Testing reweighting method for truncated Overlap fermions

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Plan

• 1. Truncated overlap fermion
• 2. Reweighting
• 3. Implementation
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1. Truncated overlap fermion

• Overlap fermion
  – Lattice chiral symmetry (Ginsparg-Wilson relation)
    \[ D_{OV} \gamma_5 + \gamma_5 D_{OV} = 2aD_{OV} \gamma_5 D_{OV} \]
    
    \[ \psi' = \psi + i \varepsilon \gamma_5 (1 - aD_{OV}) \psi \quad \iff \quad \overline{\psi}' D \psi' = \overline{\psi} D \psi \]

• Explicit construction (Neuberger overlap Dirac fermion)
  \[ D_{OV} = \frac{1}{2} (1 + \gamma_5 \text{sign}(H_W)) \]
  \[ H_W = \gamma_5 (D_W - m_{dw}) \]
  – negative mass \((0 < m_{dw} < 2)\) Wilson kernel \(D_W\)
  – Matrix Sign function

\[ \]

Hasenfraz, Laliena, Niedermayer, PLB427(1998)
Lusher, PLB428(1998)
1. Truncated overlap fermion

- Dynamical Overlap fermion
  - HMC with dynamical overlap fermion
  - Difficulty in the sign function: one needs to keep track of the low-modes of $H_w$ (reflection/reflection)
    \[ D = \frac{1}{2} \left( 1 + \gamma_s \text{sign}(H_w) \right), \quad H_w = \gamma_s (D_w - m_{dw}) \]


- Topology fixing
  - avoid/suppress appearance of near zero mode of $H_w$
  - by adding extra terms or by using an admissible gauge action.
    \[
    S_G = \left\{ \begin{array}{ll}
    \beta \sum_\infty 1 - \frac{\text{Re} Tr[P_{\mu\nu}] / 3}{1 - \frac{\text{Re} Tr[P_{\mu\nu}] / 3}{\varepsilon}} & \text{(for } 1 - \text{Re} Tr[P_{\mu\nu}] / 3 < \varepsilon) \\
    \end{array} \right.
    \]

    $\det[H_w^2 + \mu^2]$

Luscher, NPB549 (1999)
Izubuchi, Dawson (RBC) NPB ProcSuppl 106(2002)
Fukaya, Hashimoto, Hirohashi, Ogawa, Onogi; PRD73(2006)
Renfrew, Blum, Christ, Mawhinney, Vranas, PoS(Lat08)
1. Truncated overlap fermion

- **Approximate (truncated) Overlap fermion**
  - Give up exact Lattice chiral symmetry
  - Keep Better Chiral property than that of Wilson type.
  - Domain wall fermion with finite N5.
  - Truncate the approximation for the Sign function.

- **Overlap fermion construction** (approximation for sign function)
  - Domain wall type
  \[
  D_{TROV} = \epsilon^T P^\dagger \left( D_{DWF}(N_5,m_f=1) \right)^{-1} D_{DWF}(N_5,m_f) \left[ P \epsilon \rightarrow m_f + (1-m_f) D_{OV} \right]
  \]
  - Partial fraction type
  \[
  D_{TROV} = 1 + \gamma_5 H_W \left( \alpha_0 + \sum_{j=1}^N \frac{\alpha_j}{H_W + \beta_j} \right) \rightarrow 2D_{OV}
  \]
  - Continued fraction type
  \[
  D_{TROV} = 1 + \gamma_5 (\beta_0 H_W + \frac{\alpha_1}{\beta_1 H_W + \frac{\alpha_2}{\beta_2 H_W + \cdots}}) \rightarrow 2D_{OV}
  \]

Kikukawa-Noguchi’99, Borici’99, Chiu’03, Shamir, Brower’05, ….

JLQCD, TWQCD, ….

Borici’99, NrayananNeubeger’00, Edwards et al’05.
1. Truncated overlap fermion

- Here I use Domain wall type realization of overlap fermion in the HMC algorithm.
- This will smoothen the sign function. => Lowering the cost of HMC?, Topology changing?
  - S.Shaefer, PoS(Lat06)

- Lattice Chiral symmetry is explicitly broken. But it should be better than Wilson type fermions.
- Recovering Chiral symmetry at the measurement step by Reweighting method.
2. Reweighting

- We consider QCD (Nf=2)

\[ Z = \int DU \det[D_{OV}]^2 e^{-S_G[U]} \]

\[ = \int DU \det[D_{OV} / D_{TROV(1)}]^2 \det[D_{TROV(1)} / D_{TROV(2)}]^2 \cdots \]

\[ \cdots \det[D_{TROV(N_{step}-1)} / D_{TROV(N_{step})}]^2 \det[D_{TROV(N_{step})}^2 e^{-S_G[U]} \]

\[ = \int DUD\phi^+ D\phi \prod_{j=1}^{N_{step}} W(J) \exp[-S_G[U] - |D_{TROV(N_{step})}^{-1}\phi|^2] \]

\[ D_{TROV(0)} \equiv D_{OV} \quad \text{: exact sign function (numerically)} \]

\[ D_{TROV(J)} \quad \text{: truncated overlap op. (at a finite } N_5 \text{)} \]

\[ W(J) = \det[D_{TROV(J-1)} / D_{TROV(J)}] \quad \text{: reweighting factor (evaluated via noisy method)} \]

- average over ensemble generated with the truncated overlap fermion.
2. Reweighting

• Reweighting for overlap/Domain wall fermions
  – for Overlap strange quark: H.Ohki et al. (JLQCD), arXiv:1208.4185[hep-lat]

• In this conference
  • 8/2(Fri) 14:20-, RoomD: H.Fukaya et al.,
    “Overlap/Domain-wall reweighting”

• Other reweighting related talks:
  – (Mon), 18:30, Room C, W. Freeman et al.
  – (Fri), 15:00, Room B, C. Aubin et al.
  – (Mon), 16:30, RoomD, B.Leder et al.
  – (Mon), 16:50, Room D, J. Finkenrath et al.
  – Poster, S. Schaefer
3. Implementation

- HMC with truncated overlap fermion (Nf=2)
  - Domain wall operator realization
    \[
    D_{TROV} = \varepsilon^T P^\dagger \left[ D_{DWF}(N_5,m_f=1) \right]^{-1} D_{DWF}(N_5,m_f) P \varepsilon
    \]

- Final step in the reweighing factor requires the exact overlap operator.
  - Optimal Domain wall operator via Zolotarev approximation coefficients
    \[
    P \varepsilon = (P_L,0,0,\ldots,0,P_R)^T : \text{restrictor from 5D to 4D}
    \]
  - + Pulling up Low-modes (low-mode improvements)
  - => Extension to the even/odd 4d-site preconditioning (New?).
3. Implementation

- Even/odd site preconditioning with low-mode improvements

\[ D_{TROV} w = \varepsilon^T P^\dagger \left( D_{DWF(N_5,m_f=1)} \right)^{-1} D_{DWF(N_5,m_f)} \left[ P \varepsilon \right] w \]

\[ (D_{TROV})^{-1} w = \varepsilon^T P^\dagger \left( D_{DWF(N_5,m_f)} \right)^{-1} D_{DWF(N_5,m_f=1)} \left[ P \varepsilon \right] w \]

- need the inversion of \( D_{DWF} \).

\[ \tilde{D}_{DWF(N_5,m_f)} = D_{DWF(N_5,m_f)} \left( B + CM_{W5} \right)^{-1} = K - \frac{1}{2} M_{\text{hop}} \]

\[ K = 4 - m_{dw} + (1 - M_{W5})(B + CM_{W5})^{-1} \]

\( M_{W5} \): hopping in 5th direction. (extra-flavor mass matrix)

\( B = \text{diag}(b_1, b_2, \ldots, b_{N_5}), \quad C = \text{diag}(c_1, c_2, \ldots, c_{N_5}) \),

\( (b_j, c_j) : \text{improvement coefficients, } j:5\text{D-index} \)

Shamier standard Domain wall: \( b_j = a_5, c_j = 0 \)

\[ H_w = \gamma_5 \left( D_w - m_{dw} \right) \left( a_5 (D_w - m_{dw}) / 2 + 1 \right)^{-1} \]

Chiu Optimal (Shamier kernel) Domain wall: \( b_j = \frac{w_j + a_5}{2}, c_j = \frac{w_j - a_5}{2} \)

Borici Domain wall (Neuberger kernel): \( b_j = a_5, c_j = a_5 \)

Chiu Optimal (Neuberger kernel) Domain wall: \( b_j = w_j, c_j = w_j \)

General, Moebius Domain wall: \( b_j, c_j \)

3. Implementation

- Even/odd site preconditioning with low-mode improvements

Low-modes of sign kernel $H_w$

$$H_w V_k = V_k \Lambda_k, \quad V_k = (v_1, v_2, \ldots, v_k),$$

$$\Lambda_k = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_k)$$

Low-modes improvement for sign kernel $H_w$

$$H_w \rightarrow H_w^{\text{imp}} = H_w + V_k S_k V_k^\dagger$$

$$\tilde{D}_{\text{DWF}} (N_5, m_f) = K - \frac{1}{2} M_{\text{hop}} \Rightarrow \tilde{D}_D^{\text{imp}} (N_5, m_f) = K - \frac{1}{2} M_{\text{hop}} + W_k S_k^\dagger$$

Low-modes improved Domain wall

Zolotarev coefficients in $B$ and $C$ and $N_5$ are optimized with respect to $|H_w|$

$$W_k = (a_5 / 2)(D_w - m_{dw}) + 1) \gamma_5 V_k$$

$$S_k = \text{diag}(\hat{\lambda}_1 - \lambda_1, \hat{\lambda}_2 - \lambda_2, \ldots, \hat{\lambda}_k - \lambda_k)$$

$$\hat{\lambda}_j \equiv 2 \text{sign}(\lambda_j) \max_{s=1,\ldots,k} |\lambda_s|$$

$$D_{\text{DWF}} (N_5 \approx \infty, m_f) x = b \Leftrightarrow \tilde{D}_D^{\text{imp}} (N_5, m_f) \tilde{x} = b, \quad x = (B + CM_{W5})^{-1} \tilde{x}$$
3. Implementation

• Even/odd site preconditioning with low-mode improvements

\[ \tilde{D}^{\text{imp}}_{\text{DWF}}(N_5, m_f) \tilde{x} = b \]

Even/odd (4D) ordered form of the linear equation with improved DWF operator.

\[
\begin{pmatrix}
(\tilde{D}_{\text{DWF}}(N_5, m_f))_{ee} & (\tilde{D}_{\text{DWF}}(N_5, m_f))_{eo} & (W_k)_{e} \\
(\tilde{D}_{\text{DWF}}(N_5, m_f))_{oe} & (\tilde{D}_{\text{DWF}}(N_5, m_f))_{oo} & (W_k)_{o} \\
(S_k)_{e} & (S_k)_{o} & -1
\end{pmatrix}
\begin{pmatrix}
\tilde{x}_e \\
\tilde{x}_o \\
\zeta
\end{pmatrix}
= 
\begin{pmatrix}
(b_e) \\
(b_o) \\
0
\end{pmatrix}
\]

ζ : auxiliary variable

eliminating \( x_o \) and \( \zeta \)

Even/odd (4D) preconditioned form of the linear equation with improved DWF operator.

\[
\left( \tilde{D}^{\text{imp}}_{\text{DWF}}(N_5, m_f) \right)_{ee} \tilde{x}_e = \hat{b}_e
\]

\[
G_{oo} = \left( I + S_o^\dagger (\tilde{D}_{\text{DWF}})_{oo}^{-1} W_o \right)^{-1}
\]

\[
\tilde{D}^{\text{imp}}_{\text{DWF}}_{ee} = \left( \tilde{D}_{\text{DWF}} \right)_{ee} + (\tilde{D}_{\text{DWF}})_{ee}^{-1} W_e - (\tilde{D}_{\text{DWF}})_{eo} (\tilde{D}_{\text{DWF}})^{-1}_{oo} W_o \left[ S_{oo}^\dagger + S_o^\dagger (\tilde{D}_{\text{DWF}})^{-1}_{oo} (\tilde{D}_{\text{DWF}})_{oe} \right]
\]

\[
\hat{b}_e = (\tilde{D}_{\text{DWF}})_{ee}^{-1} \begin{bmatrix}
b_e - (\tilde{D}_{\text{DWF}})_{eo} (\tilde{D}_{\text{DWF}})^{-1}_{oo} W_o \\
-W_e - (\tilde{D}_{\text{DWF}})_{eo} (\tilde{D}_{\text{DWF}})^{-1}_{oo} W_o \end{bmatrix} \]

\[
\tilde{x}_e = (\tilde{D}_{\text{DWF}})_{oo}^{-1} \begin{bmatrix}
(b_e - (\tilde{D}_{\text{DWF}})_{oe} \tilde{x}_e) \\
-W_o G_{oo} \left[ S_{ee}^\dagger + S_e^\dagger (\tilde{D}_{\text{DWF}})_{oo}^{-1} (\tilde{D}_{\text{DWF}})_{oe} W_o \right] \tilde{x}_e + S_o^\dagger (\tilde{D}_{\text{DWF}})^{-1}_{oo} b_o
\end{bmatrix}
\]
4. Results

• Very preliminary

– Test on Quench configurations
  (10 configs, DBW2 gauge action beta=0.87, 8³x32)
  [ DBW2: Takaishi, PRD54(1996)1050
de Forcrand et al.(QCD-TARO), NPB577(2000)263]

– monitoring

  • 12 interior/exterior eigen values of
    \[ H_w = \gamma_5 (D_w - m_{dw})/((D_w - m_{dw})/2+1) \]

  • finite mas G.-W. relation violation:
    \[ \eta^\dagger \Delta_{GW} \eta \]
    \[ \eta : \text{Gaussian noise vector} \]
    \[ \Delta_{GW} = \{ \gamma_5, (D_{OV/TROV})^{-1} \} - \frac{2}{1 + m_f} \left[ m_f (D_{OV/TROV})^{-1} \gamma_5 (D_{OV/TROV})^{-1} + \gamma_5 \right] \]

  • exponent in reweighting factor:
    \[ dS = \left| \left( D_{TROV(j-1)} \right)^{-1} D_{TROV(j)} \eta \right|^2 - \left| \eta \right|^2 \]

  • reweighting factor:
    \[ \exp(-dS) \]
    \[ \eta : \text{Gaussian noise vector} \]

No meson spectrum measurement with reweighing....
4. Results

- meson masses $N_5=12$
  - $M_{PS} = 0.274(21)$, $M_V = 0.611(65)$
  - $M_{PS}/M_V = 0.45$
  - $\beta = 0.87$ (DBW2, quench), $8^3 \times 32$
  - $m = 0.0200$ (Mdwh=1.8), PS-channel
  - $M_{PS} = 0.2997(19)$, $M_V = 0.640(17)$
  - $\beta = 0.87$ (DBW2, quench), $8^3 \times 32$
  - $m = 0.0200$ (Mdwh=1.8), V-channel

RBC, PRD69 (2004), $16^3 \times 32$, $N_5=16$, Domain wall
$M_{PS} = 0.2997(19)$, $M_V = 0.640(17)$
4. Results

- 12 interior/exterior eigenvalues of $H_w$

Beta=0.87 (DBW2, quench), $8^3 \times 32$, $H_w$ eigenvalues (Mdwh=1.8, 12 max and 12 min)

Small $|H_w|$ in conf # 1, 2, 3, 9, 10

$\Rightarrow$ large G.-W. relation violation is expected with a fixed N5.
4. Results

- G.-W. relation violation $N_5=12, 14$, and optimal

  \[ \text{Beta}=0.87(\text{DBW2,quench}), \, 8^3\times 32, \]
  \[ \text{G-W relation violation}(m=0.02, \, M_{\text{dhw}}=1.8) \]

  \[ \eta_i^\dagger \Delta \nabla \eta_i^\dagger \eta_i \]
  
  Small $|H_w|$ in conf # 1, 2, 3, 9, 10
  \[ \Rightarrow \text{large G.-W. relation violation.} \]

  \[ \text{Optimal operator keeps the violation at the tolerance level as it should be.} \]

- G.-W. relation violation $N_5=30, 32$, and optimal

  \[ \text{Beta}=0.87(\text{DBW2,quench}), \, 8^3\times 32, \]
  \[ \text{G-W relation violation}(m=0.02, \, M_{\text{dhw}}=1.9) \]

  \[ \eta_i^\dagger \Delta \nabla \eta_i^\dagger \eta_i \]

  \[ \text{We used:} \]
  \[ m=0.02 \]
  \[ \text{optimal Zolotarev tolerance } 10^{-12} \]
  \[ \text{eigen solver tolerance } 10^{-12} \]
4. Results

- **Exponent \( dS \)**
  
  N5=12\(\rightarrow\)14 and 14\(\rightarrow\)Optimal

![Graph](image1.png)

Beta=0.87(DBW2,quench), 8\(^3\)x32, Exponent (dS) in reweighting factor exp(-dS)(m=0.02, Mdwh=1.8)

- **Exponent \( dS \)**
  
  N5=30\(\rightarrow\)32 and 32\(\rightarrow\)Optimal

![Graph](image2.png)

Beta=0.87(DBW2,quench), 8\(^3\)x32, Exponent (dS) in reweighting factor exp(-dS)(m=0.02, Mdwh=1.8)
4. Results

• Reweighing factor $\exp(-dS)$
N5=12 $\rightarrow$ 14 and 14 $\rightarrow$ optimal

Reweighting between N5=32 and optimal/ N5=14 and optimal: small eigen values in Conf #1,2,9,10.

=> large fluctuation in $\exp(-dS)$.
The factor $\exp(-dS)$ seems to be sensitive to the appearance of small eigen values.
5. Summary

• Needs methods for Lattice chiral symmetry with lower computational cost
• One possibility: Truncated/approximate overlap Dirac operator with reweighting method
• We tested:
  – Truncated overlap fermions on top of the Domain wall fermion.
  – the G.-W. relation violation and reweighting factor are investigated on quenched configurations.
  – the violation and the reweighting factor are sensitive to the small eigen values of $|Hw|$
• Further studies:
  • $dS$ must proportional to the size of lattice. How about for larger lattice?
  • How such configurations with small eigen values affect the expectation value of observables?
  • Does the HMC with the truncated Overlap fermion generate such configurations?

Thank you!
Backups

- Quench, $m=0.01$

Beta=0.87(DBW2,quench), $8^3 \times 32$, G-W relation violation ($m=0.01$, Mdwh=1.8)
• **Quench, m=0.01**

• Exponent \( dS \)

• Reweighing factor \( \exp(-dS) \)

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**Graphs:**

Left:
- \( \beta = 0.87(\text{DBW2, quench}), 8^3 \times 32 \)
- Exponent \((dS)\) in reweighting factor \(\exp(-dS)(m=0.01, \text{Mdh}=1.8)\)
- **x-axis:** conf #
- **y-axis:** \(dS\)
- **Legend:**
  - \(dS>0, N_2 = 30 \rightarrow N_2 = 32\) (2 noises)
  - \(dS<0, N_2 = 30 \rightarrow N_2 = 32\) (2 noises)
  - \(dS>0, N_2 = 32 \rightarrow N_2 = \text{optimal}\) (2 noises)
  - \(dS<0, N_2 = 32 \rightarrow N_2 = \text{optimal}\) (2 noises)

Right:
- \( \beta = 0.87(\text{DBW2, quench}), 8^3 \times 32 \)
- Reweighting factor \(\exp(-dS)(m=0.01, \text{Mdh}=1.8)\)
- **x-axis:** conf #
- **y-axis:** \(\exp(-dS)\)
- **Legend:**
  - \(N_2 = 30 \rightarrow N_2 = 32\) (2 noises)
  - \(N_2 = 32 \rightarrow N_2 = \text{optimal}\) (2 noises)