Overlap/Domain-wall reweighting

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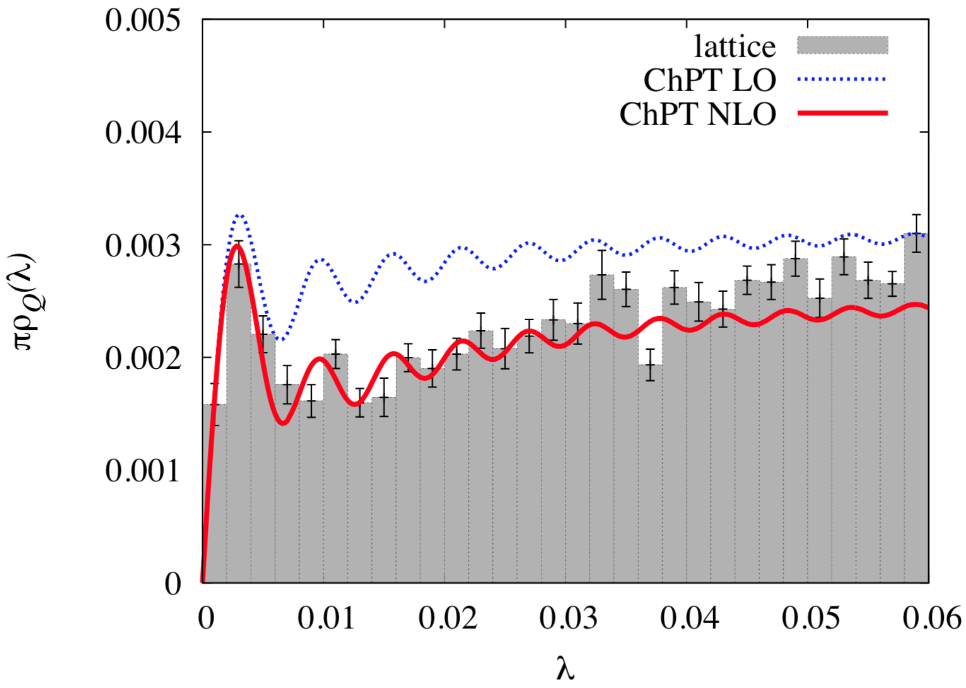
[JLQCD collaboration]

JLQCD collaboration

JLQCD (+TWQCD) collaboration
2006-2012

We have been simulating QCD with overlap quarks.



New project launched.

Simulations on bigger & finer lattices started.

Computers @KEK: SR11000 (2 TFLOPS) + BG/L (57 TFLOPS)
→ SR16000 (55 TFLOPS) + BG/Q (1.2 PFLOPS)

Lattice cut-off : 1.8 GeV → 2.4, 3.6, 4.2 GeV

Lattice size : 16^3 x48 → 32^3 x64, 48^3x96, 64^3x128

(Physical size : 1.8 fm → 2.6 fm ~ 4 fm)

Fermion action : overlap fermion→ DomainWall(Mobius) fermion

Hitachi SR16000

IBM Blue Gene/Q

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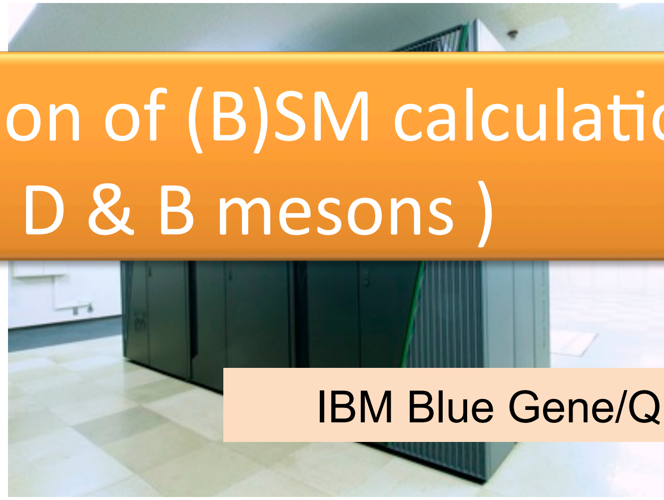
Our goal = high precision of (B)SM calculations
(in particular, D & B mesons)

Hitachi SR16000



IBM Blue Gene/Q

Overlap vs. Domain-wall

Theoretically, they are just different expressions (approximations) of the same action:

$$D_{ov} = \frac{m_0 + m}{2} + \frac{m_0 - m}{2} \gamma_5 \mathrm{sgn} H_T$$

$$D_{DW} = \frac{m_0 + m}{2} + \frac{m_0 - m}{2} \gamma_5 \frac{(1 + H_T)^n - (1 - H_T)^n}{(1 + H_T)^n - (1 - H_T)^n}$$

In this talk, let me *define*

Overlap : 10^{-8} precision of chiral symmetry

(m_{res} ~ 10 eV)

Domain-wall : 10^{-3} or less. (m_{res} ~ 1 MeV)

[cf. non-chiral D : m_{res} ~ 1 GeV.]

Overlap vs. Domain-wall

Numerical differences

Domain-wall : good for HMC.

+ cheaper numerical cost, topology tunnelings.

- chiral sym. violation, eigenvalues need

  5D eigen vectors

Overlap : good for Measurements.

+ clean analysis with exact chiral symmetry.

  recycling eigen values/vectors (for different m)

- high numerical cost, topology tunnelings difficult

  (we fixed the topology in our previous works.)

Overlap/Domain-wall reweighting

Let's use both fermions with reweighting.

HMC with domain-wall fermions

+

Measurements with overlap fermions

$$\langle O \rangle_{\text{overlap}} = \left\langle O \frac{\det D_{ov}^{N_f}}{\det D_{DW}^{N_f}} \right\rangle_{\text{DW}}$$

Ishikawa, Algorithms & machines, Monday

Exact chiral symmetry, topology changes with reasonable numericial cost.

Overlap/Domain-wall reweighting

Our goal = to find the optimal implementations for D_{DW} & D_{ov}.

$$D_{ov/DW} = \frac{m_0}{2}\left(1 + \gamma_5 \mathrm{sgn} H\right)$$

Approximation for sgn function

Kernel operator

1. D_{DW} with a reasonable numerical HMC cost, and marginal chiral condition.
2. D_{ov} with a good overlap in configurations generated by D_{DW} and good chirality

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2. Overlap vs. Domain-wall
3. Preliminary lattice results
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2. Overlap vs. Domain-wall

Domain-wall fermion [Kaplan 1992, Shamir 1993 …]

and its variations, [Borici, Chiu, Brower …]

summarized by Edwards-Heller (2000) :

$$D^5_{GDW} \equiv \begin{pmatrix} (D^1_-)^{-1}D^1_+ & -P_- & 0 & \cdots & 0 & mP_+ \\ -P_+ & (D^2_-)^{-1}D^2_+ & -P_- & 0 & \cdots & 0 \\ 0 & -P_+ & (D^3_-)^{-1}D^3_+ & -P_- & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \ddots & -P_+ & (D^{L_s-1}_-)^{-1}D^{L_{s-1}}_+ & -P_- \\ mP_- & 0 & \cdots & 0 & -P_+ & (D^{L_s}_-)^{-1}D^{L_s}_+ \end{pmatrix}$$

$$D^s_+ = 1 + b_s D_W(-M_0),\ D^s_- = 1 - c_s D_W(-M_0); \quad P_\pm = (1 \pm \gamma_5)/2$$

2. Overlap vs. Domain-wall

4D expression (with Pauli-Villars)

$$\rightarrow \quad \begin{pmatrix} D & C \\ B & A \end{pmatrix} = \begin{pmatrix} 1 & CA^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} D - CA^{-1}B (\equiv S_\chi) & 0 \\ 0 & A \end{pmatrix} \begin{pmatrix} 1 & 0 \\ A^{-1}B & 1 \end{pmatrix}$$

Note: det A = 1

$$D_{DW}{}^{4D} \equiv S_\chi^{-1}(m=1) S_\chi(m) = \frac{1+m}{2} - \frac{1-m}{2} \gamma_5 \frac{T_1^{-1} T_2^{-1} \cdots T_{L_s}^{-1} - 1}{T_1^{-1} T_2^{-1} \cdots T_{L_s}^{-1} + 1}$$

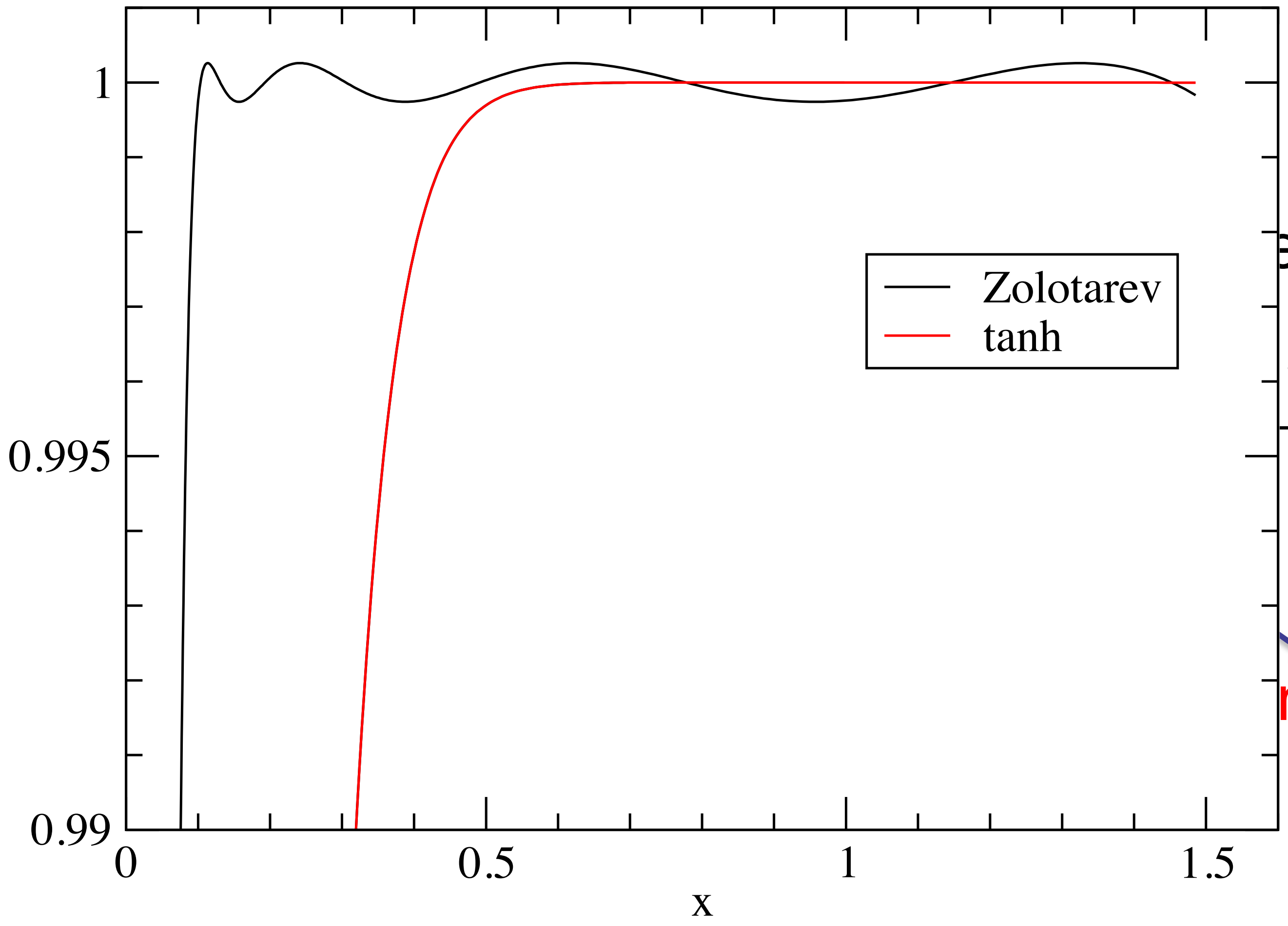
Approximation for sgn function

Kernel operator

2. Overlap vs. Domain-wall

4D expression (with Pauli-Villars)

→



$D_{DW}^{4D} \equiv$

e: det A = 1

$$\cdots T_{L_s}^{-1} - 1$$

$$\cdots T_{L_s}^{-1} + 1$$

nel operator

2. Overlap vs. Domain-wall

Overlap fermion [Neuberger 1998]

Exact treatment of the low-modes of the kernel:

$$D_{ov} = \underbrace{\frac{1}{2}\sum_{\lambda_i<\lambda_{th}} (1+\gamma_5 \mathrm{sgn}\lambda_i)\,|\lambda_i\rangle\langle\lambda_i|}_{\text{Exact low modes}} + \underbrace{D_{DW}^{4D}\left(1-\sum_{\lambda_i<\lambda_{th}}|\lambda_i\rangle\langle\lambda_i|\right)}_{\text{High modes}},$$

allows us 10^{-8} chirality with Ls=O(10).

→ Exact chiral symmetry [L¨uscher 1998]

through the Ginsparg-Wilson relation [1982] :

$$D_{ov}(0)\gamma_5 + \gamma_5 D_{ov}(0) = D_{ov}(0)\gamma_5 D_{ov}(0)/m_0.$$

2. Overlap vs. Domain-wall

Overlap/Domain-wall reweighting

$$(D_{DW}^{4D})^{-1} D_{ov} = 1 + \sum_{\lambda_i < \lambda_{th}} ((D_{DW}^{4D})^{-1} D_{ov} - 1)|\lambda_i\rangle\langle\lambda_i|$$

Only sub-volume of matrix contributes.

2. Overlap vs. Domain-wall

Overlap/Domain-wall reweighting

$$(D_{DW}^{4D})^{-1} D_{ov} = 1 + \sum_{\lambda_i < \lambda_{th}} ((D_{DW}^{4D})^{-1} D_{ov} - 1) |\lambda_i\rangle\langle\lambda_i|$$

Only sub-volume of matrix contributes.

Let's reweight them !

$$\langle O \rangle_{\text{overlap}} = \left\langle O \frac{\det D_{ov}^{N_f}}{\det D_{DW}^{N_f}} \right\rangle_{\text{DW}}$$

3. Preliminary lattice results

Domain-wall fermion for sea quarks

Our choice [T. Kaneko Tue (Chiral), S. Hashimoto, poster]

Kernel = scaled Shamir Kernel:

$$2H_T = \gamma_5 \frac{2D_W}{2+D_W}$$

Sgn function = Tanh:

$$\mathrm{sgn}_{\tanh}(2H_T) = \frac{(1+2H_T)^{L_s} - (1-2H_T)^{L_s}}{(1+2H_T)^{L_s} + (1-2H_T)^{L_s}} = \tanh(L_s \tanh^{-1}(2H_T))$$

Ls = 12

⇒ m_{res}<0.5MeV, Chiral symmetry ~ 10^{-3}

3. Preliminary lattice results

Simulation parameters

Lattice size : 16^3x32(x12) [test runs]

Symanzik gauge action with β=4.17

3 steps of stout smearing

2+1 DWF m_{ud}= 0.7 m_s, m_s ~ physical point

1/a ~ 2.4 GeV ,   L ~ 1.3 fm

(L=32(2.6fm), L=48(3.9fm) lattices running.)

[Simulated w/ Iroiro++ code, G. Cossu, poster]

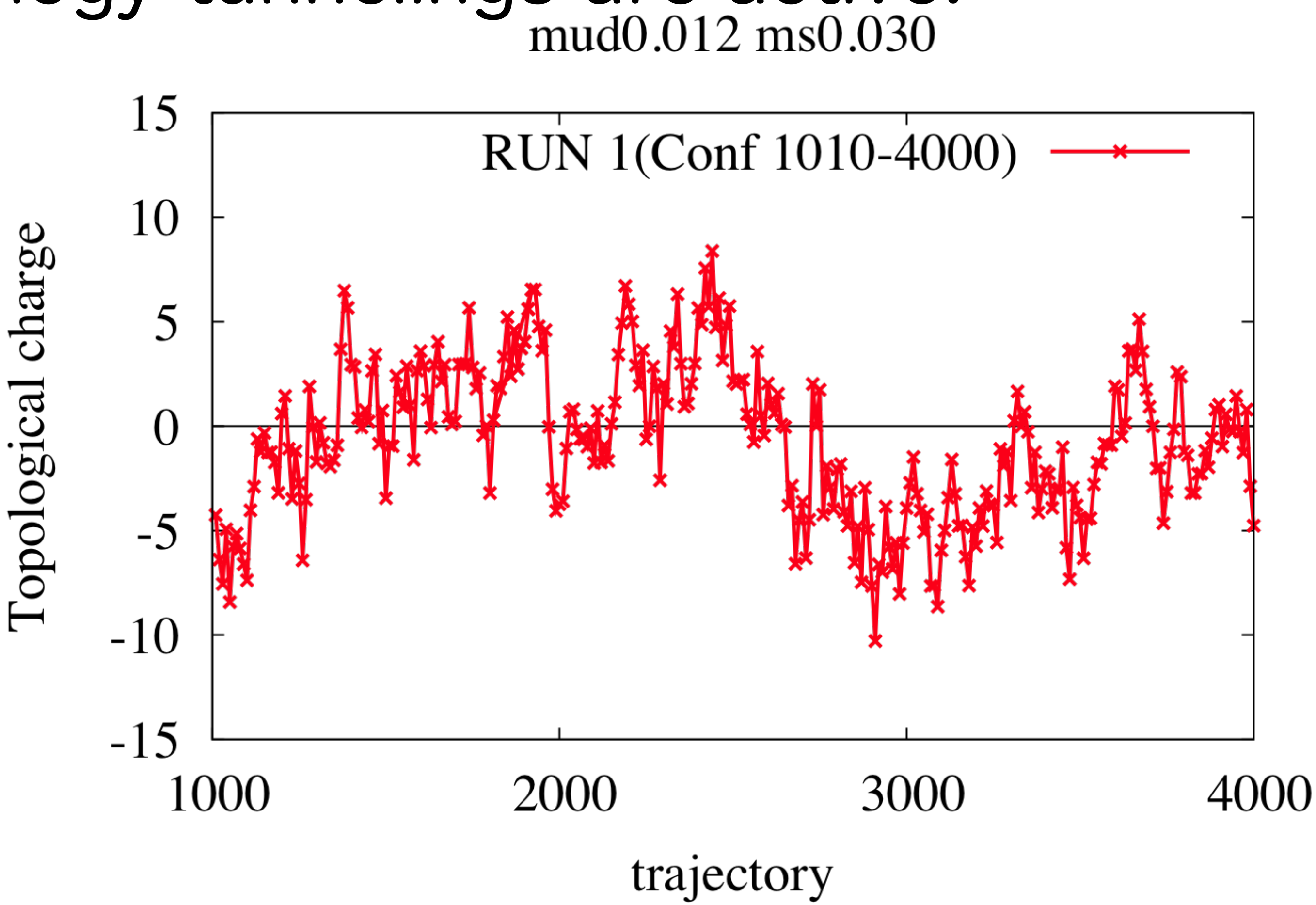
Faster than conventional DW (x4)

while reducing m_{res} to 1/10.

3. Preliminary lattice results

Domain-wall fermion for sea quarks

Topology tunnelings are active.



3. Preliminary lattice results

Overlap fermion for valence quarks

$$D_{ov} = \underbrace{\frac{1}{2}\sum_{\lambda_i<\lambda_{th}} (1+\gamma_5 \mathrm{sgn}\lambda_i)\,|\lambda_i\rangle\langle\lambda_i|}_{\text{Exact low modes}} + \underbrace{D^{4D}_{DW}\left(1-\sum_{\lambda_i<\lambda_{th}}|\lambda_i\rangle\langle\lambda_i|\right)}_{\text{High modes}},$$

We try different

1. sgn functions : Zolotarev or Tanh for D^{4D}_{DW}
2. value of threshold λ_{th} for exact treatment of low-modes of H_T,
3. Ls (5^{th} direction) .

3. Preliminary lattice results

Chiral symmetry violation

+ & - eigenpairs of $H_{ov} = \gamma_5 D_{ov}$:

$$H_{ov}|\lambda\rangle = \lambda|\lambda\rangle$$

$$\to H_{ov}\Gamma_5|\lambda\rangle = -\lambda\Gamma_5|\lambda\rangle$$

$(\Gamma_5 = \gamma_5(1 - aD_{ov}/2))$

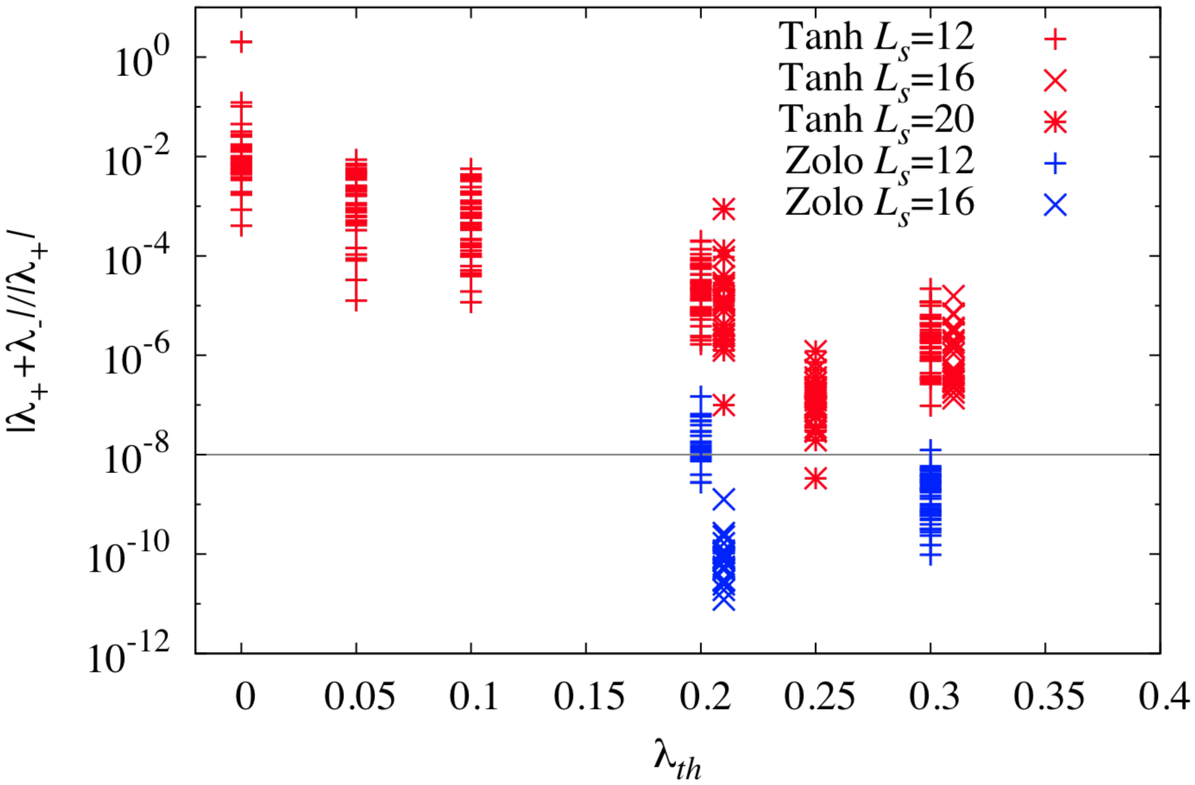
$\left|\frac{\lambda_+ + \lambda_-}{\lambda_+}\right| \simeq$ the precision of the GW relation.

$(|\lambda_{\mathrm{zero}}| - m$ as well)

3. Preliminary lattice results

Chiral symmetry : +/- degeneracy

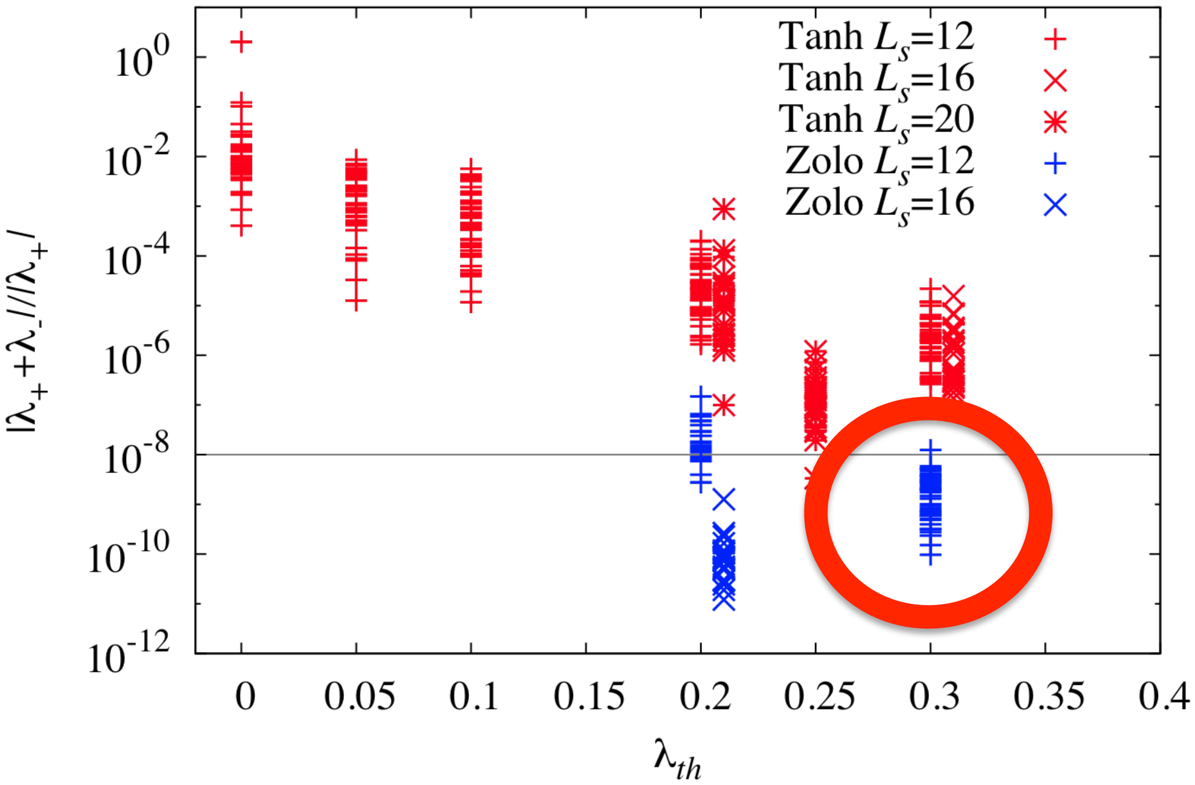
$$D_{ov} = \frac{1}{2}\sum_{\lambda_i<\lambda_{th}} (1+\gamma_5 \mathrm{sgn}\lambda_i)\,|\lambda_i\rangle\langle\lambda_i| + D_{DW}^{4D}\left(1-\sum_{\lambda_i<\lambda_{th}}|\lambda_i\rangle\langle\lambda_i|\right)$$



3. Preliminary lattice results

Chiral symmetry : +/- degeneracy

$$D_{ov} = \frac{1}{2} \sum_{\lambda_i < \lambda_{th}} (1 + \gamma_5 \mathrm{sgn}\lambda_i) |\lambda_i\rangle\langle\lambda_i| + D_{DW}^{4D} \left(1 - \sum_{\lambda_i < \lambda_{th}} |\lambda_i\rangle\langle\lambda_i|\right)$$



Our choise :

$$\mathrm{Zolotarev}[0.3, 1.65]$$

$$\lambda_{\mathrm{th}} = 0.3,$$

$$L_s = 12.$$

3. Preliminary lattice results

Reweighting factor

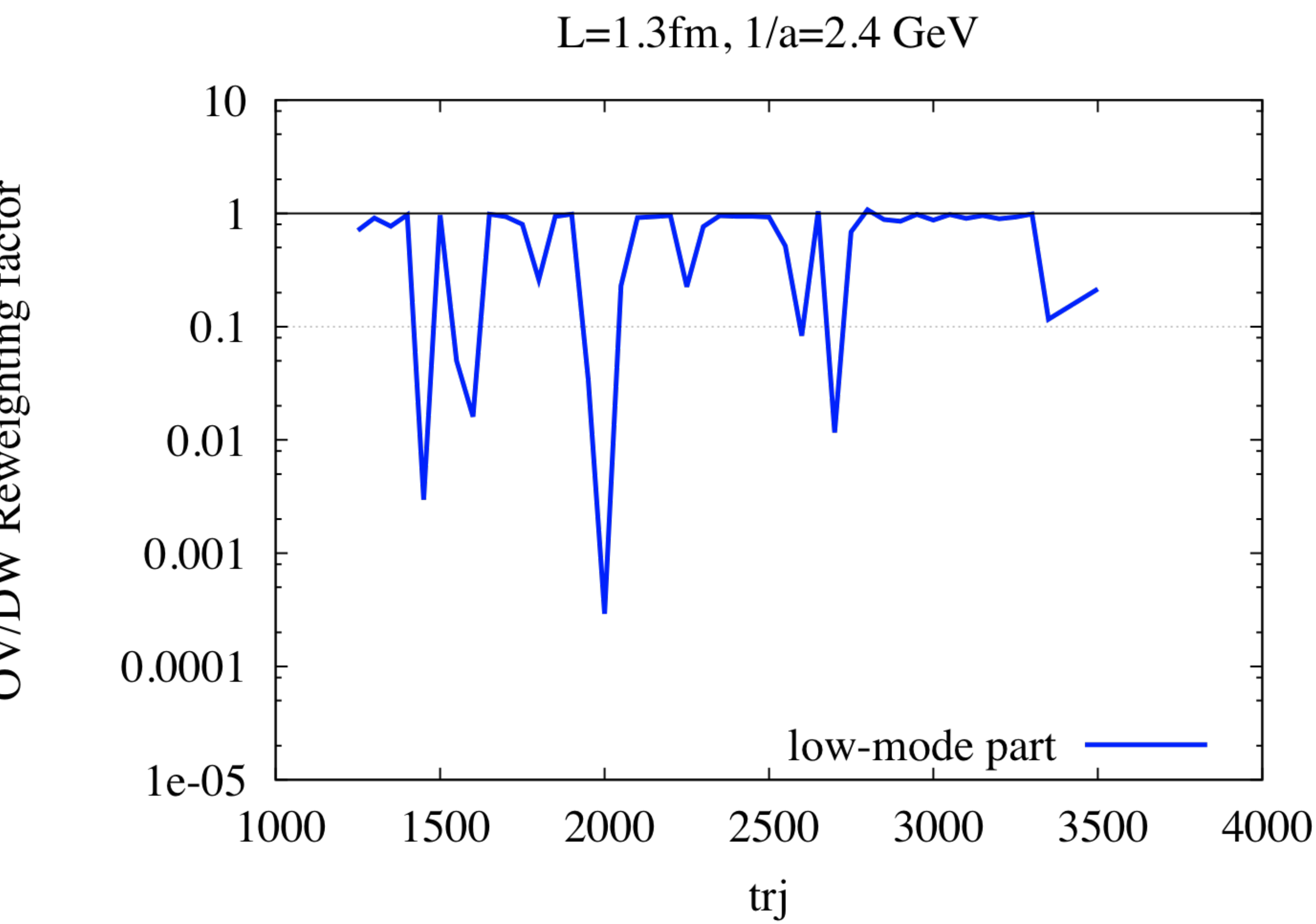
$$D_{ov} = \text{Zolotarev},\ L_s = 12,\ \text{exact lowmodes}\ (\lambda_{th} = 0.3),$$
$$D_{DW} = \text{Tanh with}\ L_s = 12,\ \text{w/o lowmode precond.},$$

$$R = \left(\frac{\det \gamma_5 D_{ov}(m_{ud})}{\det \gamma_5 D_{DW}(m_{ud})}\right)^2 \frac{\det \gamma_5 D_{ov}(m_s)}{\det \gamma_5 D_{DW}(m_s)}$$
$$= \prod_{i=1}^{100} \left(\frac{\lambda_i^{ov}(m_{ud})}{\lambda_i^{DW}(m_{ud})}\right)^2 \left(\frac{\lambda_i^{ov}(m_s)}{\lambda_i^{DW}(m_s)}\right) \times \text{high-mode part}$$

High mode part is stochastically estimated with 60 - 300 Gaussian noises.

3. Preliminary lattice results

Results (with 46 confs separated by 50 trj)



3. Preliminary lattice results

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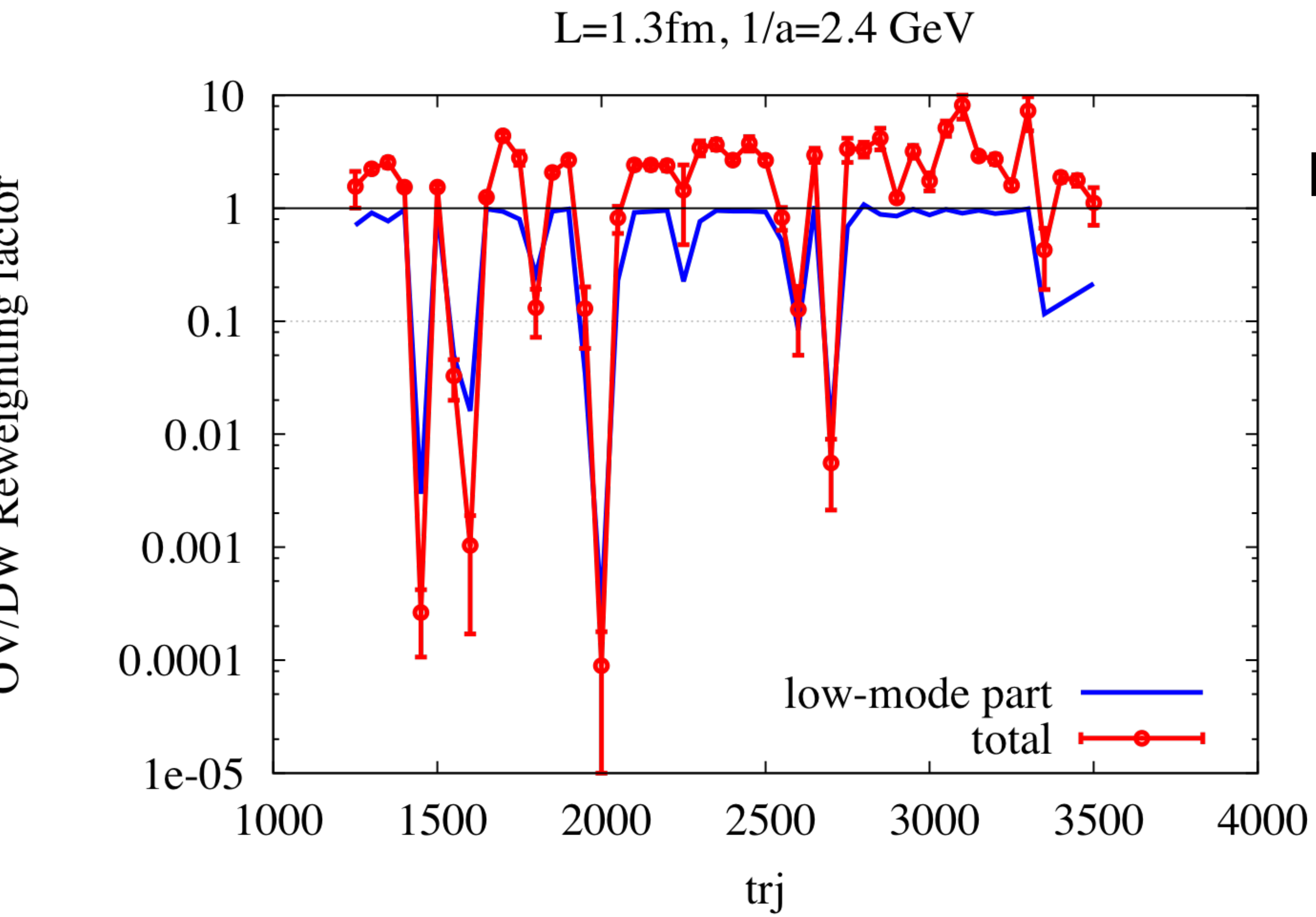


For 80 % of confs,

R = 1~ 4.

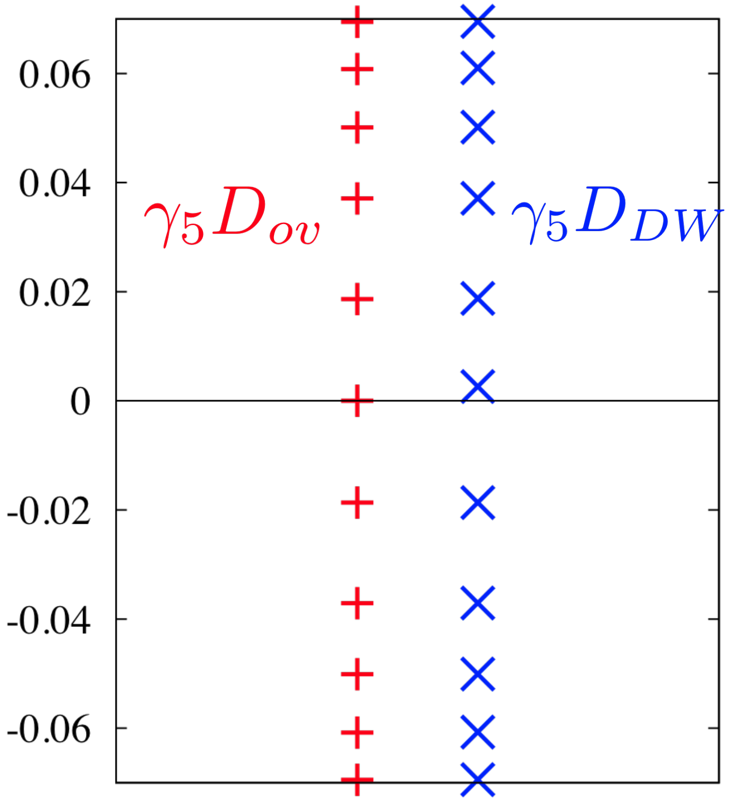
but for 20%,

R is VERY small.

3. Preliminary lattice results

Mismatch in topological charge ?

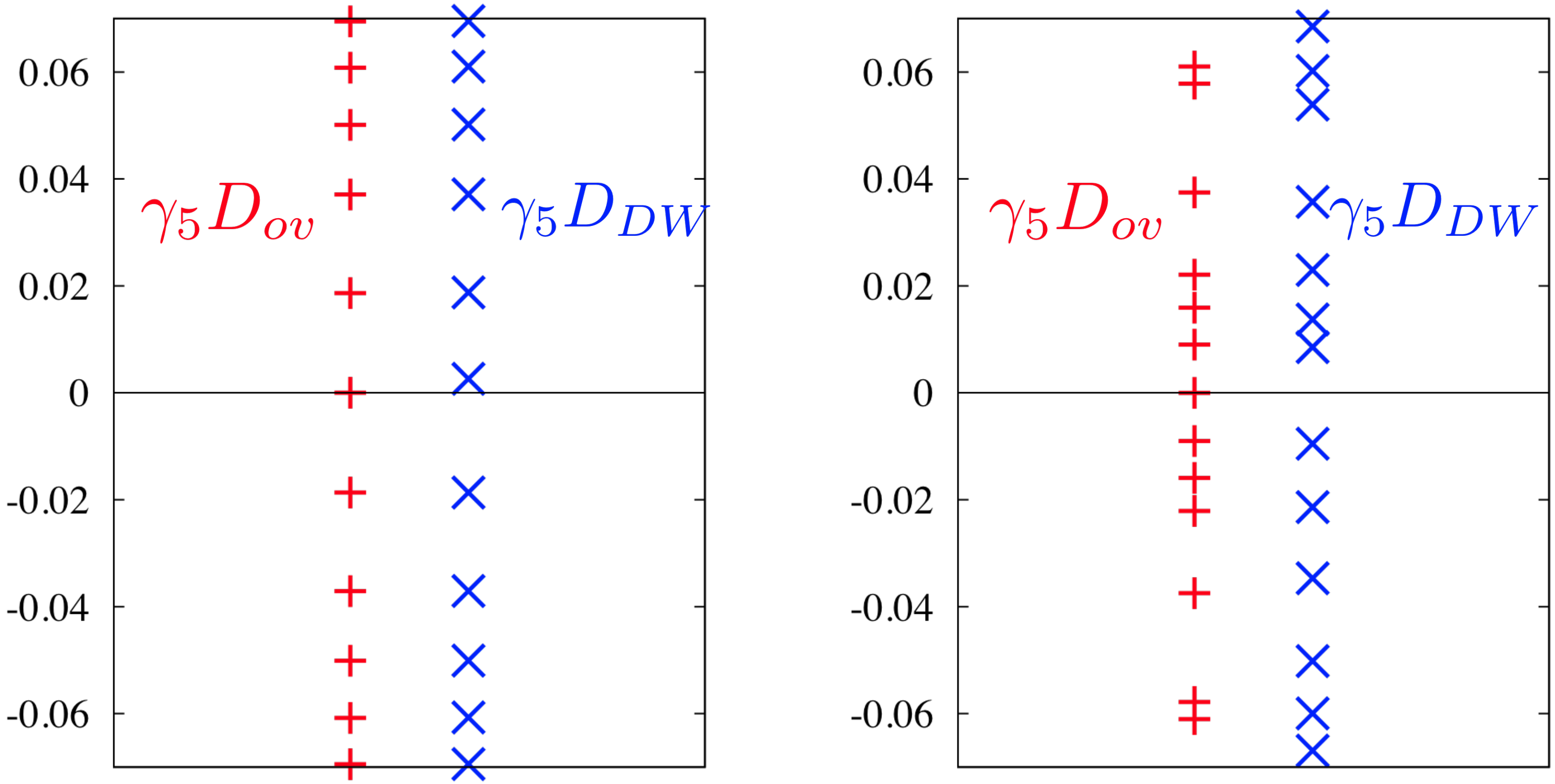
Conf1400 [R=1.54(6)]



3. Preliminary lattice results

Mismatch in topological charge ?

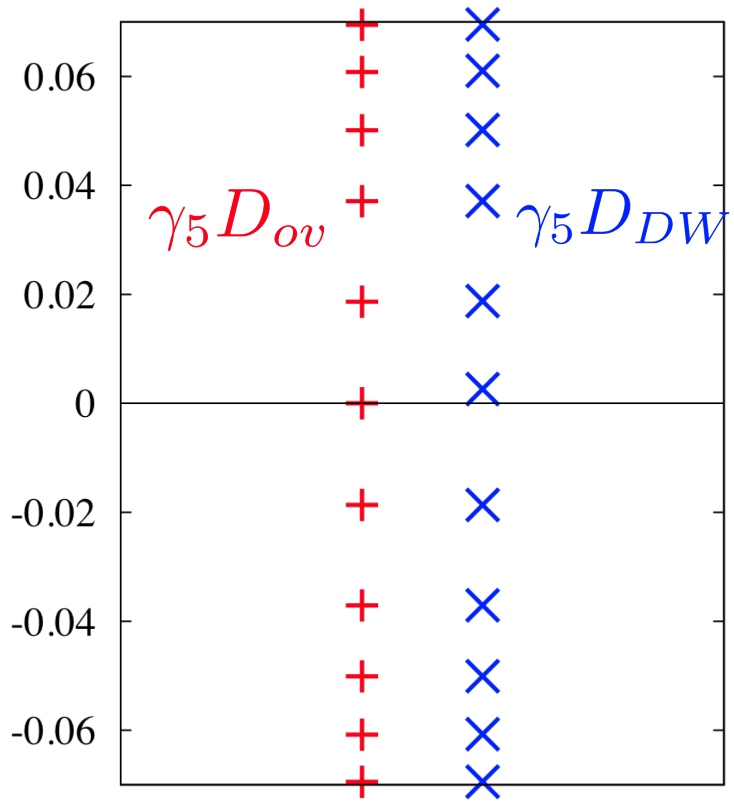
Conf1400 [R=1.54(6)]　　Conf2000 [R=0.00009(8)]



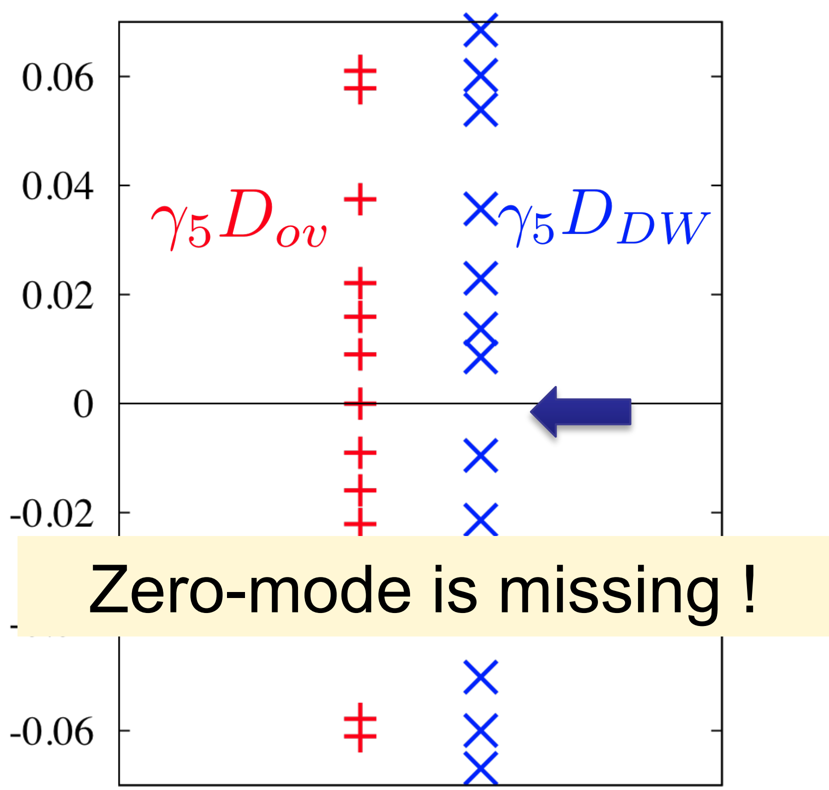
3. Preliminary lattice results

Mismatch in topological charge ?

Conf1400 [R=1.54(6)]



Conf2000 [R=0.00009(8)]



4. Summary

D_{ov} and D_{DW} are just different expressions (approximations) of the same operator:

$$D_{ov} = \frac{m_0+m}{2} + \frac{m_0-m}{2}\gamma_5 \mathrm{sgn} H_T$$

$$D_{DW} = \frac{m_0+m}{2} + \frac{m_0-m}{2}\gamma_5 \frac{(1+H_T)^n-(1-H_T)^n}{(1+H_T)^n-(1-H_T)^n}$$

1. Reweighting using

$$D_{ov} = \text{Zolotarev, } L_s = 12, \text{ exact lowmodes } (\lambda_{th} = 0.3),$$

$$D_{DW} = \text{Tanh with } L_s = 12, \text{ w/o lowmode precond.},$$

gives R~O(1) in 80 % configurations.

2. But R is very small when D_{DW} misses topological zero-modes.

4. Summary

To do

1. Any way to avoid mismatches in topology ?
2. Larger volume
3. Smaller quark mass

Other directions :

4. Loosen chirality of sea quarks
5. Isospin breaking effects
6. mixed action

…

Backup slide 1

of the kernel low-modes

$$D_{ov} = \underbrace{\frac{1}{2}\sum_{\lambda_i<\lambda_{th}} (1+\gamma_5 \mathrm{sgn}\lambda_i)\,|\lambda_i\rangle\langle\lambda_i|}_{\text{Exact low modes}} + \underbrace{D_{DW}^{4D}\left(1-\sum_{\lambda_i<\lambda_{th}} |\lambda_i\rangle\langle\lambda_i|\right)}_{\text{High modes}},$$

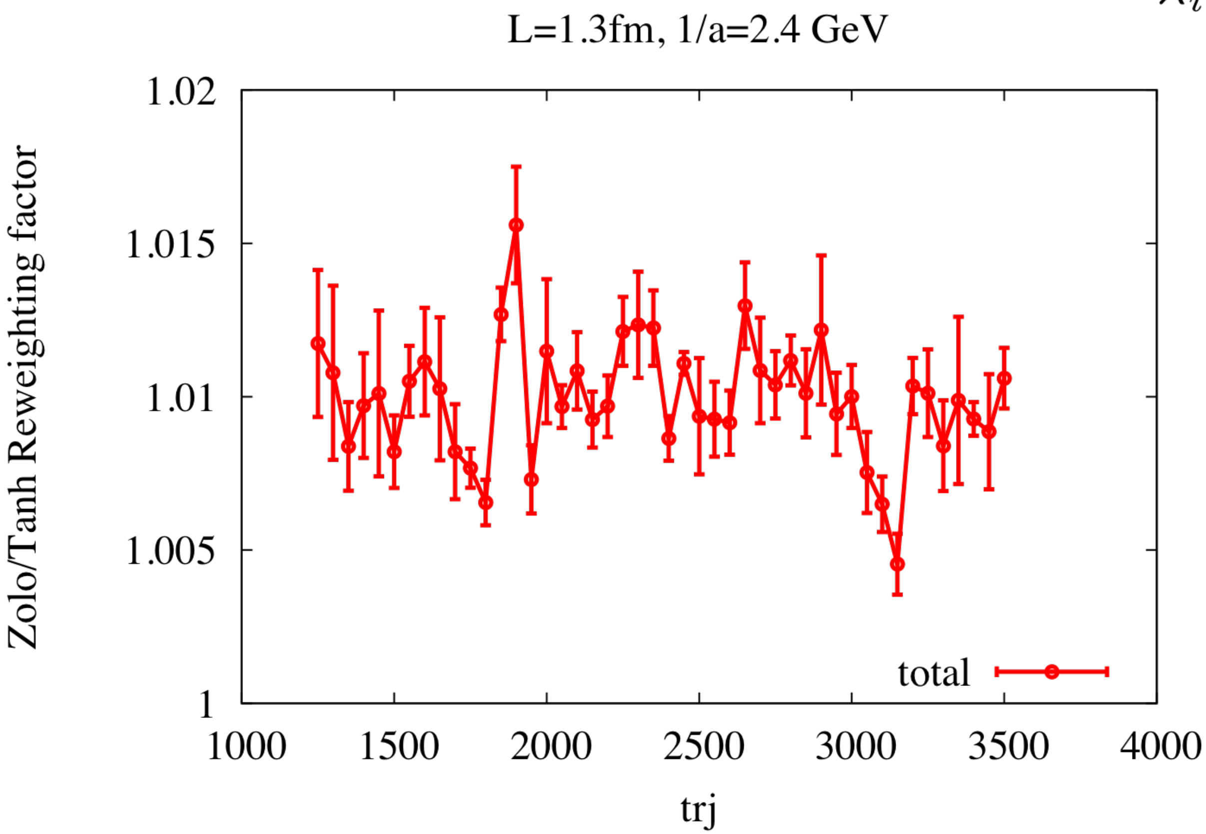
below 0.3, we need

Ls = 16 → ~ 30
Ls = 32 → ~ 300
Ls = 48 → ~ 2400

Backup slide 2

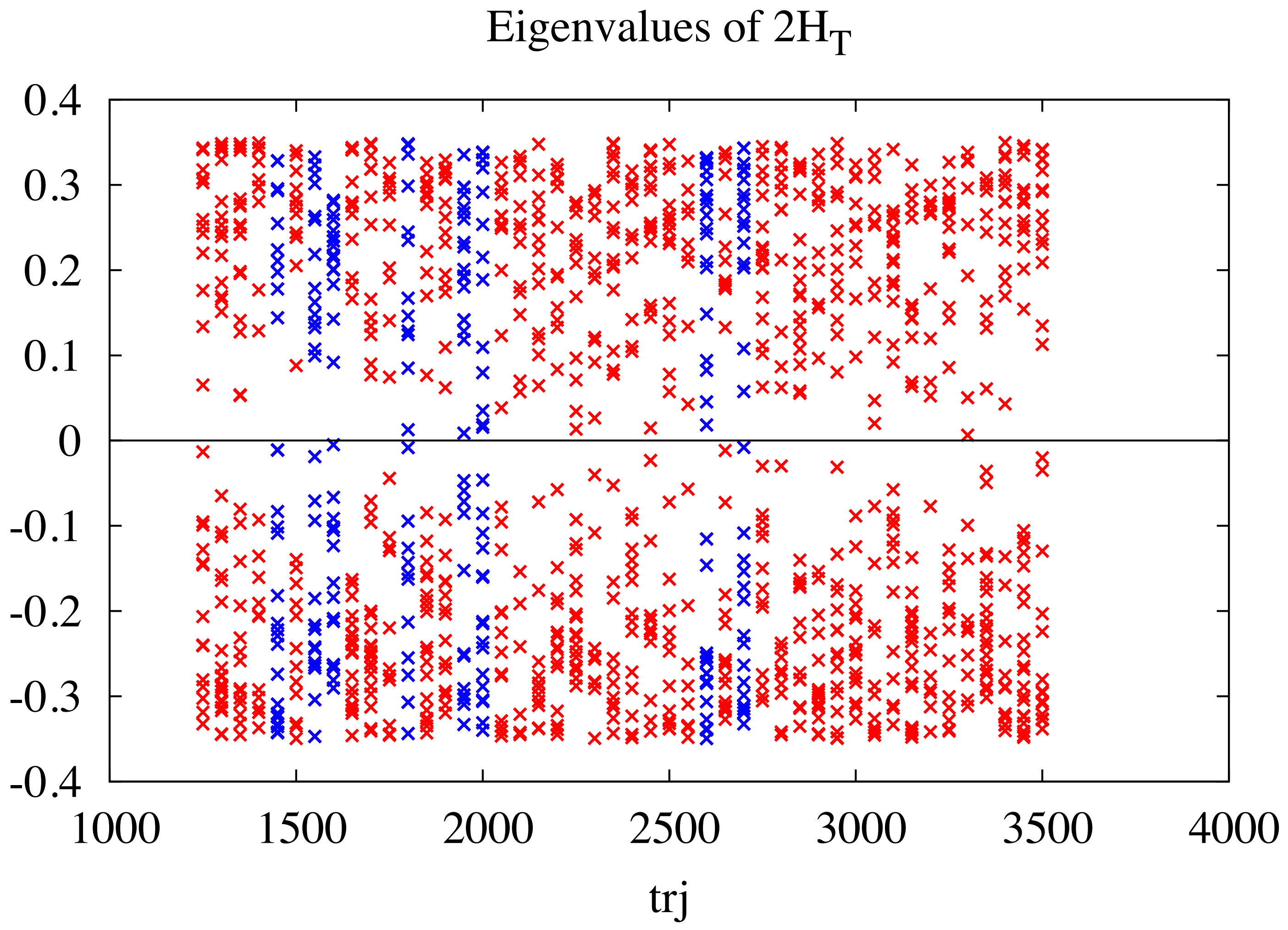
Reweighting factor of Zolo/Tanh

$$\frac{D_{ov}^{\mathrm{Zolo}}(\lambda_{th}=0.3)}{D_{ov}^{\mathrm{Tanh}}(\lambda_{th}=0.3)} = 1 + ((D_{DW}^{Tanh})^{-1} D_{DW}^{Zolo} - 1)(1 - \sum_{\lambda_i<\lambda_{th}} |\lambda_i\rangle\langle)\lambda_i|$$



Backup slide 3

Correlation with kernel eigenvalues ?



Generalized 5d implementation

– After an unitary transformation,

$$
D_\chi^5 \equiv \left(\begin{array}{c|ccccc}
P_- - mP_+ & -T_1^{-1} & 0 & \cdots & \cdots & 0 \\
\hline
0 & 1 & T_2^{-1} & 0 & \cdots & 0 \\
\vdots & 0 & 1 & T_3^{-1} & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & \cdots & 0 & 1 & T_{L_s-1}^{-1} \\
-T_{L_s}^{-1}(P_+ - mP_-) & 0 & \cdots & \cdots & 0 & 1
\end{array}\right)
$$

$$
T_s^{-1} \equiv -(Q_-^s)^{-1} Q_+^{-1}, \quad Q_\pm^s = (D_-^s)^{-1} D_+^s P_\mp - P_\pm
$$

– Then, Schur complement

$$
\begin{pmatrix} D & C \\ B & A \end{pmatrix} = \begin{pmatrix} 1 & CA^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} D - CA^{-1}B (\equiv S_\chi) & 0 \\ 0 & A \end{pmatrix} \begin{pmatrix} 1 & 0 \\ A^{-1}B & 1 \end{pmatrix}
$$

Note: det A = 1

Generalized 5d implementation

$$S_{GDW} = \sum_x \bar{\psi} D^5_{GDW} \psi$$

Edwards-Heller (2000)

$$D^5_{GDW} \equiv \begin{pmatrix} (D^1_-)^{-1} D^1_+ & -P_- & 0 & \cdots & 0 & mP_+ \\ -P_+ & (D^2_-)^{-1} D^2_+ & -P_- & 0 & \cdots & 0 \\ 0 & -P_+ & (D^3_-)^{-1} D^3_+ & -P_- & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \ddots & -P_+ & (D^{L_s-1}_-)^{-1} D^{L_s-1}_+ & -P_- \\ mP_- & 0 & \cdots & 0 & -P_+ & (D^{L_s}_-)^{-1} D^{L_s}_+ \end{pmatrix}$$

$$D^s_+ = 1 + b_s D_W(-M_0),\ D^s_- = 1 - c_s D_W(-M_0); \quad P_\pm = (1 \pm \gamma_5)/2$$

4D effective operator

– det A =1 doesn't contribute to path integ.

$$S_\chi(m) = -(1+T_1^{-1}T_2^{-1}\cdots T_{L_s}^{-1})\gamma_5\left[\frac{1+m}{2} - \frac{1-m}{2}\gamma_5\frac{T_1^{-1}T_2^{-1}\cdots T_{L_s}^{-1}-1}{T_1^{-1}T_2^{-1}\cdots T_{L_s}^{-1}+1}\right]$$

– Combining with Pauli-Villars (m=1),

$$D^{(4)} \equiv S_\chi^{-1}(m=1)S_\chi(m) = \frac{1+m}{2} - \frac{1-m}{2}\gamma_5\underbrace{\frac{T_1^{-1}T_2^{-1}\cdots T_{L_s}^{-1}-1}{T_1^{-1}T_2^{-1}\cdots T_{L_s}^{-1}+1}}$$

- Looks similar to overlap

$$\mathrm{sgn}^{(approx)} = \frac{1-\prod_s T_s}{1+\prod_s T_s}$$

may approximate the sign function