients

$$b(V) \text{ and } c(\Delta M, V) \text{ with } \Delta M = m_2 - m_1$$

Fluctuation of the reweighting factor - 2

unimpr. Wilson-Fermions - $(0.834\,\mathrm{fm})^4$ - $(1.18\,\mathrm{fm})^4$ - $(1.67\,\mathrm{fm})^4$ - with $a = 0.0521(7)$
$m_1 : m_{PS} = 752$ MeV and $m_2 : m_{PS} = 387$ MeV





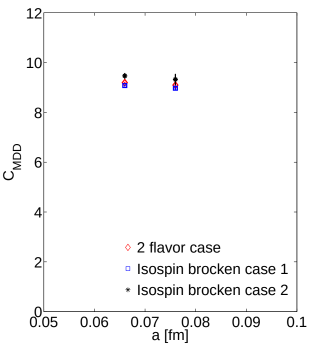
$c(\Delta M, V) = C_{mdd} \cdot V^{0.88} \Delta M^2$ $\qquad$ $b(V) = B_{mdd} \cdot V$

while x_0 has a weak V dependence (expected $x_0 \underset{V\to\infty}{\longrightarrow} m_2$)

parametrization of fluctuation
$\sigma^2 = b(V)(m - x_0(V))^2 + c(\Delta M, V)$

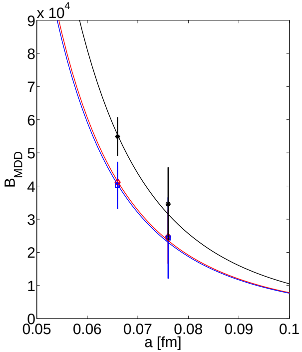
Fluctuation of the reweighting factor - 3

$$c(\Delta M, V) = C_{mdd}(a) \cdot (a^4 V)^{0.88} \Delta M^2$$



$$C_{mdd}(a) = \mathcal{C}_{MDD}$$

$$b(V) = B_{mdd}(a) \cdot a^4 V$$



$$B_{mdd}(a) = \mathcal{B}_{MDD} \cdot a^{-4}$$

with $\chi^2 \in [0.01, 0.08]$

Cost compare to the DD-HMC

Cost of DD-HMC:

− Solver iteration:(N_{iter})
iteration number increases if m_q decreases
(conventional $1/m_q$ (CG), very small increase using Multi Grid)

− Step size of trajectory: (N_0)
step size increase for $m_q \to 0$ to avoid large spikes
$\longrightarrow$ *Cost per configuration:* $cost(m) = 2 \cdot N_{tr/cnfg} N_{iter}(m) N_0(m)$

Cost of mass reweighting:

+ Reduction of stochastic variance:
$N_{rew} \sim 60$ inversions per reweighting factor
$\longrightarrow$ *Cost of a mass reweighting:* $cost_{mrew} = N_{rew} N_{iter}(m_{12})$

+ Ensemble fluctuations via reweighting:
$e^{\sigma^2(\Delta M,V)}$ correction with $\sigma^2(\Delta M, V)$ the ensemble fluctuations
(rough overestimated!!! ignores correlation with the observable)

Cost for the 2-flavor mass–degenerated case @m_2:

	DD-HMC	MDD-HMC	"+"mass-reweighting
X	1	$\frac{\text{cost}(m_1)+\text{cost}_{mrew}}{\text{cost}(m_2)}$	$e^{\sigma^2(\Delta M,V)}$ cost(MDD)/cost(DD)
A5	1	$0.76 + 0.06$	$e^{0.78} \cdot 0.82 = 1.79$
E6	1	$0.41 + 0.10$	$e^{3.92} \cdot 0.51 = 27.01$

Comparision with Isospin reweighting

Isospin-breaking with $\sum m_{q,ensemble} = \sum m_{q,rew}$ $(\Delta m = m_d - m_u)$
Scaling :

$$\sigma_4^2 = \Delta m^4 \cdot \text{var}\left\{ Tr\left(\frac{1}{D^2}\right)\right\} = \frac{A_4 \Delta m^4 V}{m_q^2}$$

Isospin-breaking with $\sum m_{q,ensemble} \neq \sum m_{q,rew}$
Scaling :

$$\sigma_2^2 = \Delta m^2 \cdot \text{var}\left\{ Tr\left(\frac{1}{D}\right)\right\} = A_2 \Delta m^2 V$$

$\rightarrow$ dependence of $1/m_q$ hidden for large enough m_q (?)

MDD-HMC $m_1 = m_u$ and $m_2 = m_d$
Scaling :

$$\sigma_{MDD}^2 = a(m - x_0)^2 + c \overset{m=x_0}{=} C_{mdd} V^{0.88} \Delta M^2$$

assume: dependence of $1/m_q$ hidden for large enough m_q (?)

@physical masses: $\Rightarrow \Delta m \sim m_q$

$$\frac{\sigma_4^2}{\sigma_{MDD}^2} = \frac{A_4}{C_{mdd}} V^{0.12}$$

with $\frac{A_4}{C_{mdd}} = 1.62$ (if σ_{MDD}^2 has no $1/m_q$ dependence)

Conclusion

Results:

MDD-Algorithm:

- stabilization of simulation by setting IR-modes to a higher mass
  $\rightarrow$ smaller m_q accessible than for DD-HMC
- using reweighting to get correct Boltzmann-weight
  $\longrightarrow m_u \neq m_d$ possible
- fluctuations scales "slightly" with the volume $\sim V^{0.88}$
- future improvements of algorithm:
  $\rightarrow$ recursive DD (with $D_b(m_u), \hat{D}_b(m_{ud}), \hat{D}(m_d)$)
  $\rightarrow$ MPre to stabilizes forces further

Prospects:

- tool for precision physics on the lattice (need controll of the fluctuations)
- MDD-algorithm is (can be) effectiv for simulation towards physical point

[J.F.,Knechtli,Leder (2013)]