Testing reweighting method for truncated Overlap fermions

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Plan

- 1. Truncated overlap fermion
- 2. Reweighting
- 3. Implementation
- 4. Results
- 5. Summary

1. Truncated overlap fermion

- Overlap fermion
  - Lattice chiral symmetry (Ginsparg-Wilson relation)

$$D_{OV}\gamma_5 + \gamma_5 D_{OV} = 2aD_{OV}\gamma_5 D_{OV}$$

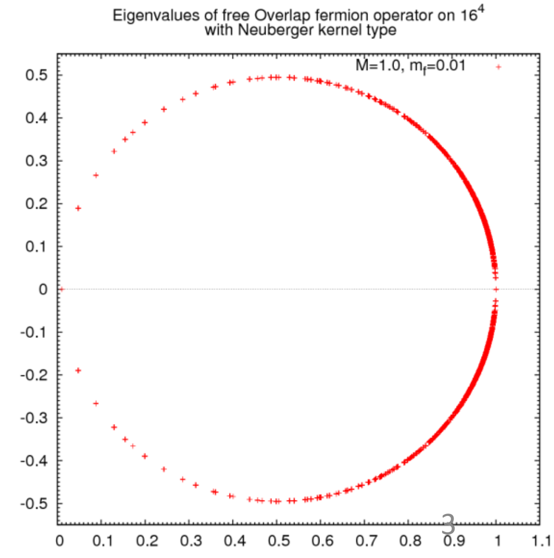
Hasenfraz,Laliena, Niedermayer,PLB427(1998)
Lusher, PLB428(1998)

$$\psi' = \psi + i\varepsilon\gamma_5(1 - aD_{OV})\psi \qquad \Leftrightarrow \overline{\psi}' D\psi' = \overline{\psi} D\psi$$
$$\overline{\psi}' = \overline{\psi} + i\varepsilon\overline{\psi}(1 - aD_{OV})\gamma_5$$

- Explicit contruction (Neuberger overlap Dirac fermion)

$$D_{OV} = \frac{1}{2}\left(1 + \gamma_5 \mathrm{sign}(H_W)\right), \quad H_W = \gamma_5(D_W - m_{dw})$$

  - negative mass (0<m_{dw}<2) Wilson kernel D_W
  - Matrix Sign function
  -



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 (refrection/reflaction)

$$D = \frac{1}{2}\left(1 + \gamma_5 \mathrm{sign}(H_W)\right), \quad H_W = \gamma_5 (D_W - m_{dw})$$

Fodor,Katz,Szabo, JHEP 08(2004),NPB ProcSuppl 140(2005),JHEP 01(2006),
DeGrand, Shafer, PRD71(2005),PRD72(2005),PoS(Lat05),
Cundy, Krieg, Arnold, Frommer, Lippert, Schilling, NPB ProcSuppl 140(2005),
Cundy, Krieg, Lippert PoS(Lat05).

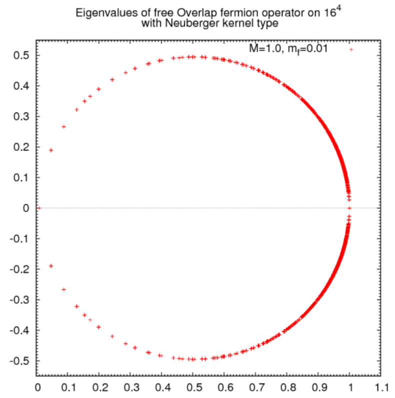
  - Topology fixing
    - avoid/suppress appearance of near zero mode of H_w
    - by adding extra terms or by using an admissible gauge action.

$$S_G = \begin{cases} \beta \sum \dfrac{1 - \mathrm{Re}\,Tr[P_{\mu\nu}]/3}{1 - (1 - \mathrm{Re}\,Tr[P_{\mu\nu}]/3)/\varepsilon} & (\text{for}\, 1 - \mathrm{Re}\,Tr[P_{\mu\nu}]/3 < \varepsilon) \\ \infty & \end{cases}$$

$$\det[{H_W}^2 + \mu^2]$$

Luscher, NPB549 (1999)
Izubuchi, Dawson (RBC) NPB ProcSuppl 106(2002)
Bietenholz, Jansen, Nagai, Necco, Scorzato, Shcheredin, JHEP 0603 (2006)
Fukaya, Hashimoto, Hirohashi, Ogawa, Onogi; PRD73(2006)
JLQCD: Fukaya et al. PRD74(2006),
Vranas, PRD74(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

$$D_{TROV} = \varepsilon^T P^\dagger \left[\left(D_{DWF(N_5, m_f=1)} \right)^{-1} D_{DWF(N_5, m_f)} \right] P \varepsilon \xrightarrow[N_5 \to \infty]{} m_f + (1 - m_f) D_{OV}$$

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

  - Partial fraction type

$$D_{TROV} = 1 + \gamma_5 H_W \left(\alpha_0 + \sum_{j=1}^{N} \frac{\alpha_j}{H_W + \beta_j} \right) \xrightarrow[N \to \infty]{} 2 D_{OV}$$

JLQCD, TWQCD,….

  - Continued fraction type

$$D_{TROV} = 1 + \gamma_5 (\beta_0 H_W + \cfrac{\alpha_1}{\beta_1 H_W + \cfrac{\alpha_2}{\beta_1 H_W + \cfrac{\alpha_3}{\ddots + \cfrac{\ddots \alpha_{2N}}{}}}}) \xrightarrow[N \to \infty]{} 2 D_{OV}$$

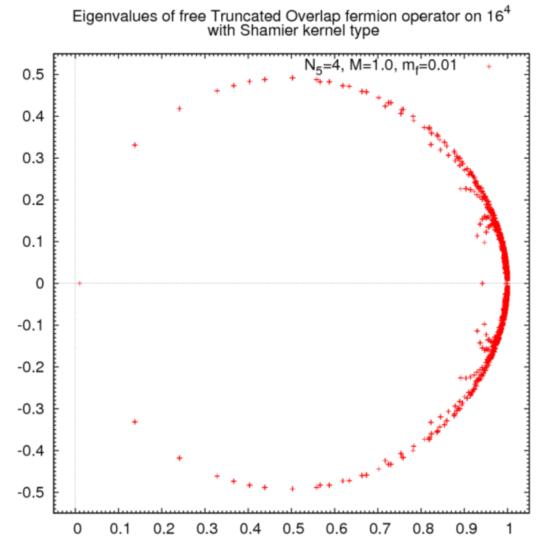
Borici'99, NrayananNeubeger'00, Edwards et al'05.

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?
  - c.f. Nf=2 Dynamical Domain wall simulation:

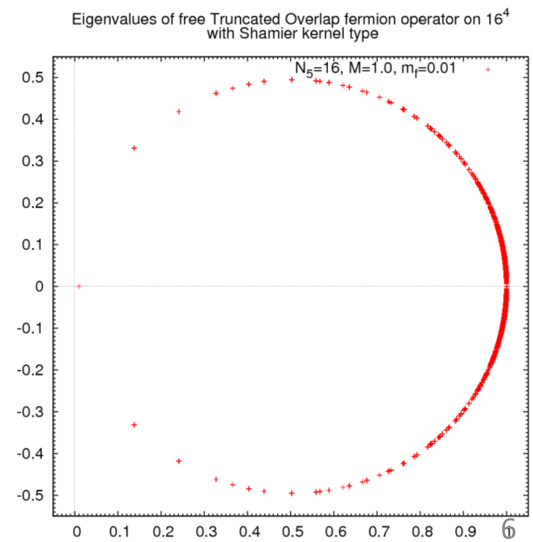
    Y.Aoki et al., PRD72(2005)

    S.Shaefer, PoS(Lat06)



Trunc'd OV with DWF kernel(N5=4)

- 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)

$$Z = \int DU \det\left[D_{OV}\right]^2 e^{-S_G[U]}$$
$$= \int DU \det\left[D_{OV} / D_{TROV(1)}\right]^2 \det\left[D_{TROV(1)} / D_{TROV(2)}\right]^2 \cdots$$
$$\cdots \det\left[D_{TROV(Nstep-1)} / D_{TROV(Nstep)}\right]^2 \det\left[D_{TROV(Nstep)}\right]^2 e^{-S_G[U]}$$
$$= \int DUD\phi^\dagger D\phi \prod_{j=1}^{Nstep} W_{(J)} \exp\left[-S_G[U] - |D_{TROV(Nstep)}{}^{-1}\phi|^2\right]$$

$D_{TROV(0)} \equiv D_{OV}$: exact sign function (numerically)

$D_{TROV(J)}$: truncated overlap op. (at a finite N_5)

$W_{(J)} = \det\left[D_{TROV(J-1)} / D_{TROV(J)}\right]^2$: reweighting factor (evaluated via noisy method)

  – average over ensemble generated with the truncated overlap fermion.

$$\langle O \rangle = \frac{\int DUO[U] \det\left[D_{OV}\right]^2 e^{-S_G[U]}}{\int DU \det\left[D_{OV}\right]^2 e^{-S_G[U]}} = \left\langle O \prod_{j=1}^{Nstep} W_{(J)} \right\rangle_{TROV(Nstep)} \Big/ \left\langle \prod_{j=1}^{Nstep} W_{(J)} \right\rangle_{TROV(Nstep)}$$

$$\langle X \rangle_{TROV(Nstep)} \equiv \frac{\int DUX[U] \det\left[D_{TROV(Nstep)}\right]^2 e^{-S_G[U]}}{\int DU \det\left[D_{TROV(Nstep)}\right]^2 e^{-S_G[U]}}$$

2. Reweighting

- Reweighting for overlap/Domain wall fermions
  - for Domain wall, Chirality improvement : T.Ishikawa, Y.Aoki, T.Izubuchi(RBC-UKQCD), PoS(Lat09)035.
  - for Overlap in epsilon regime: T.DeGrand, PRD78(2008)117504.
  - for Overlap strange quark: H.Ohki et al.(JLQCD) , arXiv:1208.4185[hep-lat]
  - for Domain wall, change mass: Q.Liu et al (RBC-UKQCD), PRD87(2013)054503.

  - 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

A.Borici, hep-lat/0402035
A.Allkoci, A.Borici, PoS(Lat05)099

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

$P\varepsilon = \left(P_L, 0, 0, \cdots, 0, P_R\right)^T$: restrictor from 5D to 4D

- Final step in the reweighing factor requires the exact overlap operator.
  - Optimal Domain wall operator via Zolotarev approximation coefficients

T.-W. Chiu, PRL 90,071601(2003)

  - + Pulling up Low-modes (low-mode improvements)

P.Hernandez, K.Jansen,M.Luscher, [hep-lat/0007015]
K.Jansen, K.Nagai, JHEP12(2003)038

  - => Extension to the even/odd 4d-site precoditioning (New?).

3. Implementation

- Even/odd site preconditioning with low-mode improvements

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

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

- need the inversion of $D_{DWF.}$

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

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

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

$B = \mathrm{diag}(b_1, b_2, \cdots, b_{N_5}),\quad C = \mathrm{diag}(c_1, c_2, \cdots, c_{N_5}),$

$(b_j, c_j$: improvement coefficients, j : 5D-index)

Shamier standard Domain wall: $b_j = a_5, c_j = 0$

$$H_W = \gamma_5 (D_W - m_{dw})(a_5 (D_W - m_{dw})/2 + 1)^{-1}$$

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

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

$$H_W = \gamma_5 D_W$$

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

Gneral, Moebius Domain wall: b_j, c_j

R.Brower,H.Neff,K.Orginos, [arXiv:1206.5214];
Nucl.Phys. ProcSuppl.153(2006)191

3. Implementation

- Even/odd site preconditioning with low-mode improvements

Low-modes of sign kernel *Hw*

$$H_W V_k = V_k \Lambda_k, \quad V_k = (v_1, v_2, \cdots, v_k),$$
$$\Lambda_k = \mathrm{diag}(\lambda_1, \lambda_2, \cdots, \lambda_k)$$

Low-modes improvement for sign kernel *Hw*

$$H_W \to H_W^{imp} = H_W + V_k S_k V_{\mathrm{k}}^{\dagger}$$

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

Low-modes improved Domain wall

Zolotarev coefficients in *B* and *C* and N_5 are optimized with respect to |Hw|

$$W_k = ((a_5/2)(D_W - m_{dw}) + 1)\gamma_5 V_k$$
$$S_k = \mathrm{diag}(\hat{\lambda}_1 - \lambda_1, \hat{\lambda}_2 - \lambda_2, \cdots, \hat{\lambda}_k - \lambda_k)$$
$$\hat{\lambda}_j \equiv 2\mathrm{sign}(\lambda_j) \max_{s=1,\cdots,k} |\lambda_s|$$

$$D_{DWF(N_5 \approx \infty, m_f)} x = b \Leftrightarrow \tilde{D}^{imp}_{DWF(N_5,m_f)} \tilde{x} = b, x = (B + CM_{W5})^{-1} \tilde{x}$$

3. Implementation

- Even/odd site preconditioning with low-mode improvements

$$\tilde{D}^{imp}_{DWF(N_5,m_f)}\tilde{x} = b \qquad \tilde{D}^{imp}_{DWF(N_5,m_f)} = \tilde{D}_{DWF(N_5,m_f)} + W_k S_k^\dagger$$

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

$$\begin{pmatrix} \left(\tilde{D}_{DWF(N_5,m_f)}\right)_{ee} & \left(\tilde{D}_{DWF(N_5,m_f)}\right)_{eo} & \left(W_k\right)_e \\ \left(\tilde{D}_{DWF(N_5,m_f)}\right)_{oe} & \left(\tilde{D}_{DWF(N_5,m_f)}\right)_{oo} & \left(W_k\right)_o \\ \left(S_k^\dagger\right)_e & \left(S_k^\dagger\right)_o & -1 \end{pmatrix} \begin{pmatrix} \tilde{x}_e \\ \tilde{x}_o \\ \zeta \end{pmatrix} = \begin{pmatrix} b_e \\ b_o \\ 0 \end{pmatrix}$$

ζ : auxiliary variable

eliminating x_o and ζ

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

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

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

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

$$\hat{b}_e = \left(\tilde{D}_{DWF}\right)_{ee}^{-1}\left[\begin{array}{l} b_e - \left(\tilde{D}_{DWF}\right)_{eo}\left(\tilde{D}_{DWF}\right)_{oo}^{-1} b_o \\ -\left(W_e - \left(\tilde{D}_{DWF}\right)_{eo}\left(\tilde{D}_{DWF}\right)_{oo}^{-1}W_o\right)G_{oo}S_o^\dagger\left(\tilde{D}_{DWF}\right)_{oo}^{-1} b_o \end{array}\right]$$

$$\tilde{x}_o = \left(\tilde{D}_{DWF}\right)_{oo}^{-1}\left[\begin{array}{l} b_o - \left(\tilde{D}_{DWF}\right)_{oe}\tilde{x}_e \\ -W_o G_{oo}\left\{\left(S_e^\dagger - S_o^\dagger\left(\tilde{D}_{DWF}\right)_{oo}^{-1}\left(\tilde{D}_{DWF}\right)_{oe}W_o\right)\tilde{x}_e + S_o^\dagger\left(\tilde{D}_{DWF}\right)_{oo}^{-1} b_o\right\} \end{array}\right]$$

4. Results

- Very preliminary
  - Test on Quench configurations
    (10 configs, DBW2 gauge action beta=0.87, 8^3x32)

[explored by Y.Aoki et al.(RBC), PRD69(2004)074504]

[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: $\dfrac{\eta^\dagger \Delta_{GW} \eta}{\eta^\dagger \eta}$ $\quad \eta:$ Gaussian noise vector

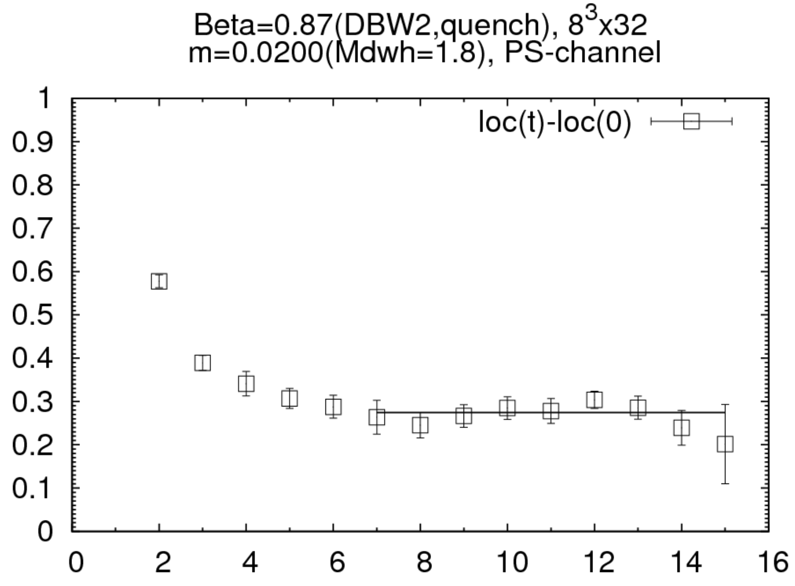
$$\Delta_{GW} \equiv \left\{ \gamma_5, \ (D_{OV/TROV})^{-1} \right\} - \frac{2}{1+m_f} \left[m_f (D_{OV/TROV})^{-1} \gamma_5 (D_{OV/TROV})^{-1} + \gamma_5 \right]$$

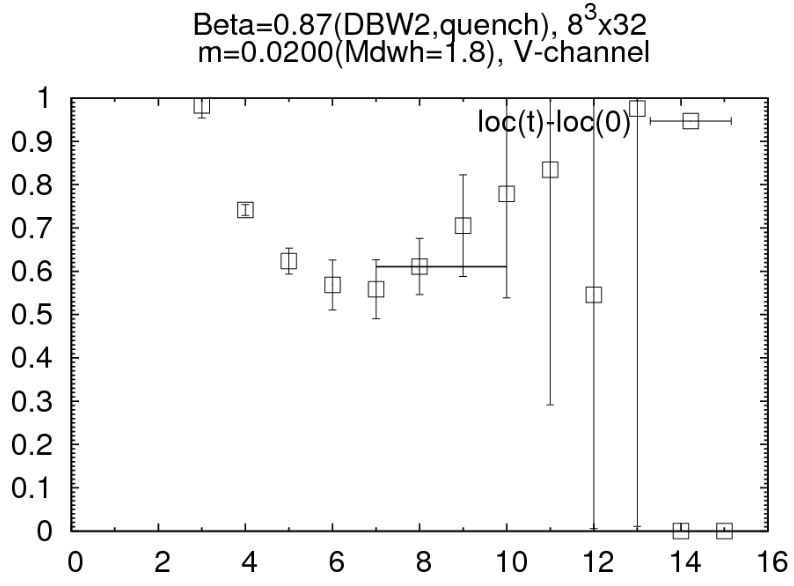
    - exponent in reweighting factor : $dS \equiv \left| (D_{TROV(j-1)})^{-1} D_{TROV(j)} \eta \right|^2 - |\eta|^2$
    - reweighting factor : $\exp(-dS)$ $\quad \eta:$ Gaussian noise vector

No meson spectrum measurement with reweighing….

4. Results

- meson masses N_5=12



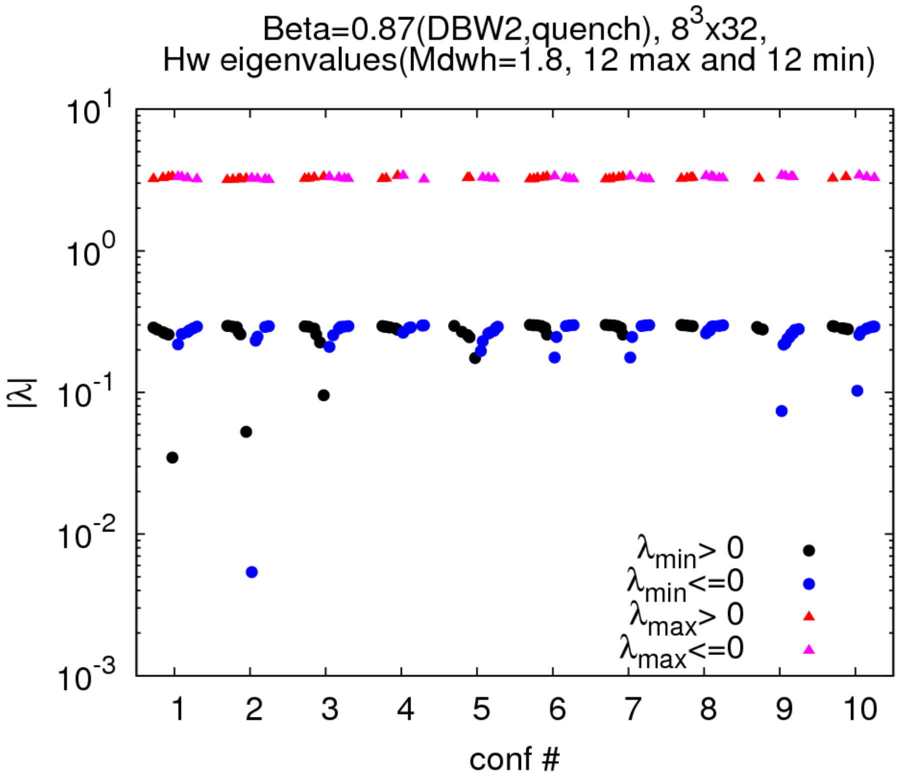


- M_{PS}= 0.274(21), M_V=0.611(65)
- M_{PS}/M_V=0.45

RBC,PRD69(2004), 16^3x32, N_5=16,Domain wall
M_{PS}= 0.2997(19), M_V=0.640(17)

4. Results

- 12 interior/exterior eigen vaules of *Hw*

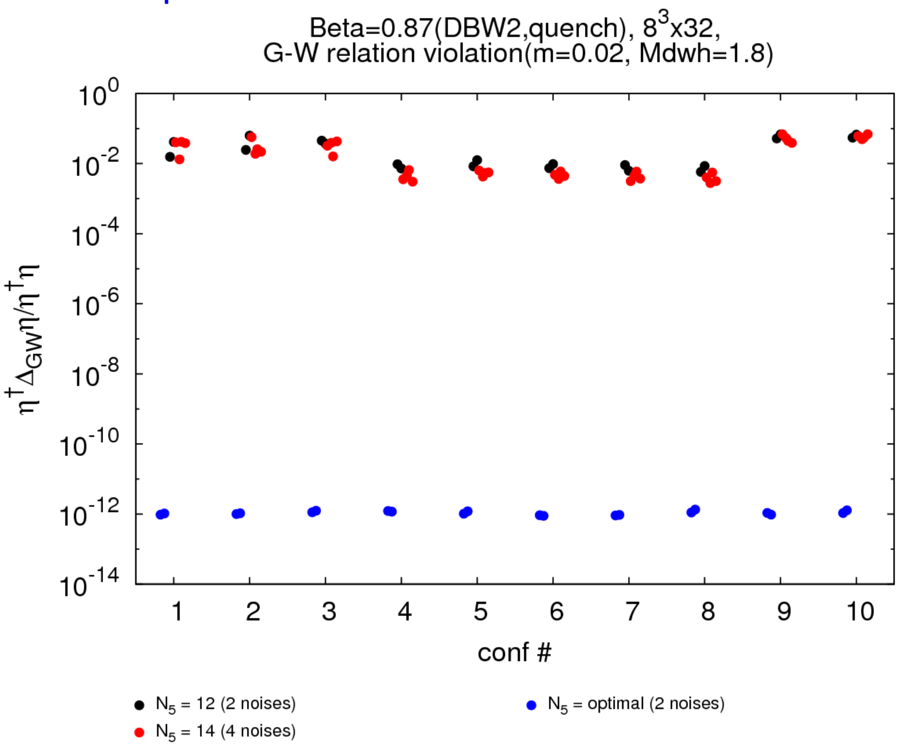


Small |Hw| in conf # 1,2,3,9 10

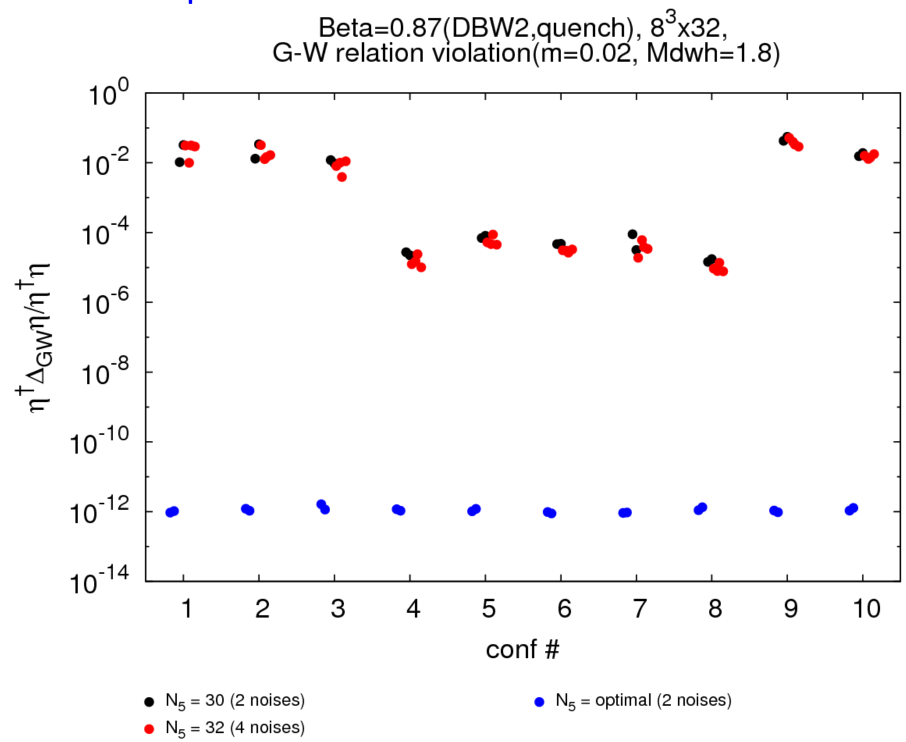
$\Rightarrow$ large G.-W. relation violation is expected with a fixed N5.

4. Results

- G.-W. relation violation N5=12,14, and optimal



- G.-W. relation violation N5=30,32, and optimal



Small |Hw| in conf # 1,2,3, 9, 10
$\Rightarrow$ large G.-W. relation violation.

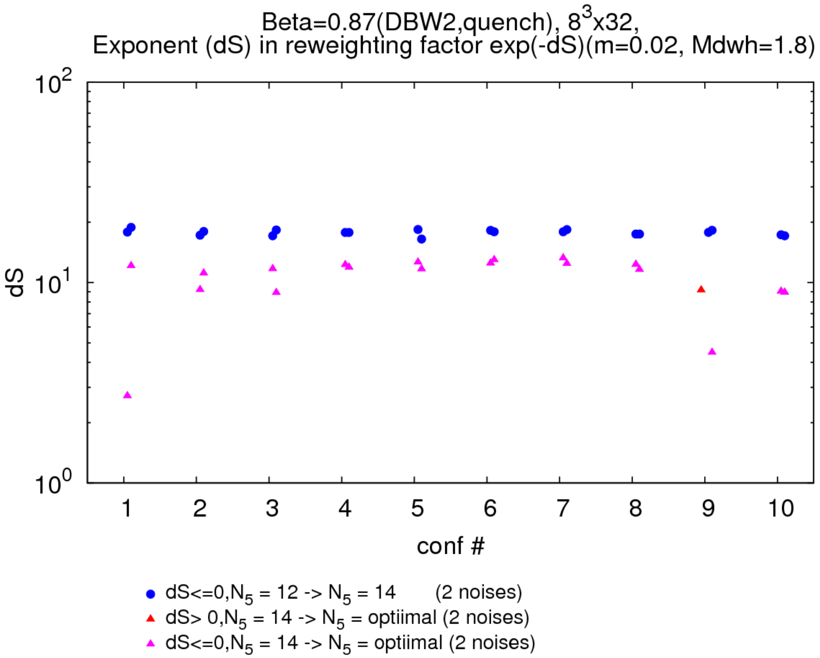
Optimal operator keeps the violation at the tolerance level as it should be.

We used:
m=0.02
optimal Zolotarev tolerance 10^{-12}
eigen solver tolerance 10^{-12}

4. Results

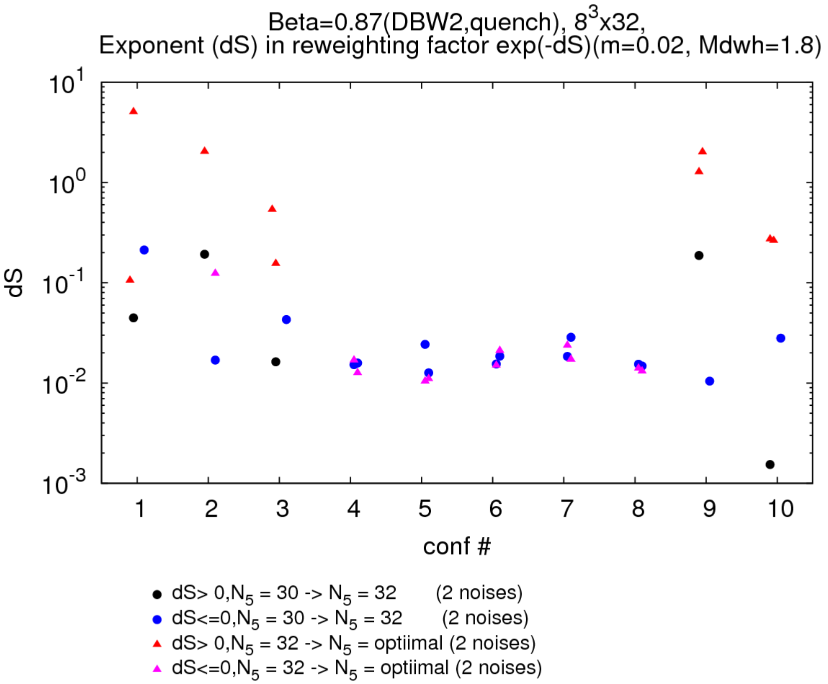
- Exponent *dS*

  N5=12->14 and 14->Optimal



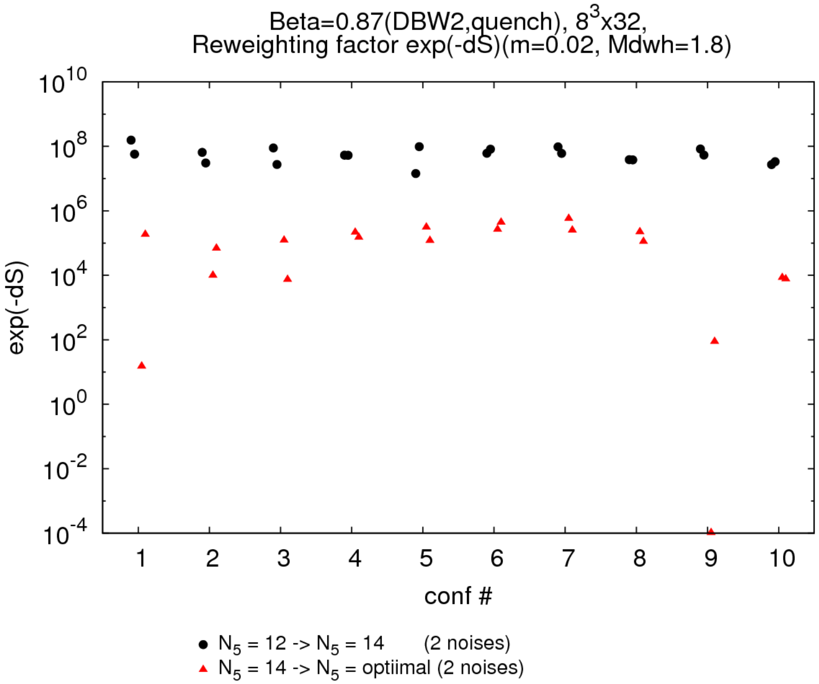
- Exponent *dS*

  N5=30->32 and 32->Optimal

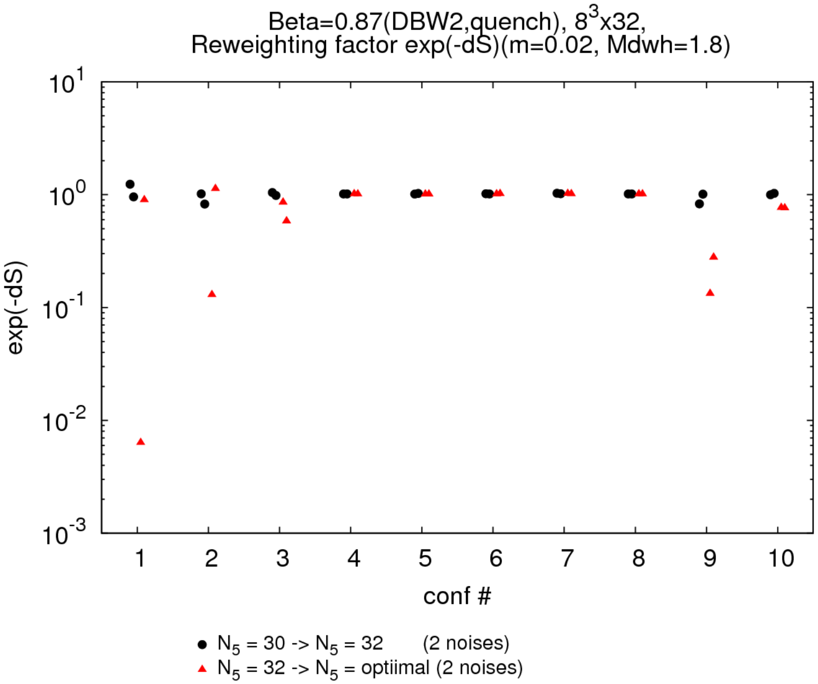


4. Results

- Reweighing factor exp(-*dS*)
  N5=12->14 and 14 -> optimal



- Reweighing factor exp(-*dS*)
  N5=30->32 and 32 -> 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

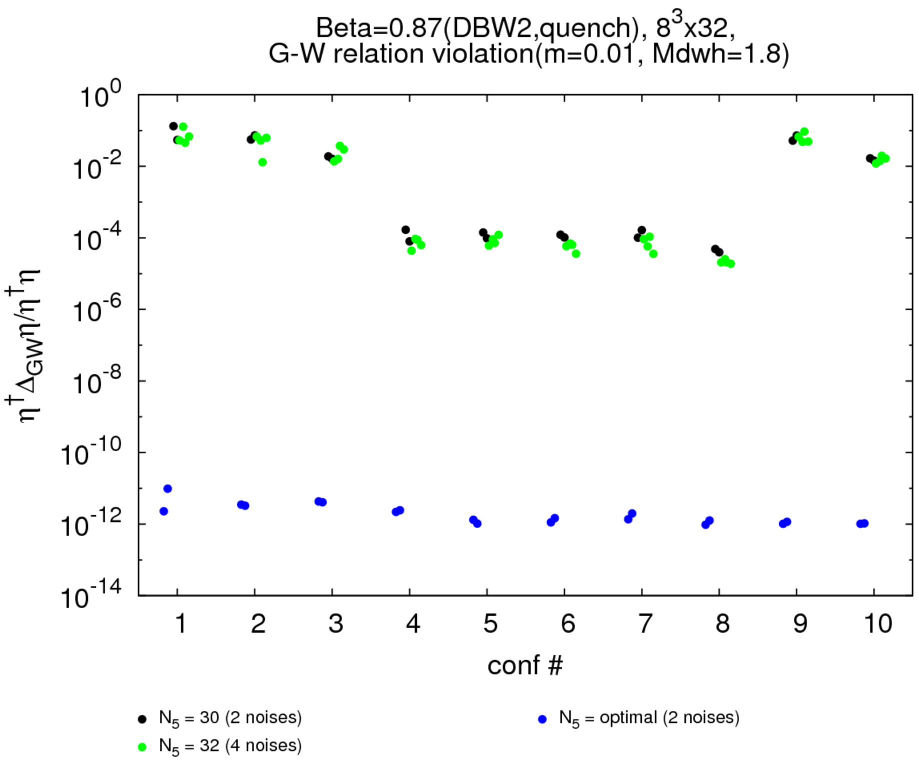
- Needs methods for Lattice chiral symmetry with lower computational cost
- One possibility: Truncated/approximate overlap Dirac operator with reweighting method
- We tested:
  - Truncated overlap fermions on top of the Domain wall fermion.
  - the G.-W. relation violation and reweighting factor are 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

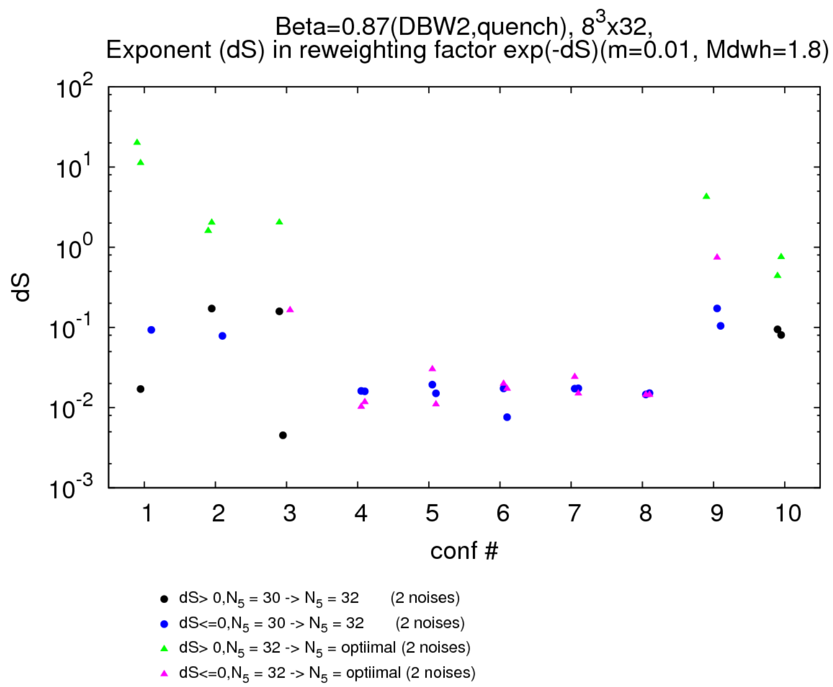
- G.-W. relation violation



Backups

- Quench, m=0.01

- Exponent *dS*



- Reweighing factor exp(-*dS*)