# Lattice Simulations with Domain Wall Fermions

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for RBC/UKQCD collaborations

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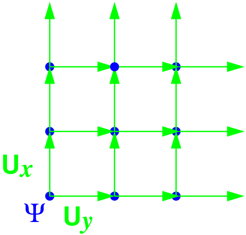
Quantum ChromoDynamics (QCD): Theory of strong interaction which governs interaction between quarks and gluons.
In contrast to Quantum Electrodynamics (QED), The effective coupling of QCD decreases in high energy, hence is calculable by hand, but not in low energy. $\rightarrow$ Nonperturbative techniques such as lattice QCD is needed for *ab initio* calculations. $(\psi(x), A_\mu(x)) \rightarrow (\psi(n), U_\mu(n) = \exp(-iA_\mu))$




$$Z = \int [dU] \det(\not{D} + m) e^{-(S_g)}$$
$$= \int [dU][d\bar{\psi}][d\psi] \ \exp[-(S_g + S_f)]$$
$$S_f = \bar{\psi}(D^\dagger D)^{-1}\psi, \qquad S_{eff} = S_g + S_f$$
$$S_g = \beta \sum \left[ (U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x) \right]$$

Current "typical" calculation: $V = 64^3 \times 128$, rank(D) $\sim 10^{10}$, nonzero element per row $= \sim 10^2$

# Different discretizations in Lattice QCD

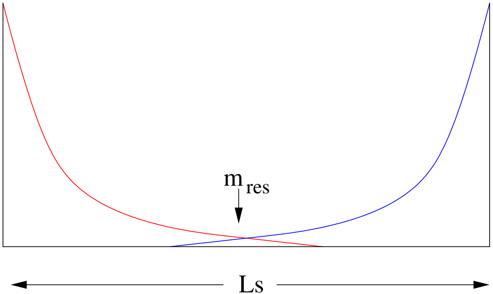
Basic problem/motivation: Naive discretization

$$(\partial_\mu + iA_\mu)\psi(x) \to \frac{(U_\mu(x)\psi(x+\mu) - U^\dagger_\mu(x-\mu)\psi(x-\mu))}{2a}$$

turns $p$ into $\sin(p)$. $2^4 = 16$ particles instead of 1 (doubler).
It is impossible to have a chirally invariant, doubler-free, local, translationally invariant, real bilinear fermion action on the lattice (Nielsen-Ninomiya no-go theorem).
Various solutions:

- Wilson Fermion: Add Laplacian-like term $-\frac{a}{2}\Delta\psi(x) = -\frac{a}{2}\sum_\mu[\psi(x+a\hat{\mu}) + \psi(x-a\hat{\mu}) - 2\psi(x)]$ Additive mass renormalization → fine tuning needed.
- Twisted Wilson Fermion: massless 2-flavor Wilson fermion + $m_l + i\mu_l\tau^3\gamma^5$
- Staggered (Kogut-Susskind) fermion: $\psi \to \psi\Pi_{i=1\dots4}\gamma_i^{x_i}$ turns the action into 4 degenrate "particles" with 4 poles each. Keep only 1 spinor per site, interpret remaining 4 poles as 4 degenerate fermions ($\gamma_\mu(x) \to (-1)^{(\sum_{\nu<\mu} x_\nu)}$) Chiral symmetry only partially preserved. 1 of 15 "pions" is a Goldstone pion. Special ChPT(Staggered ChPT, SChPT) to deal with taste breaking better.

- Domain Wall Fermion(DWF)/Mobius/Overlap fermions: Dirac operator in 5D with repeating gauge field in 4D




Residual symmetry breaking term well represented by a mass term for low enenegy quantities.

$$m'_{\rm res}(m_f) = \frac{\langle 0|J^a_{5q}|\pi\rangle}{\langle 0|J^a_5|\pi\rangle} \sim e^{-L_s}$$

$J^a_{5q}$ : mid-point($s = L_s/2$) pseudoscalar density
$J^a_5$: physical pseudoscalar density($s = 0, L_s - 1$)
Satisfies Ginsparg-Wilson relation$\{D, \gamma_5\} = aD\gamma_5 D$ exactly or approximately. Can be used to define a lattice equivalent of chiral symmetry (Lüscher).

# DWF/Mobius/Overlap Fermion arXiv:1206.5214, 1411.5728

$$D_{Mob}(M, m_f) = \begin{pmatrix} D_+ & -D_- P_- & & & & mD_- P_+ \\ -D_- P_+ & D_+ & -D_- P_- & & & \\ & -D_- P_+ & D_+ & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ mD_- P_- & & & & -D_- P_+ & D_+ \end{pmatrix}$$

$$D_w(M)_{xx'} = M + 4 - \frac{1}{2}\left[(1-\gamma_\mu)\mathbf{U}_\mu(x)\delta_{x+\mu,x'} + (1+\gamma_\mu)\mathbf{U}_\mu{}^\dagger(y)\delta_{x-\mu,y}\right]$$

$$D_+ = bD_W(M) + 1,\ D_- = (1 - cD_W(M))$$

$$S_{DWF} = \bar{\psi} D_{GDW}(M, m_f)\psi,\ D_{GDW}(M, m_f) = (D_-)^{-1} D_{mob} =$$

$$\begin{pmatrix} \tilde{D} & P_- & & & & m_f P_+ \\ -P_+ & \tilde{D} & -P_- & & & \\ & -P_+ & \tilde{D} & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ m_f P_- & & & & -P_+ & \tilde{D} \end{pmatrix}$$

$$P_\pm = \frac{1}{2}(1 \pm \gamma_5), \qquad \tilde{D} = (D_-)^{-1} D_+$$

$$q_R(x) = P_+\psi(x, Ls-1), q_L(x) = P_-\psi(x,0)$$
$$\bar{q}_R(x) = \bar{\psi}(x, Ls-1)P_-, \bar{q}_L(x) = \bar{\psi}(x,0)P_+$$
$$\mathcal{P} = \begin{pmatrix} P_- & P_+ & & 0 \\ 0 & P_- & P_+ & \\ & \ddots & P_- & P_+ \\ P_+ & & 0 & P_- \end{pmatrix}, \mathcal{P}^{-1} = \begin{pmatrix} P_- & 0 & & P_+ \\ P_+ & P_- & 0 & \\ & \ddots & \ddots & 0 \\ & & P_+ & P_- \end{pmatrix}$$
$$Q_s = (\mathcal{P}^{-1}\psi)_s = P_-\psi_s + P_+\psi_{s-1}, \bar{Q}_s = (\bar{\psi}R_5\mathcal{P}^{-1})_s = \bar{\psi}_{L_s-s}P_- + \bar{\psi}_{L_s-s+1}P_+$$
$$\chi = \mathcal{P}^{-1}\psi$$
$$S = \bar{\psi}D_{GDW}\psi = \bar{\psi}Q_- Q_-^{-1}\gamma_5 D_{GDW}\mathcal{P}\mathcal{P}^{-1}\psi$$
$$= \bar{\chi}D^5_\chi\chi, \tilde{H} = \gamma_5\tilde{D},$$
$$Q_- = \tilde{H}P_- - P_+ = \gamma_5 D_-^{-1}\left[D_+P_- - D_-P_+\right]$$
$$Q_+ = \tilde{H}P_+ + P_- = \gamma_5 D_-^{-1}\left[D_+P_+ + D_-P_-\right]$$
$$T^{-1} = -Q_-^{-1}Q_+ = -\left[D_+P_- - D_-P_+\right]^{-1}\left[D_+P_+ + D_-P_-\right]$$
$$= -[H_M - 1]^{-1}[H_M + 1], H_M = \gamma_5\frac{(b+c)D_W}{2+(b-c)D_W}$$

$$Q_\pm P_\pm = \tilde{D} P_\pm, \qquad Q_\pm P_\mp = -\tilde{D} P_\mp$$

$$D^5_\chi = Q_-^{-1} \begin{pmatrix} Q_-(P_- - m_f P_+) & Q_+ & & & 0 \\ 0 & Q_- & Q_+ & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & Q_- & Q_+ \\ Q_+(P_+ - m_f P_-) & & \cdots & 0 & Q_- \end{pmatrix}$$

$$= \begin{pmatrix} (P_- - m_f P_+) & -T^{-1} & & & 0 \\ 0 & 1 & -T^{-1} & & \\ & & \ddots & \ddots & \ddots \\ & & \ddots & 1 & -T^{-1} \\ -T^{-1}(P_+ - m_f P_-) & & \cdots & 0 & 1 \end{pmatrix}$$

$$S_\chi(m_f) = (P_- - m_f P_+) - (T^{-1})^{Ls}(P_+ - m_f P_-)$$

$$D_{ov}(m_f) = S_\chi^{-1}(1) S_\chi(m_f) = \frac{1+m_f}{2} + \frac{1-m_f}{2}\gamma_5 \frac{T^{-Ls}-1}{T^{-Ls}+1}$$

# Surface propagator: $\tilde{D}_{ov}^{-1}$

$$D_{ov}(m_f)^{-1} = S_\chi(1)S_\chi(m_f)^{-1} = \left[D^5_\chi(1)^{-1}D^5_\chi(m_f)\right]_{00}$$

$$\tilde{D}_{ov}(m_f)^{-1} = \frac{1}{1-m_f}\left[D_{ov}(m_f)^{-1} - 1\right]$$

$$= \frac{1}{1-m_f}\left[\mathcal{P}^{-1}D^5_{GDW}(m_f)^{-1}D^5_{GDW}(1)\mathcal{P} - 1\right]_{00}$$

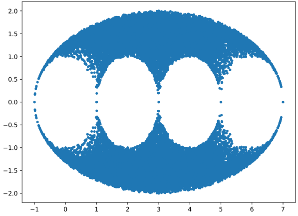
$$= \frac{1}{1-m_f}\left[\mathcal{P}^{-1}D^5_{GDW}(m_f)^{-1}(D^5_{GDW}(1) - D^5_{GDW}(m_f))\mathcal{P}\right]_{00}$$

$$\left[D^5_{GDW}(1) - D^5_{GDW}(m_f)\right]_{ij} = (1-m_f)\left[P_-\delta_{i,Ls-1}\delta j, 0 + P_+\delta_{i,0}\delta j, Ls-1\right]$$

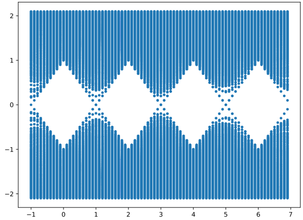
$$\tilde{D}_{ov}(m_f)^{-1} = \left[\mathcal{P}^{-1}D^5_{GDW}(m_f)^{-1}R_5\mathcal{P}\right]_{00}$$

# Spectrum of Free Field Wilson and Effective Overlap Operators

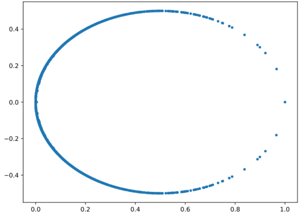
$D_w(M_5 = 1)$




$H_w$

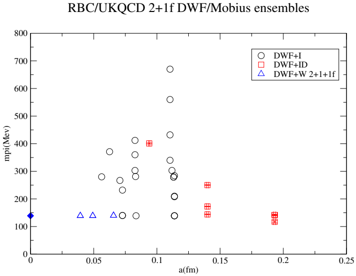


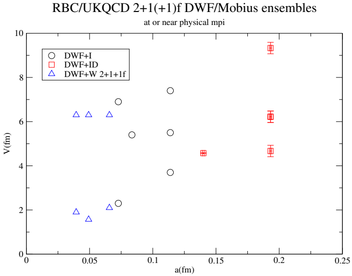

$D_{ov}$




$(D_{ov} - 1)(D_{ov}^\dagger - 1) \sim 1$ (GW relation)

# RBC/UKQCD dynamical Ensembles




DWF+I: Iwasaki gauge action

DWF+ID: Iwasaki + Dislocation Suppressing Determinant Ratio (DSDR): Supresses the chiral symmetry breaking on larger lattice spacing.

$$S_{DSDR}(m_D, m'_D) = \frac{H_W(-M_5)^2 + m_D^2}{H_W(-M_5)^2 + m_D'^2}$$

# Dynamical ensemble generation with DWF

Disadvantage:

- Expensive (flops $\sim \times L_s$ )
- Residual symmetry breaking
- Breakdown of surface mode

Advantage:

- Well optimized dslashes are more performant compared to 4d ones
- Zero mode protected: No exceptional configuration. Simuating at physical point directly, eliminating chiral extrapolation
- Careful tuning of DWF specific parameters ($L_s, M_5$) and gauge action can reduce needed $L_s$ significantly.
- Change of gauge action and/or smearing also possible

# Performance of optimized 4d/5d operators in Grid (From 8 node (64 rank) OLCF Frontier, total mflops/s )

| L | Wilson | DWF4 ($Ls = 12$) | Staggered(3link+1link) | 4d Laplace |
|---|---|---|---|---|
| 8 | 1014634.1 | 10315774.9 | 345519.8 | 3770537.5 |
| 12 | 4844813.5 | 30062324.5 | 1747031.9 | 17422228.8 |
| 16 | 13219328.2 | 50326855.0 | 4885087.8 | 41278240.6 |
| 24 | 30887201.4 | 66882645.2 | 14789298.3 | 77047214.9 |
| 32 | 39483267.7 | 76135253.4 | 24723868.7 | 89981018.2 |

DWF dslash performance often significantly larger, because of the imbalnce between computing and communication (latency/bandwidth) capability of GPU nodes.

# DWF 2+1+1 flavor, physical ensemble program

Parameter $(\beta, m_l, m_s, m_c \cdots)$ tuning done on small volume. Duplicated to create starting lattice for the production run

- Wilson gauge action, Mobius$(b + c = 2, Ls = 12, 16)$
- $96^3 \times 192, 1/a \sim 3$Gev : started on Frontier
- $128^3 \times (\sim 288), 1/a \sim 4$Gev : started on Frontier
- $160^3 \times (\sim 384), 1/a \sim 5$Gev

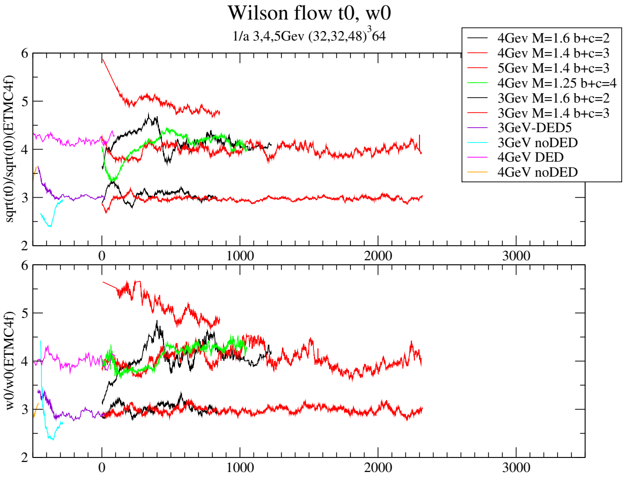
# Observables for ensemble generation parameter tuning

- Residual mass: Should be low enough to reach desired physical mass.
- $H_W(-M_5) = \gamma_5 D_W(-M_5)$ (spectral flow)

$$T^{-1} = -[H_M - 1]^{-1}[H_M + 1], H_M = \frac{\gamma_5 (b+c) D_W(-M_5)}{2 + (b-c) D_W(-M_5)}$$

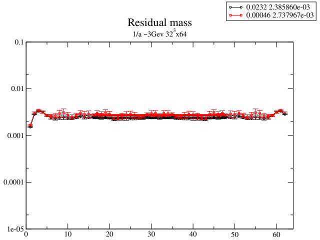
  Scan eigenvalues of $H_W(-M_5)$. Choose $M_5$ to be a region with low density of zero modes for $H_W$.

  Caveat: near zero modes of $H_W(-M_5)$ are necessary to change topology.
- Measure for lattice spacing: Glounic($w_0, t_0 \dots$) or Hadronic (masses..): Smaller lattice spacing error preferred.

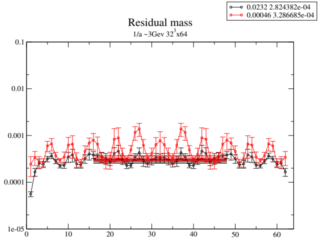



Dislocation Enhancing Determinant(DED): Similar to DSDR, but to encourage dislocation for finer ensembles For each ensemble tuning, you (mostly) just had to tune $\beta$

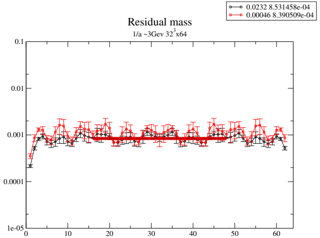
# Residual mass on $1/a \sim 3$Gev 2+1+1f ensemble



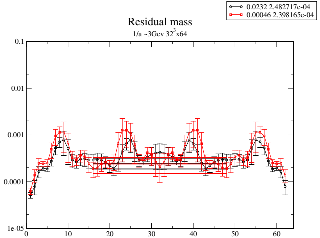

$M_5 = 1.8, b + c = 1, m_{res} \sim 10$Mev




$M_5 = 1.4, b + c = 3, m_{res} \sim 0.9$Mev

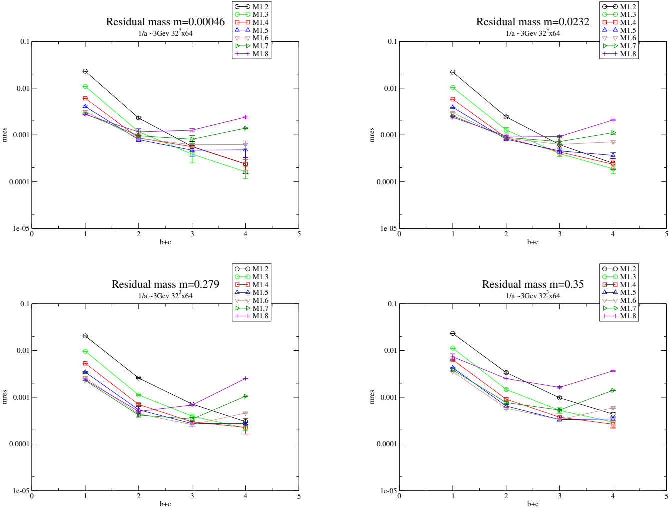



$M_5 = 1.6, b + c = 2, m_{res} \sim 3$Mev



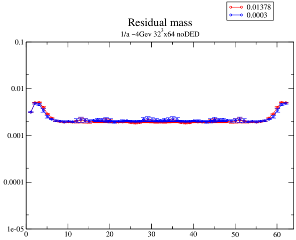

$M_5 = 1.2, b + c = 4, m_{res} \sim 0.9$Mev

# Residual mass on $1/a \sim 3$Gev 2+1+1f ensemble(cont.)

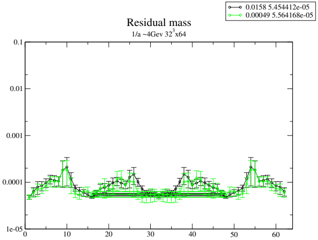



Tuning of $M_5$ makes a significant difference in controlling residual mass with the same $Ls$. Same tuning persistes from $m_f \sim$ 1Mev to 1Gev.

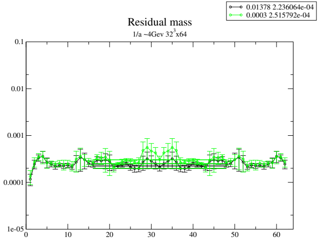
# Balance study of residual mass on $1/a \sim$ 4Gev 2+1+1f ensemble



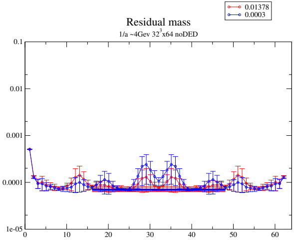

$M_5 = 1.8, b + c = 1, m_{res} \sim$ 10Mev




$M_5 = 1.4, b + c = 3, m_{res} \sim$ 0.2Mev

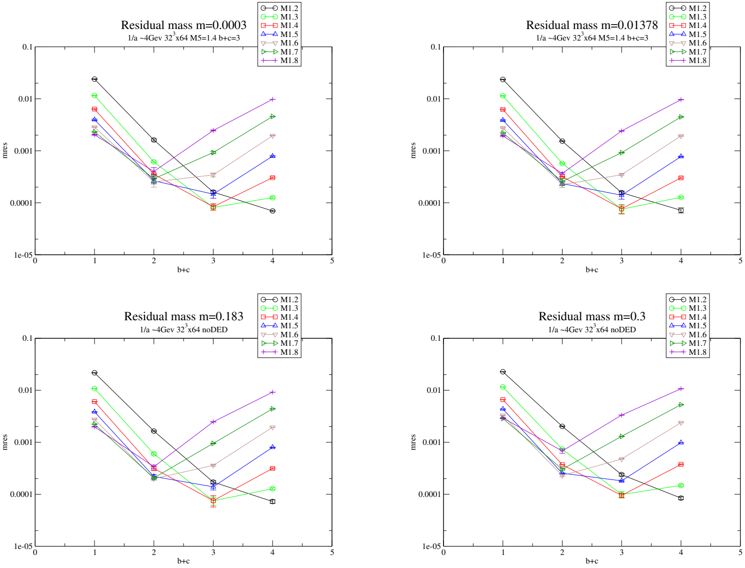



$M_5 = 1.6, b + c = 2, m_{res} \sim$1Mev




$M_5 = 1.2, b + c = 4, m_{res} \sim$ 0.2Mev

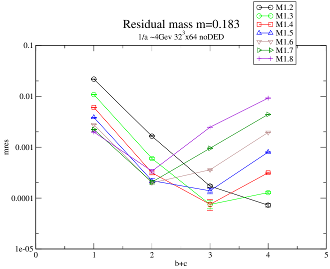
# Residual masses for 2+1+1f $1/a \sim$ 4Gev Wilson ensemble

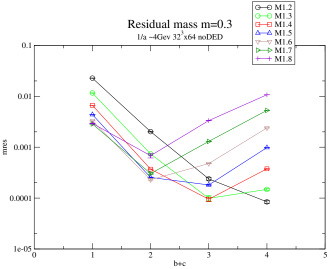



Tuning the same as 3Gev

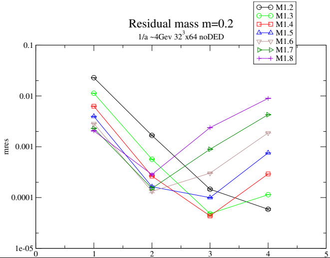
Residual masses for 2+1+1f $1/a \sim$ 4Gev Wilson ensemble, $m_f \sim$ 800Mev, 1.2Gev

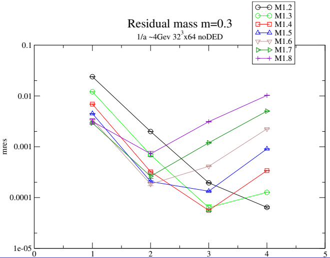
$M_5 = 1.4, b + c = 3$



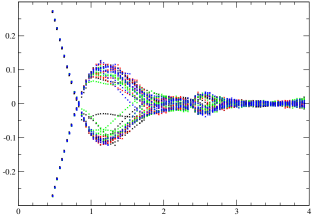

$M_5 = 1.6, b + c = 2$

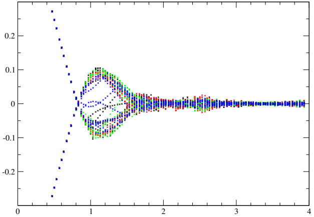


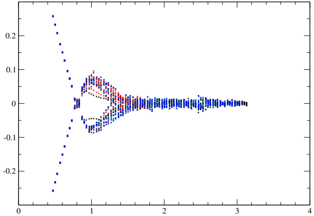



# Spectral flow for $1/a \sim 4$Gev

$$(M_5, b+c) = (1.6, 2), (1.4, 3), (1.2, 4)$$

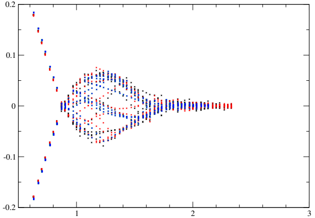


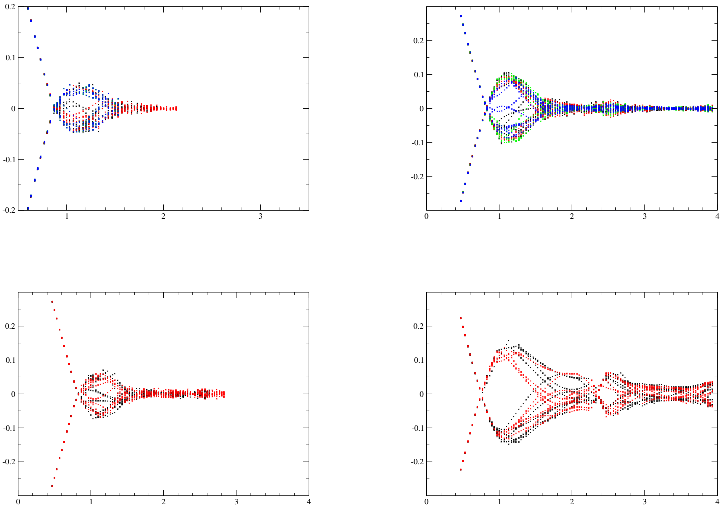
# Spectral flow for $1/a \sim 3\text{Gev}$

$$(M_5, b+c) = (1.6, 2), (1.4, 3)$$

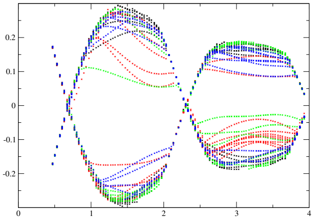


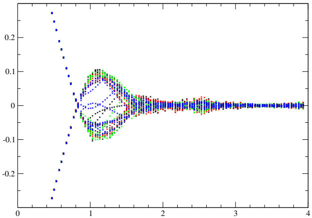
# Wilson vs. Tree-level Symazik gauge action

2+1+1f $1/a \sim$3,4Gev

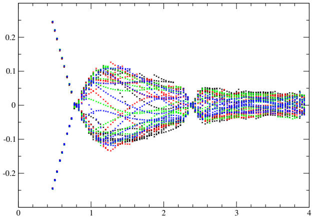


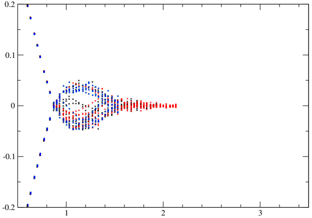
## Wilson $1/a \sim 3.8$Gev vs. 2+1+1f $1/a \sim 4$Gev



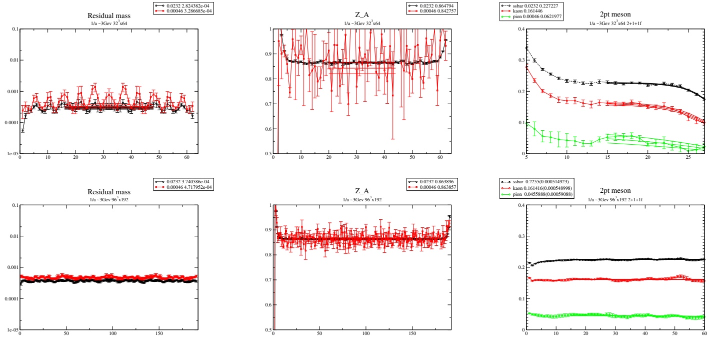




## 2+1f, $1/a \sim 2.8$Gev (Iwasaki) vs. 2+1+1f $1/a \sim 3$Gev



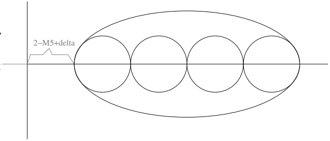



# Large volme measurement of residual mass, $Z_a$, meson spectrum



# Discussions

- $M_5$ dependence of the residual mass: For the real eigenvalues $\delta$ of $D_W(0)$, $H_T = \frac{-M_5+\delta}{2-M_5+\delta}$




- Domain Wall Fermion formalism provides means to control chiral symmetry breaking inherent in Lattice QCD indepdent of lattice spacing, which enables simulations near or at physical masses.
- The numerical cost from 5-dimensional formalism ($Ls$) can be controlled by various means, given a range of lattice spacing needed for the study.
- Spectrum of Hermitian Wilson operator($H_w(-M_5)$), as well as measurement of residual mass and lattice spacing are among useful tools in ensemble tuning.

Thank you!
Questions?