Scaling and Properties of 1/a = 1 GeV, 2+1 Flavor Mobius Domain Wall Fermion Ensembles

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Robert Mawhinney
Columbia University
RBC and UKQCD Collaborations

The RBC & UKQCD collaborations

BNL and RBRC

Mattia Bruno
Tomomi Ishikawa
Taku Izubuchi
Chulwoo Jung
Christoph Lehner
Meifeng Lin
Taichi Kawanai
Hiroshi Ohki
Shigemi Ohta (KEK)
Amarjit Soni
Sergey Syritsyn

CERN

Marina Marinkovic

Columbia University

Ziyuan Bai
Norman Christ
Luchang Jin
Christopher Kelly
Bob Mawhinney
Greg McGlynn
David Murphy
Jiqun Tu

University of Connecticut

Tom Blum

Edinburgh University

Peter Boyle
Guido Cossu
Luigi Del Debbio
Richard Kenway
Julia Kettle
Ava Khamseh
Brian Pendleton
Antonin Portelli
Oliver Witzel
Azusa Yamaguchi

KEK

Julien Frison

Peking University

Xu Feng

Plymouth University

Nicolas Garron

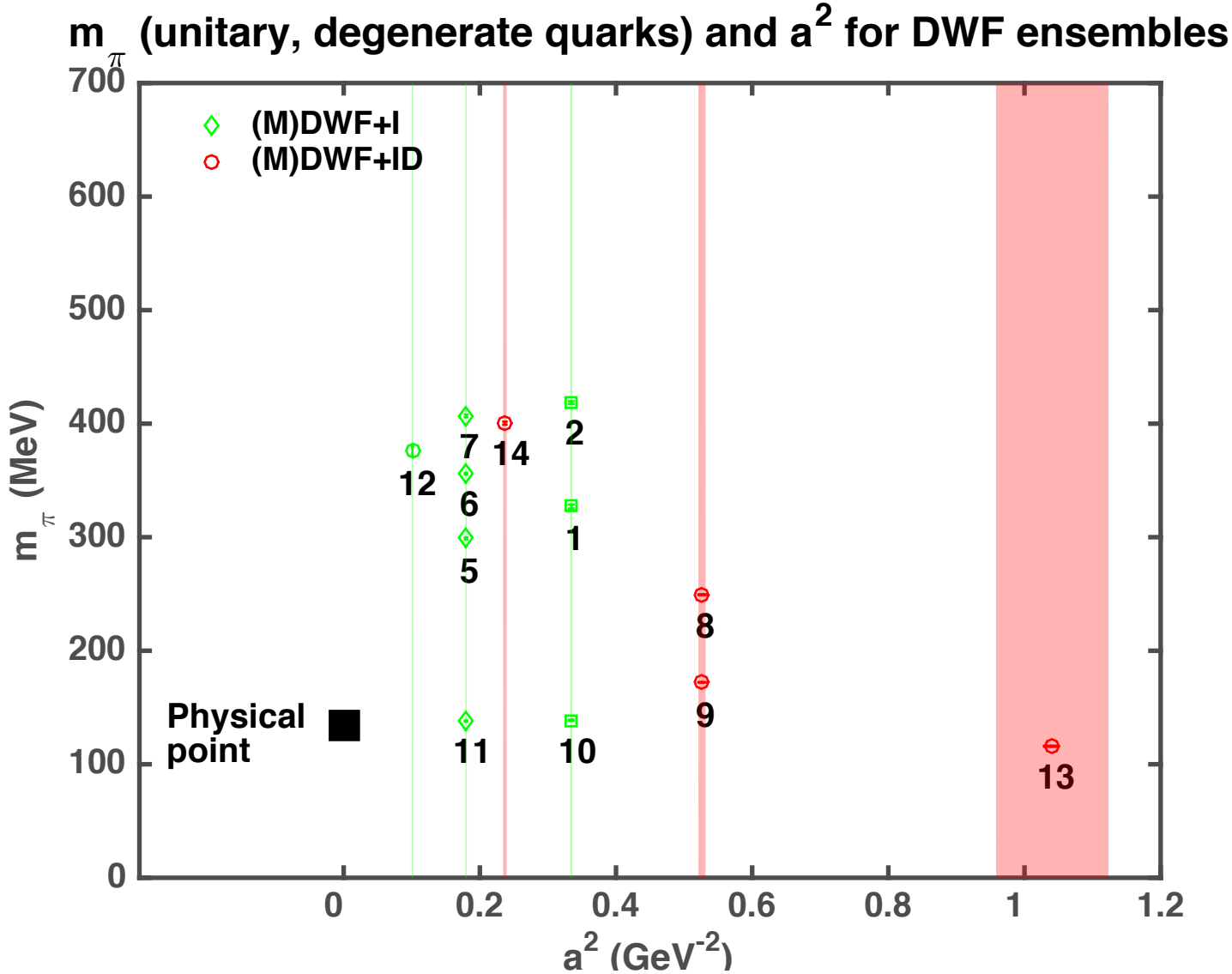
University of Southampton

Jonathan Flynn
Vera Guelpers
James Harrison
Andreas Juettner
Andrew Lawson
Edwin Lizarazo
Chris Sachrajda
Francesco Sanfilippo
Matthew Spraggs
Tobias Tsang

York University (Toronto)

Renwick Hudspith

RBC/UKQCD 2+1 Flavor DWF Ensembles

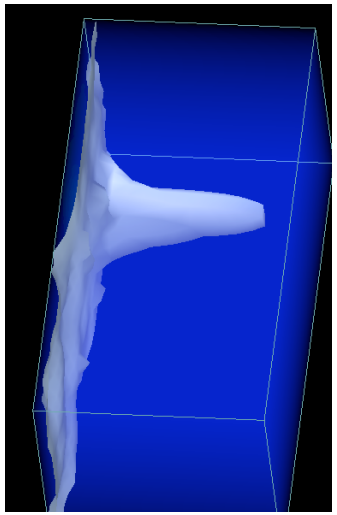


Balancing m_{res} and Topological Tunneling for DWF

- The propagation of light modes between the five-dimensional boundaries is controlled by the eigenvalues of the transfer matrix, H_T

$$H_T = \gamma_5 D_W(M) \frac{1}{2 + (b_i - c_i) D_W(M)}$$

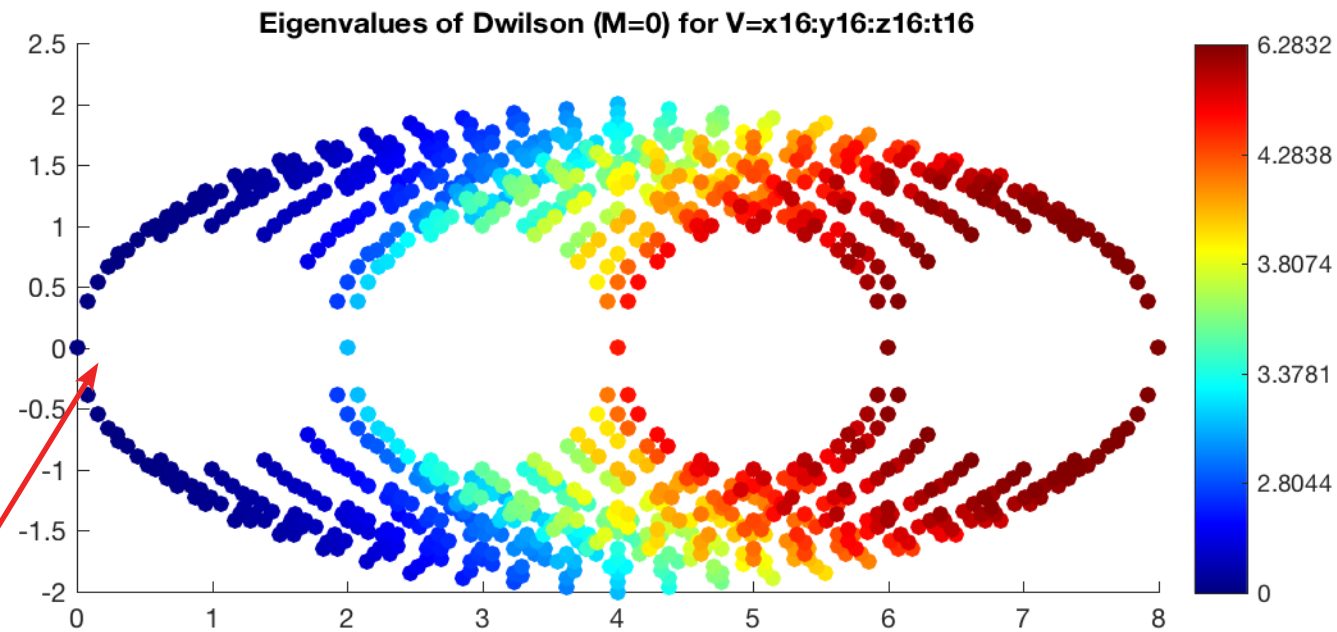
- Zeros of $D_w(M)$ produce modes not bound to the five-dimensional boundaries
- These zeros occur when the gauge fields are changing topology (picture from PRD 77 (2008) 014509)



- Refer to this type of localized fluctuation in the gauge fields as a dislocation.
- For a given L_s, dislocations increase the size of the residual mass, m_{res}.

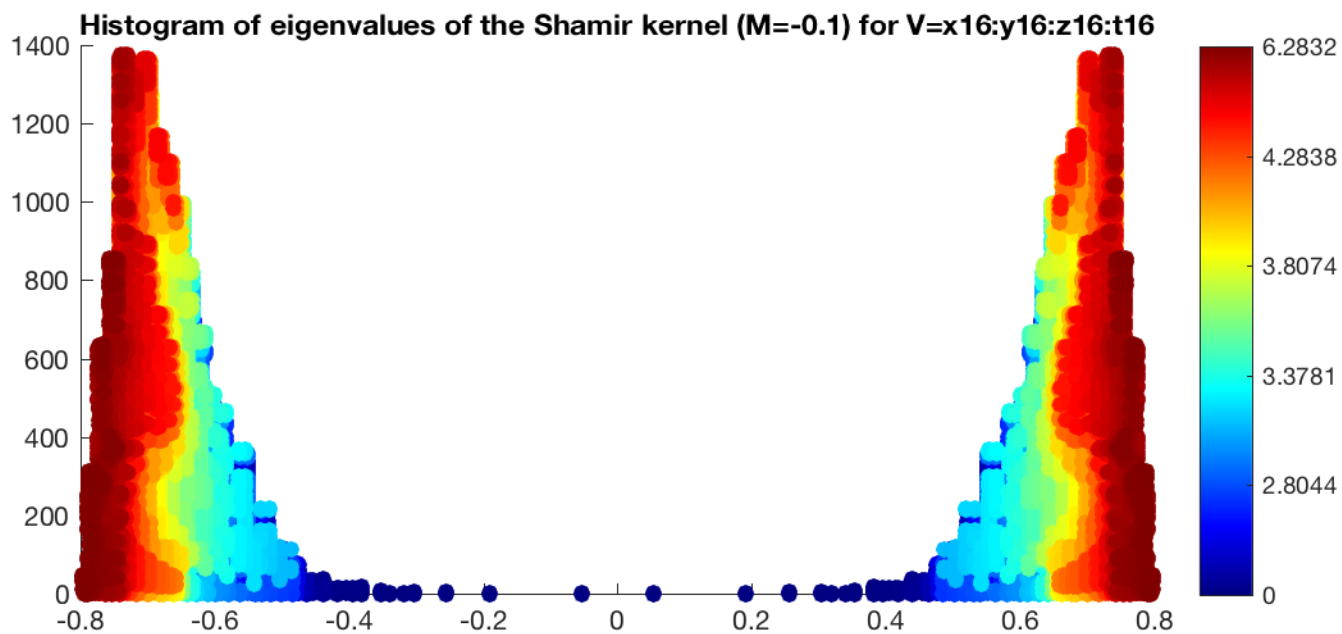
Free Field on a 16^4 lattice

Complex eigenvalues of $D_w(0)$



$\boxed{m = -0.1}$

Eigenvalues of $H_T(-0.1)$



Choices of Action

- For 1/a in range 1.5 - 2.5 GeV, Iwasaki gauge action suppresses dislocations sufficiently with 2+1 flavors of fermions to allow physical light quark masses to be reached.

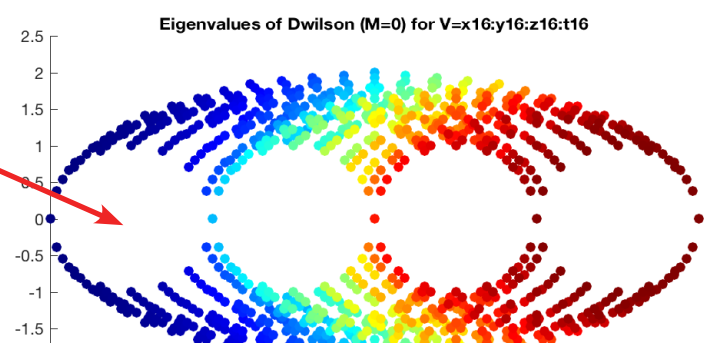
  * 1/a = 1.73 GeV: L_s = 24 for MDWF (b+c=2) gives $m_{res} = 0.45\ m_{ud}$

  * 1/a = 2.31 GeV: L_s = 12 for MDWF (b+c=2) gives $m_{res} = 0.32\ m_{ud}$

- For stronger couplings, add the Dislocation Suppressing Determinant Ratio (DSDR) to suppress topological tunneling

$$\det\left(\frac{D_W^\dagger(M)D_W(M)+\varepsilon_f^2}{D_W^\dagger(M)D_W(M)+\varepsilon_b^2}\right)=\prod_\lambda \frac{\lambda^2+\varepsilon_f^2}{\lambda^2+\varepsilon_b^2} \qquad \varepsilon_f < \varepsilon_b$$

choose
$M = -M_5$

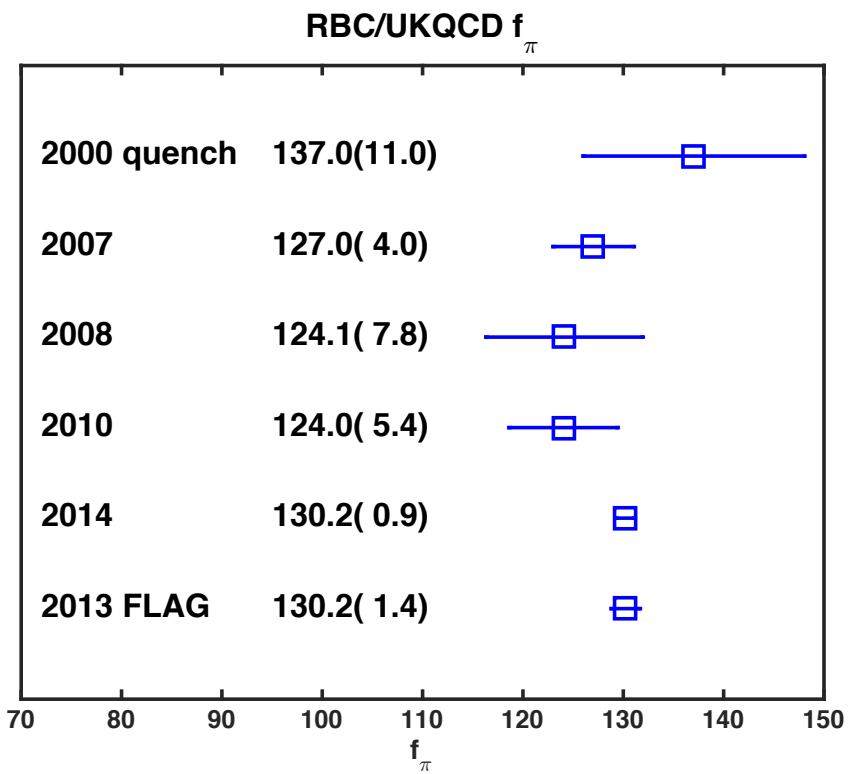


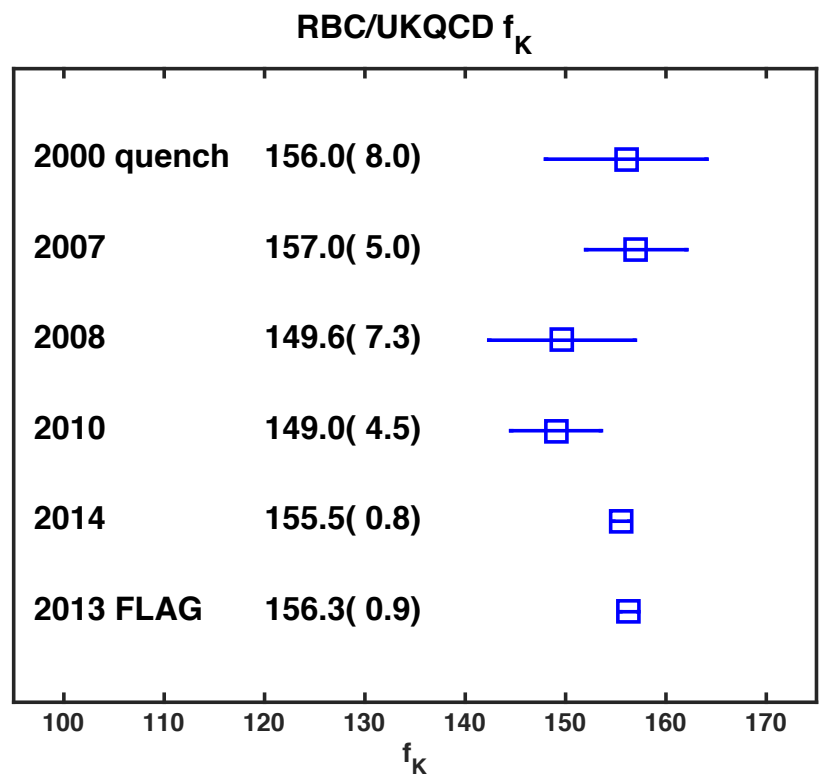
  * 1/a = 1.35 GeV: L_s = 12 for MDWF (b+c=32/12) gives $m_{res} = 0.95\ m_{ud}$

Essentially Physical Quark Mass Ensembles

- Use SU(2) ChPT to make small extrapolation (arXiv:1411.7017).
- Inputs: m_π, m_K and m_Ω. Outputs: f_π and f_K. Overweight physical pt. ensembles

Quantity	Physical Value	Ens. 10 Value	Deviation	Ens. 11 Value	Deviation
m_π/m_K	0.2723	0.2790	2.4%	0.2742	0.7%
m_π/m_Ω	0.0807	0.0830	2.8%	0.0822	1.9%
m_K/m_Ω	0.2964	0.2974	0.3%	0.2998	1.2%

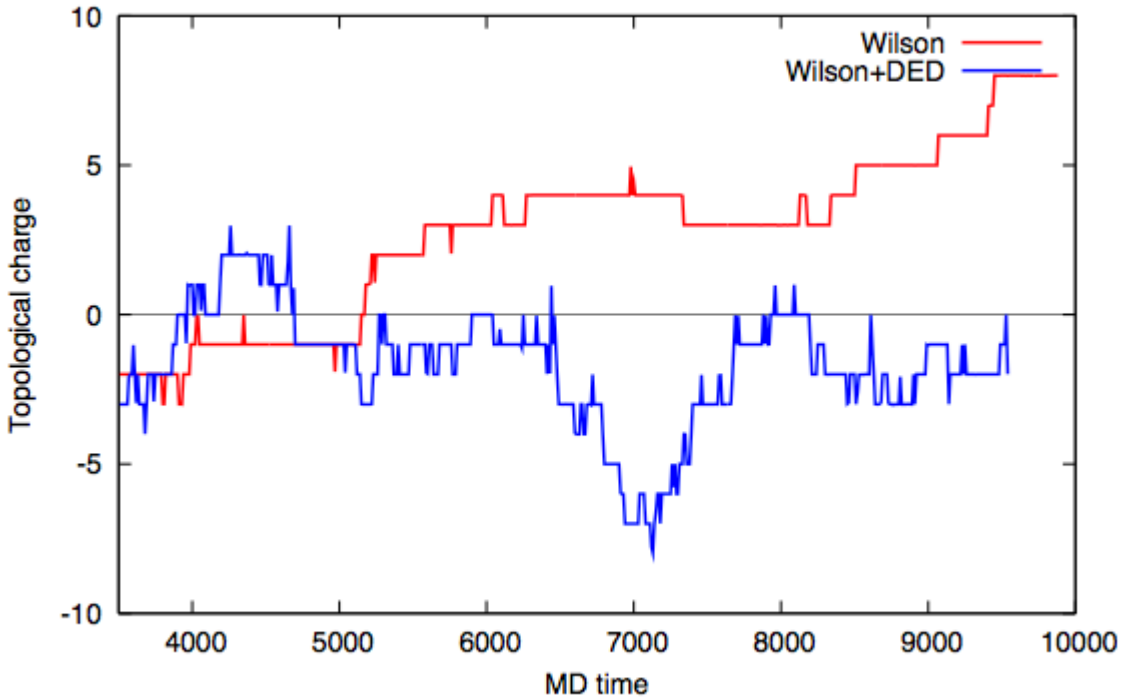


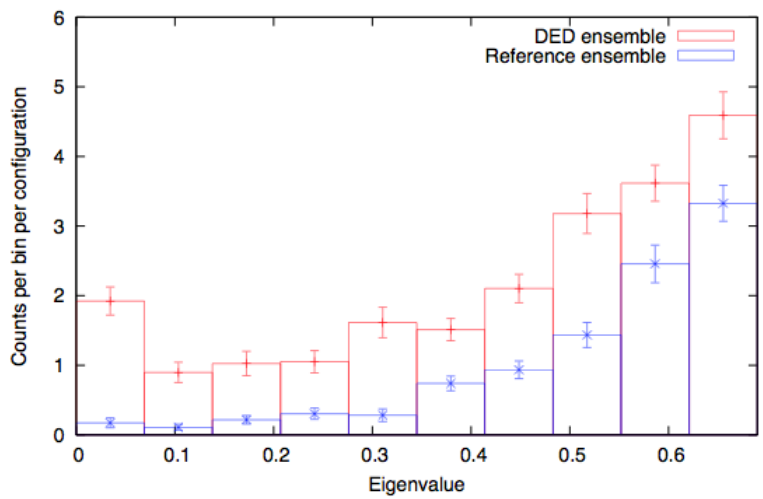


Choices of Action for 1/a ≥ 3 GeV

- Topological tunneling rate falls dramatically with lattice spacing
  - * Switching from Iwasaki to Wilson gauge action helps
  - * How to do more?
- Do the opposite of DSDR term: Dislocation Enhancing Determinant (DED)
- Try DSDR with $\varepsilon_f > \varepsilon_b$. Shift in β (to larger values) suppresses tunneling almost as much as inverse determinant improves it.
- Choose a rational function of $D_W(M)$ which falls off faster for larger eigenvalues. Still effects dislocations, but has less effect on physical modes and should reduce the β shift. (Greg McGlynn)
  - * Normal pseudofermion action in RHMC: $S = \phi^\dagger R_b(B) R_f(F)^2 R_b(B) \phi$
  - * For DWF, choose: $R_f(x) \approx x^{-1/4} \quad R_b(x) \approx x^{1/4}$
  - * For DED term, choose: $R_f(x) = 1, \quad R_b(x) = 1 - \frac{a}{x+b_1} + \frac{a}{x+b_2}$
  - * This gives: $\det[R_b(M_{prec}^\dagger M_{prec}(-M_5))^{-2}] = \prod_\lambda \left(1 - \frac{a}{\lambda+b_1} + \frac{a}{\lambda+b_2}\right)^{-2}$
  - * For large values of λ_H, this falls like $1 + \mathcal{O}(\lambda_H^{-4})$

Quenched Test of DED with 1/a = 4.55 GeV





2+1+1 Flavor DWF + DED with 1/a ≈ 3 GeV

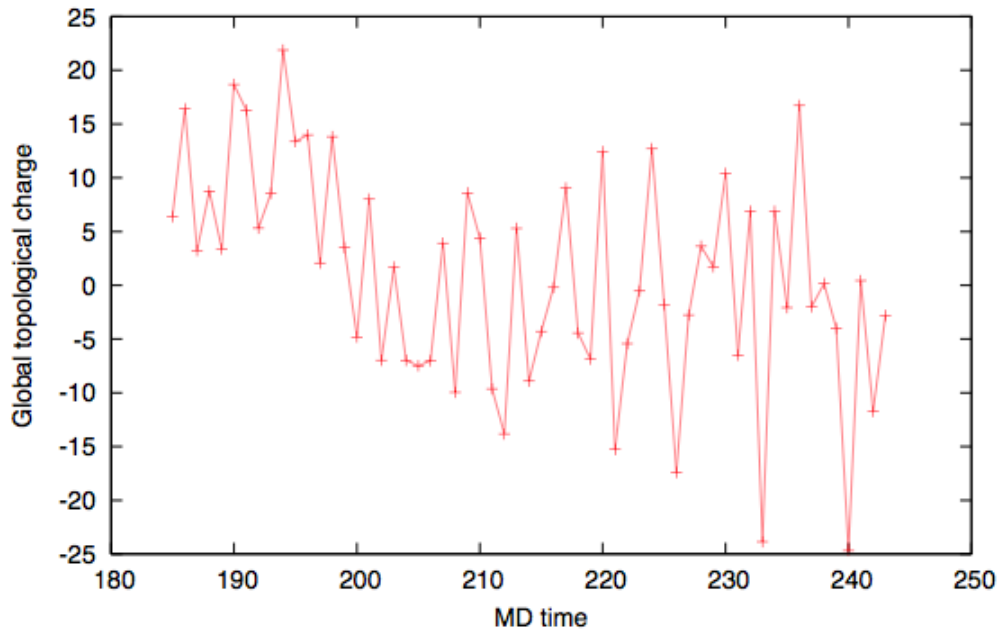


Figure 33: Evolution of the global topological charge on the $80 \times 80 \times 96 \times 192$ ensemble.

	Time (seconds)	Fraction of total
Gauge action	5800	11.6%
Light quark ($L_s = 14$)	18000	36.1%
$L_s = 32/Ls = 14$ correction determinant	1600	3.3%
$L_s = 32$ strange and charm quarks	24200	48.5%
DED	170	0.3%
Trajectory	50000	100.0%

Table 16: Timings for trajectory 243 of the $80 \times 80 \times 96 \times 192$ 2+1+1 flavor ensemble on a 12,288-node partition of a Blue Gene/Q machine.

Greg McGlynn, Ph.D. Thesis, April 2016

2+1+1 Flavor DWF + DED + zMobius Molecular Dynammics

- zMobius: a variant of Mobius DWF with complex coefficients (Izubuchi, et. al.) allowing reduced L_s
  - * Here we find $L_s = 14$ zMDWF is a good approximation to $L_s = 32$ MDWF
  - * CG iteration counts rise because preconditioning less effective.
- McGlynn implemented an idea of Brower and Orginos to do MD at reduced L_s

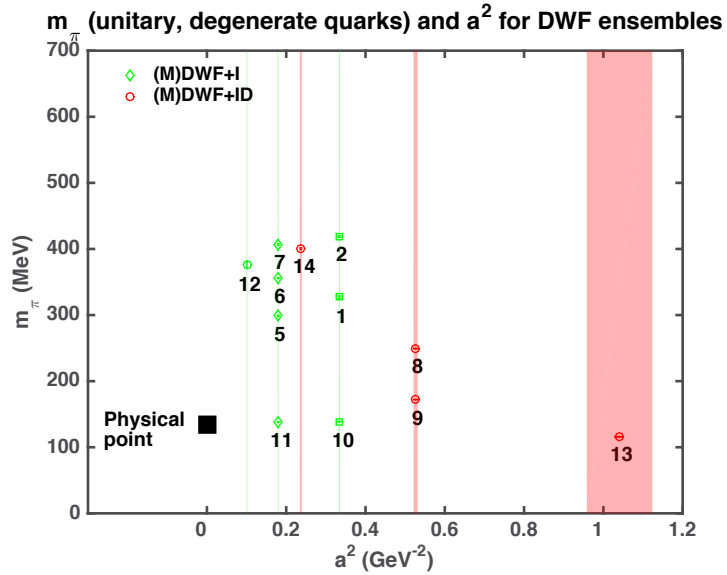
$$\det\left[\frac{D_{DW}(m,L_s)}{D_{DW}(1,L_s)}\right]_{5D} = \det[D_{ov}(L_s)]_{4D}$$
$$= \det[D_{ov}(L'_s)]_{4D} \times \det\left[\frac{D_{ov}(L_s)}{D_{ov}(L'_s)}\right]_{4D}$$
$$= \det\left[\frac{D_{DW}(m,L'_s)}{D_{DW}(1,L'_s)}\right]_{5D} \times \det\left[\frac{D_{ov}(L_s)}{D_{ov}(L'_s)}\right]_{4D}$$

Use zMDWF here to have an accurate, small L_s approximation to original determinant

This is a small correction. Not necessary to include in MD, only include in accept/reject step

A 32^3 test ensemble is 2× faster with zMobius

2+1 Flavor Iwasaki + DSDR (M)DWF ensembles



- Original DSDR ensemble had 1/a = 1.37(1) GeV, m_π = 170 MeV and V = $(4.7\ \text{fm})^3$
  - * Another ensemble, with G-parity boundary conditions, generated for K –› ππ matrix elements calculations with m_π = 170 MeV
- For HotQCD thermodynamics study of the QCD phase transition with MDWF quarks, two T=0 DSDR ensembles were generated at 1/a = 0.98(4) and 2.02(1) GeV (PRL 113 (2014) no.8 082001).
- Global fits show small $O(a^2)$ errors for MDWF ensembles, even at 1/a = 1 GeV.

SU(2) ChPT Fits to m_{PS} and f_{PS}

- We can simultaneously fit lattice data for different lattice spacings, actions and volumes using expansions of the form (SU(2) NLO example):

$$
\begin{aligned}
(m_{ll}^{\mathbf{e}})^2 &= \chi_l^{\mathbf{e}} + \chi_l^{\mathbf{e}} \cdot \left\{ \frac{16}{f^2}\Big((2L_8^{(2)} - L_5^{(2)}) + 2(2L_6^{(2)} - L_4^{(2)})\Big)\chi_l^{\mathbf{e}} + \frac{1}{16\pi^2 f^2}\chi_l^{\mathbf{e}} \log\frac{\chi_l^{\mathbf{e}}}{\Lambda_\chi^2} \right\} \\
f_{ll}^{\mathbf{e}} &= f\left[1 + c_f (a^{\mathbf{e}})^2\right] + f \cdot \left\{ \frac{8}{f^2}(2L_4^{(2)} + L_5^{(2)})\chi_l^{\mathbf{e}} - \frac{\chi_l^{\mathbf{e}}}{8\pi^2 f^2}\log\frac{\chi_l^{\mathbf{e}}}{\Lambda_\chi^2} \right\}
\end{aligned}
$$

with

$$
\chi_l^{\mathbf{e}} = \frac{Z_l^{\mathbf{e}}}{R_a^{\mathbf{e}}} \frac{B^{\mathbf{1}} \widetilde{m}_l^{\mathbf{e}}}{(a^{\mathbf{e}})^2}
$$

- At NNLO order, using codes from Bijnens and collaborators, we fit to

$$
X(\tilde{m}_q, L, a^2) \simeq X_0 \left(1 + \underbrace{X^{\mathrm{NLO}}(\tilde{m}_q) + X^{\mathrm{NNLO}}(\tilde{m}_q)}_{\text{NNLO Continuum PQChPT}} + \underbrace{\Delta_X^{\mathrm{NLO}}(\tilde{m}_q, L)}_{\text{NLO FV corrections}} + \underbrace{c_X a^2}_{\text{Lattice spacing}} \right)
$$

- For SU(2), we use m_π, m_K and m_Ω to set the scale.
- There are different a^2 corrections to the decay constants for I and ID actions.
- Heavy quark ChPT used for light quark extrapolation of kaon.
- ${t_0}^{1/2}$ and w_0 are also fit using a linear chiral ansatz.

Scaling Errors for f_π and f_K

- Fits use different $O(a^2)$ coefficients for Iwasaki and Iwasaki+DSDR actions
- Results for these coefficients from PRD 93 054502 (2016):

	NLO (370 MeV cut)	NNLO (450 MeV cut)
Iwasaki f_π a^2 coeff.	0.059(47) GeV^2	0.065(45) GeV^2
DSDR f_π a^2 coeff.	-0.013(17) GeV^2	0.012(16) GeV^2
Iwasaki f_K a^2 coeff.	0.049(39) GeV^2	0.069(36) GeV^2
DSDR f_K a^2 coeff.	-0.005(15) GeV^2	0.019(15) GeV^2

- For 1/a = 1 GeV, percent scaling error:

	NLO (370 MeV cut)	NNLO (450 MeV cut)
Iwasaki f_π	6 ± 5%	7 ± 5%
DSDR f_π	-1 ± 2%	1 ± 2%
Iwasaki f_K	5 ± 4%	7 ± 4%
DSDR f_K	-1 ± 2%	2 ± 2%

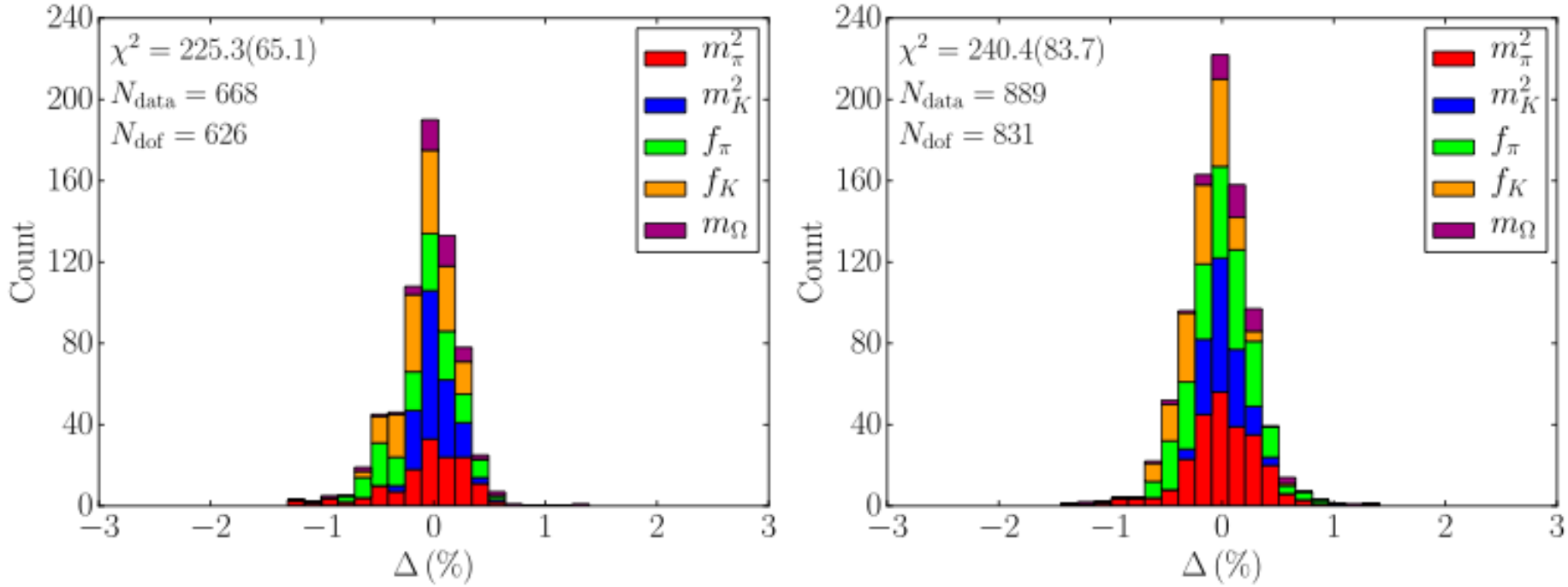
- Canonical scaling errors should be $(a\Lambda^{(3)}_{QCD})^2 \sim (330\,\mathrm{MeV}/980\,\mathrm{MeV})^2 \sim 0.11$.
- 2+1 flavor physical quark mass simulations at strong coupling well behaved.

Scaling Errors For More Observables

- We have preliminary fits with more observables, including the $\pi\pi$ I=2 scattering length (David Murphy)
- Show results for SU(2) NNLO fits with pseudoscalar masses below 450 MeV

	Iwasaki a^2 coefficient	DSDR a^2 coefficient
f_π	0.070±0.041	0.022±0.017
f_K	0.079±0.034	0.030±0.014
$t_0^{1/2}$	-0.017±0.041	-0.021±0.020
w_0	-0.117±0.360	-0.039±0.018
a_0^2 (I=2 pi-pi scattering)	-0.15±0.33	-0.04±0.45

Fit Quality



(a) NLO, $m_\pi^{\rm cut} = 370\,{\rm MeV}$ (b) NNLO, $m_\pi^{\rm cut} = 450\,{\rm MeV}$

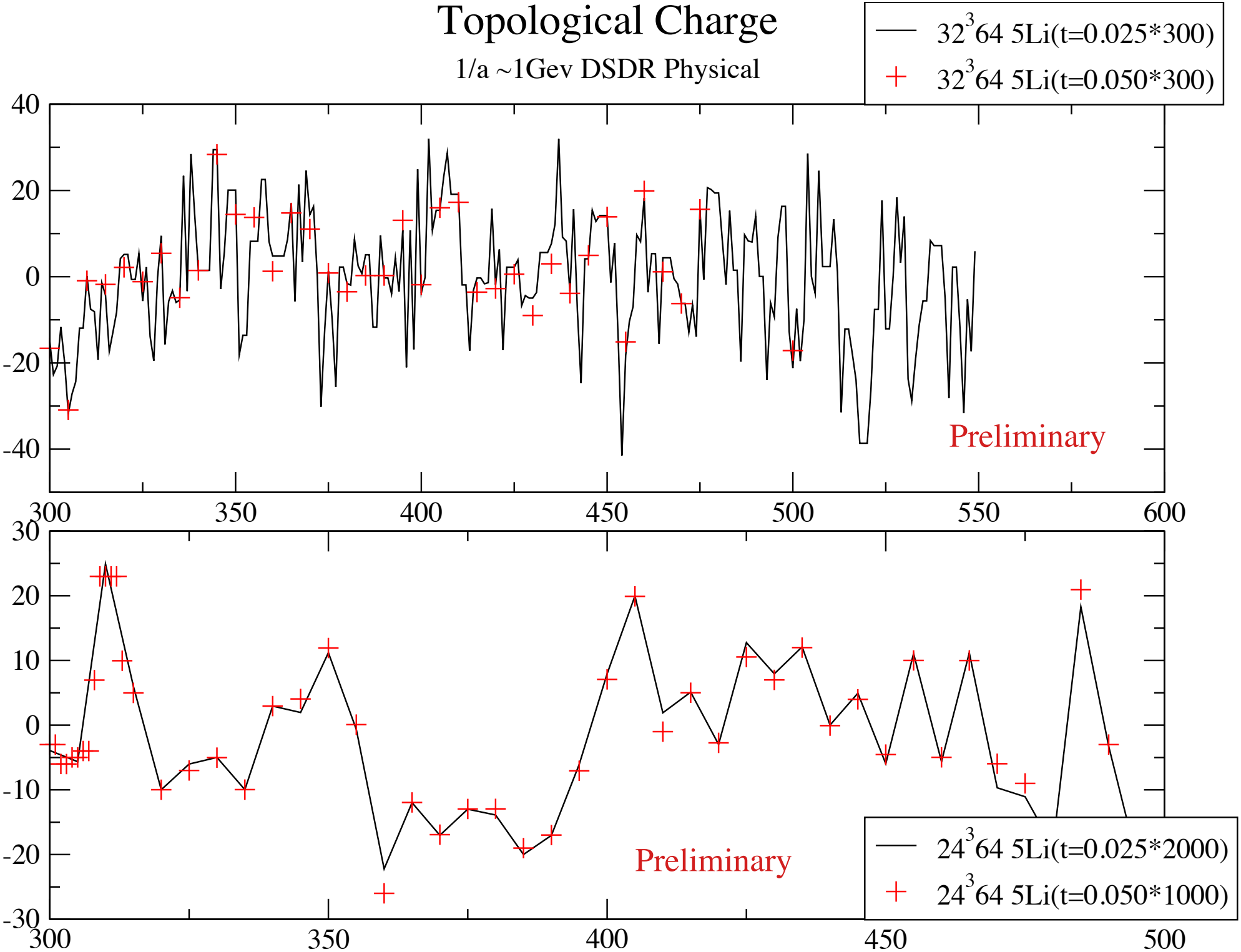
- Have 3 DSDR ensembles plus the requirement that Iwasaki and DSDR actions have common continuum limit, so linear fit in a^2 has to match 4 conditions.
- Deviations between fits and data are almost all below 1%.
- Argues against any measureable contribution from higher orders in a.

1 GeV Ensembles

- Evidence presented shows that we have an action that allows strong coupling simulations with 2+1 flavors at physical quark masses
  - Small a^2 corrections
  - Rapid topological tunneling
  - No execeptional configurations
  - Good chiral symmery properties from MDWF
- We expect these ensembles will be very useful for
  - Studying finite volume effects for QCD and QCD+QED physics, like g-2
  - Developing and testing methods at physical quark masses
  - Measurements requiring large statistics and/or good topological sampling.
- We are generating 3 ensembles with 1/a = 1 GeV
  - 24^3: physical volume is $(4.8\ \mathrm{fm})^3$, $m_\pi L = 3.4$
  - 32^3: physical volume is $(6.4\ \mathrm{fm})^3$, $m_\pi L = 4.5$
  - 48^3: physical volume is $(9.6\ \mathrm{fm})^3$, $m_\pi L = 6.7$

Topological Charge

1/a ~1Gev DSDR Physical



Preliminary Measurements on 24^3 1 GeV Ensemble

- To date, have measured on 41 configurations. Input quark masses for this ensemble came from our global chiral fits.
- Using 1/a = 0.981 GeV (from global chiral fit) can convert lattice results to physical units.

L	24
T	64
L_s	24
β	1.633
am_l	0.00107
am_h	0.0850

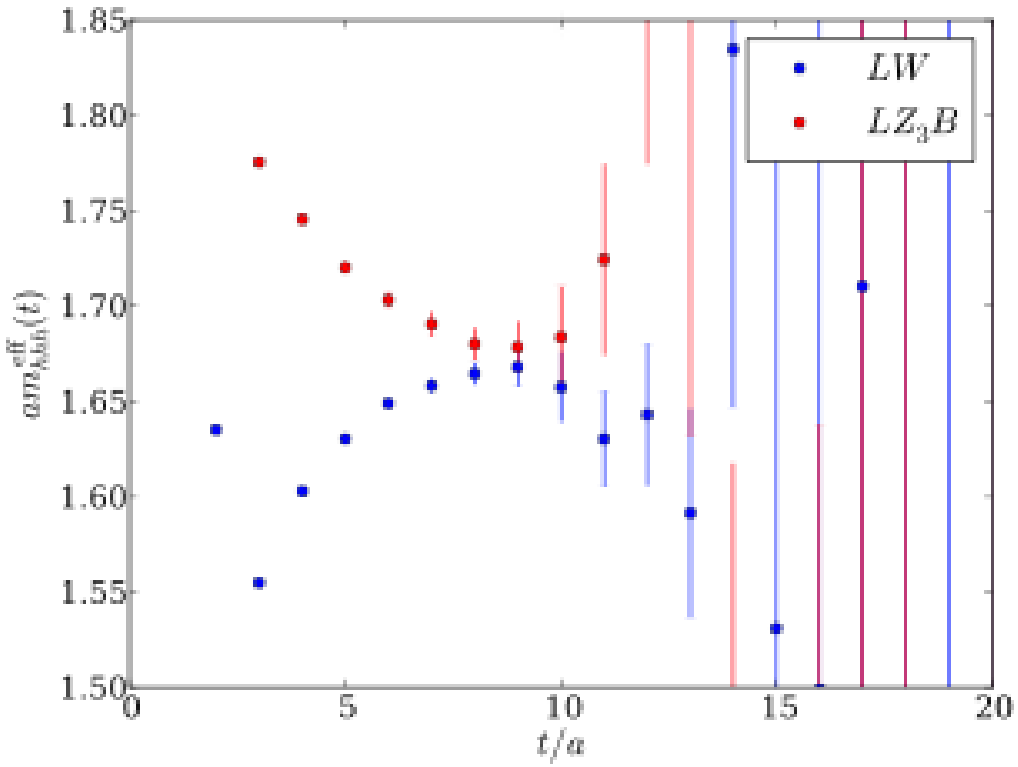
Table 1: Ensemble parameters

Observable	aX	X (MeV)
$m'_{\rm res}(m_l)$	0.002291(15)	—
m_π	0.14011(35)	137.4(3)
m_K	0.50455(46)	495.0(5)
m_Ω	1.6777(59)	1645.8(5.8)
f_π	0.13076(27)	128.3(3)
f_K	0.15880(31)	155.8(3)
f_K/f_π	1.2144(30)	—

- Previous global fits showed small $O(a^2)$ scaling deviations and the close agreement of f_π and f_K with experiment further supports this.

Omega Baryon Effective Mass on 24^3 1 GeV Ensemble

- Two sources: Coulomb gauge fixed wall source and 8 smaller Coulomb gauge fixed wall sources.
- Preliminary results from 41 configurations.
- Good agreement between the two sources.



Conclusions

- The DSDR term has allowed us to simulate domain wall fermions on coarse lattices.
- DSDR Used for K –› ππ (with G-parity boundary conditions) and also for finite temperature QCD studies with $N_T = 8$.
- Adding a DED term enhances topological tunneling and we have a large volume, 2+1+1 flavor, 1/a = 3 GeV DWF ensemble showing good tunneling.
- Global chiral fits have revealed that our Iwasaki+DSDR ensembles have small a^2 scaling violations.
- We are currently generating 1/a = 1GeV ensembles with physical volumes of $(4.8\ \mathrm{fm})^3$, $(6.4\ \mathrm{fm})^3$, and $(9.6\ \mathrm{fm})^3$.
- These coarse lattices will allow studies of finite volume effects for a variety of observables.
- Physical 2+1 flavor ensembles with size $24^3 \times 64 \times 24$ useful for high statistics and exploring techniques.