Application of Domain Decomposition to the Evaluation of Fermion Determinant Ratios

Lattice 2012 - Cairns

Jacob Finkenrath

with Francesco Knechtli and Björn Leder

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BERGISCHE UNIVERSITÄT WUPPERTAL

Outline

Aim

Apply techniques of Partially Stochastic Multi-Step (PSMS) algorithm to Mass - Reweighting

Idea of PSMS algorithm [J.F.,Knechtli,Leder (2012)]

- decoupling of pure gauge- and fermion-weight
  $\rightarrow$ proposal by a pure gauge update
  $\rightarrow$ weighted by the fermion determinant given by the ratio operator $M = D^{-1}_{(U_{new},m)} D_{(U_{old},m)}$

- Metropolis accept-reject step with probability
  $\min\left\{1, \det(M^\dagger M)^{-1}\right\} \rightarrow \min\left\{1, e^{-\eta^\dagger(M^\dagger M - 1)\eta}\right\}$
  $\rightarrow$ ensemble + stochastic fluctuations

- Domain Decomposition (DD) helps:
  hierachical filter, reduces stochastic noise

Outline - Mass Reweighting

Aim: Calculate Mass Reweighting factor

$$W = \det[\underbrace{D^{-1}(m_2)D(m_1)}_{=:M}]^{-2} \rightarrow \frac{1}{N_{hit}} \sum_{i=1}^{N_{hit}} e^{-\eta_i^\dagger (M^\dagger M - 1)\eta_i}$$

for m_1 mass of ensemble and m_2 target mass ($\Delta m = m_1 - m_2$)

$\Rightarrow$ leads to stochastic on top of ensemble fluctuations

$\rightarrow$ reduce this noise by

- interpolation in the mass [Hasenfratz,Hoffmann,Schaefer(2008)]
  $\longrightarrow D(m_2)/D(m_1) = D(m_2)/D(m_{inter}) \cdots D(m_{inter})/D(m_1)$
- Domain Decomposition [Lüscher (2005)]
  $\longrightarrow \det D = \det \hat{D}_{Schur} \cdot \prod \det D_{blk}$
- Correlation with the plaquette[Hasenfratz,Hoffmann,Schaefer(2008)]
  $\longrightarrow -\beta S_W + \ln\det D^2 = -\beta' S_W + \left(\ln\det D^2 - \delta\beta S_W\right)$

$\rightarrow$ test on following CLS ensembles:

$N_f = 2$ O(a) impr. Wilson fermions at $\beta = 5.3$ ($a = 0.066$ fm)

$\kappa_1 \sim m_{PS} = 440$ MeV $\kappa_2 \sim m_{PS} = 310$ MeV

Volumes: $V_1 = 48 \times 24^3$ $V_2 = 64 \times 32^3$

Stochastic fluctuations - Motivation

Mass-Reweighting factor is known, if the spectrum of $D(m_2)$ is known

$$\det M^{-1} = \prod_{i=1}^{12V} \frac{\lambda_{i(D(m_2))}}{\lambda_{i(D(m_2))} + \Delta m}$$

$\rightarrow$ only small $\lambda_i \lesssim \Delta m$ contribute (IR-modes)

use Wilson-Dirac-Operator: $M = 1 + \Delta m \cdot D^{-1}(m_2)$

$$\lambda(M) = 1 + \Delta m \cdot \lambda(D^{-1}(m_2)) \;\Rightarrow\; \lambda(M) > 1$$

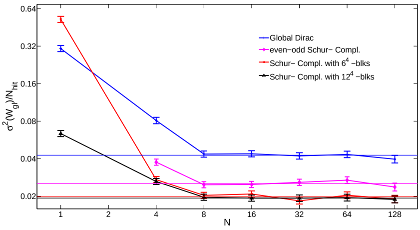
$\rightarrow$ every eigenvalue contributes to the stochastic fluctuations
(also UV-modes !!!)

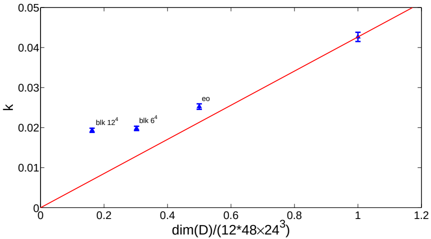
Can Domain Decomposition reduce the fluctuations ?

Domain Decomposition applied to Mass Reweighting

$$W = W_{gl} \cdot \prod_{k=1}^{N_{blk}} \frac{\det D_k^2(m_2)}{\det D_k^2(m_1)}, \quad W_{gl} = \prod_{i=1}^{N} \left\{ \frac{1}{N_{hit}} \sum_{j=1}^{N_{hit}} e^{-\eta_{i,j}^\dagger (\hat{M}_i^\dagger \hat{M}_i - 1)\eta_{i,j}} \right\}$$

stochastic fluctuations for one cnfg (48×24^3)





$\#$ inversions $= N \cdot N_{hit} = 640$

$\rightarrow$ stochastic noise: $\frac{\sigma^2_{stoc}}{N_{hit}} \propto \frac{k(V,\Delta m)}{N \cdot N_{hit}}$

$\rightarrow$ DD 2 times more efficient

$\Rightarrow$ small blocks are sufficient to eat noise of UV-modes

Mass Reweighting in measurements

Observable

$$< \mathrm{O} >_{m_2} = \frac{< \mathrm{O}W >_{m_1}}{< W >_{m_1}}$$

Total Variance of Observable

$$\mathsf{var}(\mathrm{O}) \sim \frac{\delta \mathrm{O}^2}{N_{cnfg}} \tau_{corr} \left(\frac{\mathsf{var}(W)}{< W >^2} + 1 \right)$$

[Liu,Christ,Jung(2012)]+[Y.Aoki et al.(2011)]

Mass-reweighting factor destributed like log-normal distribution

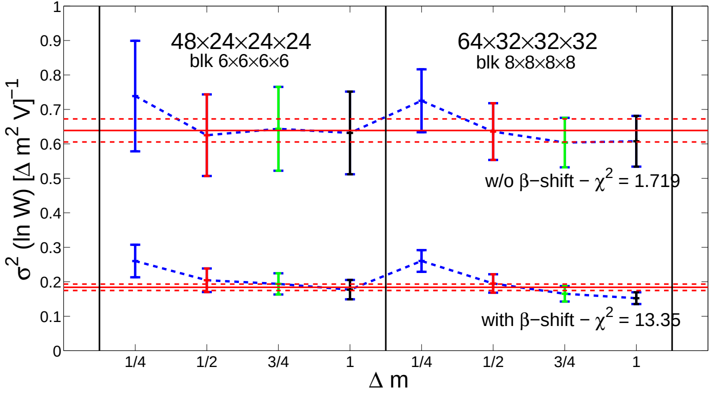
$$\rho(W) \sim \frac{1}{W} \exp\left\{ -\frac{(\ln W - \mu)^2}{2\sigma^2} \right\}$$

then it is straightforward

$$\left(\frac{\mathsf{var}(W)}{< W >^2} + 1 \right) = e^{\sigma^2}$$

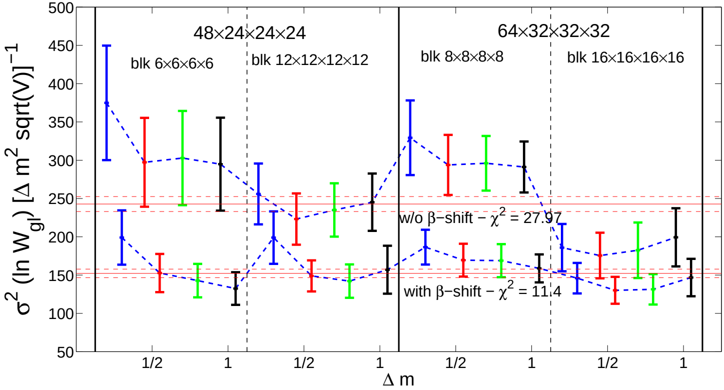
with $\sigma^2 = \mathsf{var}(\ln W)$

Mass and Volume dependence of fluctuations



$$\sigma^2 \propto \Delta m^2 \cdot V$$

Mass and Volume dependence of gl. Schur-Compl.



$$\sigma^2 \propto \Delta m^2 \cdot \sqrt{V}$$

Mass reweighting for one flavor

Estimation of $M \in \mathbb{C}^{12V\times 12V}$

$$\frac{1}{\det M} \stackrel{?}{=} \int \mathrm{D}\eta \mathrm{D}\eta^\dagger e^{-\eta^\dagger M \eta}$$

$$\Leftrightarrow \ \mathrm{Re}(\eta^\dagger M \eta) > 0$$

compare to Root-trick [S. Aoki et al. (2012)]:

$$\frac{1}{\det M} \stackrel{?}{=} \sqrt{\int \mathrm{D}\eta \mathrm{D}\eta^\dagger e^{-\eta^\dagger M^\dagger M \eta}}$$

$$\Leftrightarrow \ \det M > 0$$

Remarks:

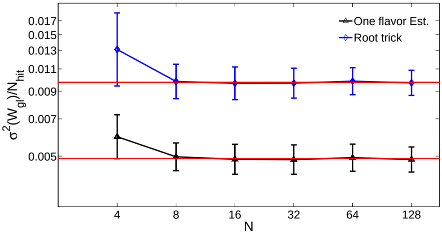
- it is possile to satisfy $\mathrm{Re}(\eta^\dagger M \eta) > 0$ with mass interpolation and DD
- stochastic fluctuations diverges for $\lambda(M + M^\dagger) < 1$
  $\rightarrow$ easy to detect (for $N_{hit} > 1$)
- application: strange quark

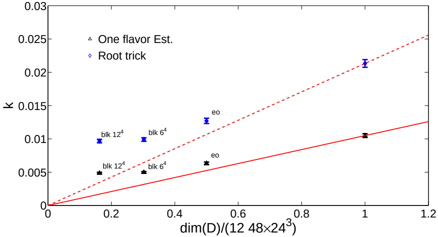
Stochastic fluctuations for one flavor mass reweighting

$$\frac{1}{\det M} \rightarrow \prod_{i=1}^{N} e^{-\eta_i^\dagger (M_i - 1)\eta_i} \rightarrow \prod_{i=1}^{N} \text{Re}\left\{ e^{-\eta_i^\dagger (M_i - 1)\eta_i} \right\}$$

$\rightarrow$ only real part of $e^{-\eta^\dagger M \eta}$ contributes ($\det M$ real)

stochastic fluctuations for one cnfg (48×24^3)





\# inversions $= N \cdot N_{hit} = 640$

$\rightarrow$ 2 times more efficient

$\Rightarrow$ Imaginary parts of $e^{-\eta^\dagger M \eta}$ produce additional noise

Conclusion

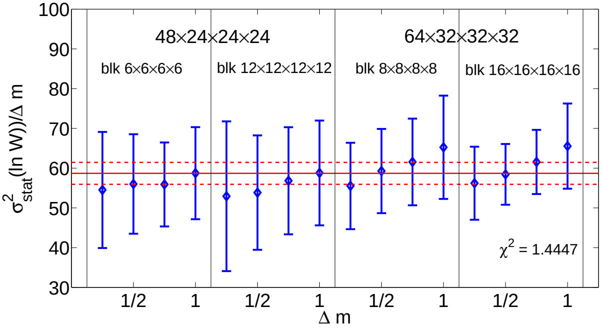
2-flavor - Mass - Reweighting:

- stochastic fluctuations:
  $\frac{\sigma^2_{stoc}}{N_{hit}} \propto \frac{k(V,\Delta m)}{N \cdot N_{hit}}$ with $k(V, \Delta m) = V \cdot \Delta m$
  DD 2 times more efficient for block size of $l \geq 1$
- ensemble fluctuations:
  $\sigma^2 \propto V \cdot \Delta m^2$ with $\left(\frac{\text{var}(W)}{<W>^2} + 1\right) = e^{\sigma^2}$
  Global Schur Complement:
  $\sigma^2_{gl} \propto \sqrt{V} \cdot \Delta m^2$

1-flavor - Mass - Reweighting:

- it is possile to satisfy Re$(\eta^\dagger M \eta) > 0$
  with Mass interpolation and Domain Decomposition
- 2 times more efficient then root-trick

Volume and mass dependence of statistical fluctuations

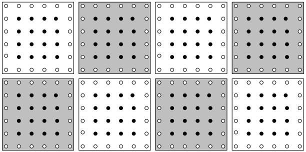


with $V/N = \text{const}$

Domain Decomposition (DD)

Division into non-overlapping blocks:

$$D = \begin{pmatrix} D_{\mathrm{bb}} & D_{\mathrm{bw}} \\ D_{\mathrm{wb}} & D_{\mathrm{ww}} \end{pmatrix}$$



Factorization [Lüscher, 2005]

$$\det(D) = \prod_{b \in \mathcal{C}} \det(D_b) \det(\hat{D})$$

short: block Dirac operators D_b (with Dirichlet boundary conditions)
long: Schur complement $\hat{D} = 1 - D_{\mathrm{bb}}^{-1} D_{\mathrm{bw}} D_{\mathrm{ww}}^{-1} D_{\mathrm{wb}}$ (block interaction)

History of Mass reweighting factor