

2+1 flavor QCD simulations with domain wall fermions and the I-DSDR gauge action

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Outline

1. Introduction/motivation
2. Topology, m_{res} and all that
3. Some new results
4. Summary

RBC / UKQCD Collaboration (taken from N. Christ's talk, 7/28)

UKQCD Collaboration

- Edinburgh
 - Rudy Arthur
 - Peter Boyle
 - Luigi del Debbio
 - Nicolas Garron
 - Chris Kelly
 - Tony Kennedy
 - Richard Kenway
 - Chris Maynard
 - Brian Pendleton
 - James Zanotti
- Southampton
 - Dirk Brommel
 - Jonathan Flynn
 - Patrick Fritzsch
 - Elaine Goode
 - Chris Sachrajda

RBC Collaboration

- Columbia
 - Norman Christ
 - Michael Endres
 - Xiao-Yong Jin
 - Matthew Lightman
 - Meifeng Lin (Yale)
 - Qi Liu
 - Robert Mawhinney
 - Hao Peng
 - Dwight Renfrew
 - Hantao Yin
- BNL
 - Michael Creutz
 - Shinji Ejiri
 - Prasad Hegde
 - Chulwoo Jung
 - Frithjof Karsch
 - Swagato Mukherjee
 - Chuan Miao
 - Peter Petreczky
 - Amarjit Soni
 - Ruth Van de Water
 - Alexander Velytsky
 - Oliver Witzel
- RBRC
 - Yasumichi Aoki
 - Tom Blum (Connecticut)
 - Saumitra Chowdhury (Connecticut)
 - Chris Dawson (Virginia)
 - Tomomi Ishikawa (Connecticut)
 - Taku Izubuchi (BNL)
 - Christoph Lehner
 - Shigemi Ohta (KEK)
 - Eigo Shintani
 - Ran Zhou (Connecticut)

Motivation Need **light quarks** and **big boxes** because

Chiral pert. theory slowly convergent

Direct $K \rightarrow \pi\pi$ decay calculations require large volume

(talks by C. Sachrajda, Q. Liu, and N. Christ)

Longstanding problems in nucleon structure calculations (g_A ,
momentum fraction, helicity fraction, form factors, ...)

EM properties of hadrons in QCD+QED (talk by T. Izubuchi)

Hadronic corrections to muon $g - 2$

...

Iwasaki-Dislocation Suppressing Determinant Ratio

(I-DSDR)

Take advantage of good chiral properties of DWF

Small quark mass, so large volume

Large lattice spacing (OK for DWF)

But residual mass gets big for conventional gauge actions

DWF and residual χ SB

The residual mass m_{res} [Furman and Shamir (1995), Blum (1998)]

A small additive shift to the bare quark mass due to finite size of the extra dimension of DWF, L_s

$$m_{\text{res}} \equiv \sum_{t \gg a} \frac{\langle J_{5q} J_5(t) \rangle}{\langle J_5 J_5(t) \rangle}$$

Falls off exponentially with L_s if gauge fields are smooth enough

[Shamir (1993); Hernandez, Jansen, Lüscher (1999); Neuberger (2000)]

$$T = \frac{1 - H}{1 + H}$$

$$H = \frac{1}{2 + D_W(-M_5)} \gamma_5 D_W(-M_5)$$

unless T has a **unit eigenvalue**

Low modes of D_W and explicit χ SB in DWF

Low modes of Wilson (DWF) Dirac operator near $(+)$ – M_5 responsible for χ symmetry breaking in DWF Edwards, Heller, Narayanan (1999); Hernandez, Jansen, Lüscher (2000); Orginos (RBC Collaboration) (2002); Hernandez, Jansen, Nagai (2002); A. Aoki, *et al* (RBC Collaboration) (2004);

Low modes $\rightarrow m_{\text{res}} \sim 1/L_s$ [Golterman and Shamir (2003); RBC (2007)]

Low modes supported by “dislocations”, or small lattice artifact “instantons”

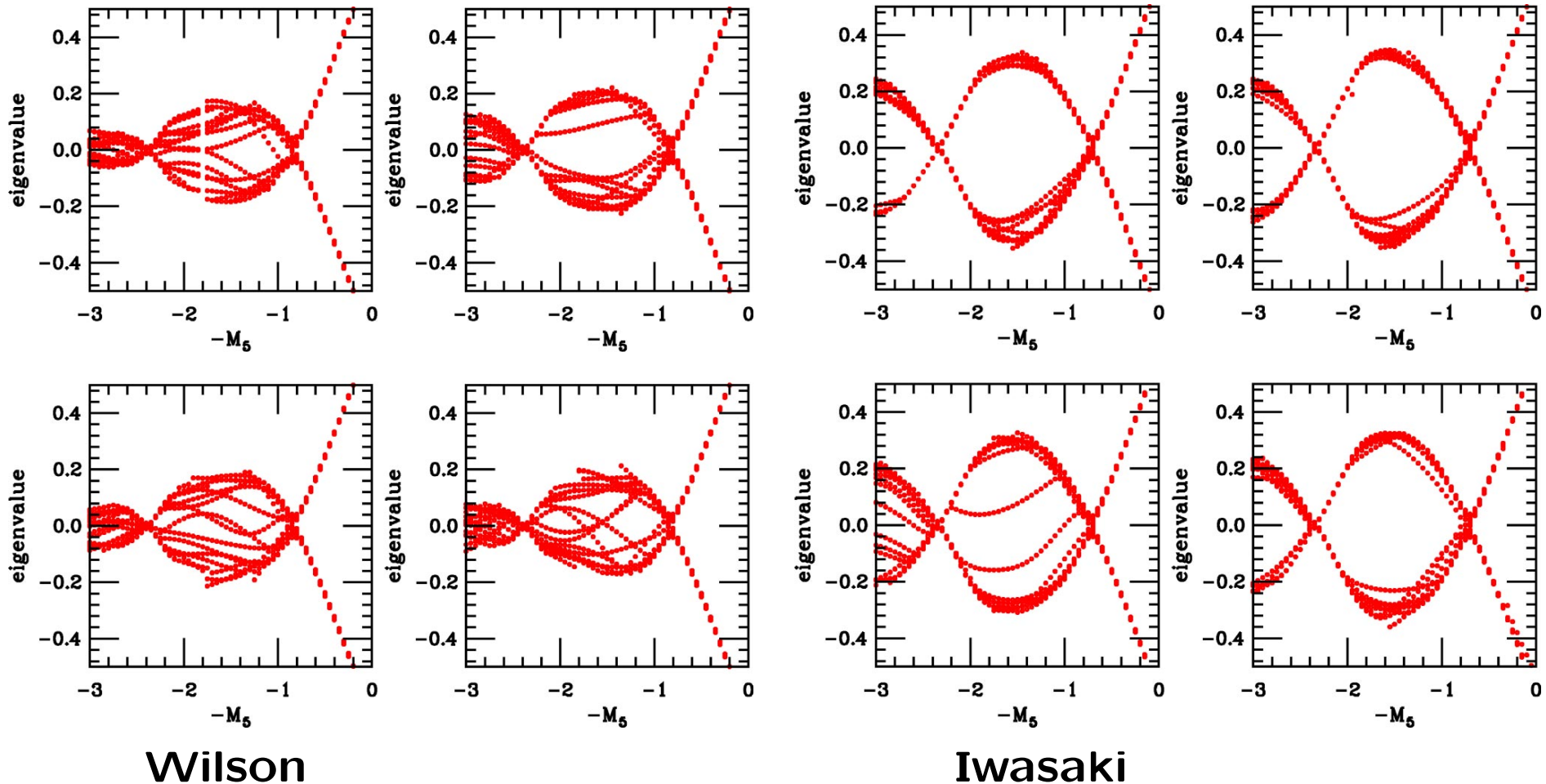
Suppress dislocations \rightarrow reduce χ SB

These dislocations, with large topological charge density, are topology-changing gauge configurations, and cause a complete reordering of the (Dirac) spectrum: χ SB

Low modes of D_W (Quenched, $a^{-1} \approx 2$ GeV)

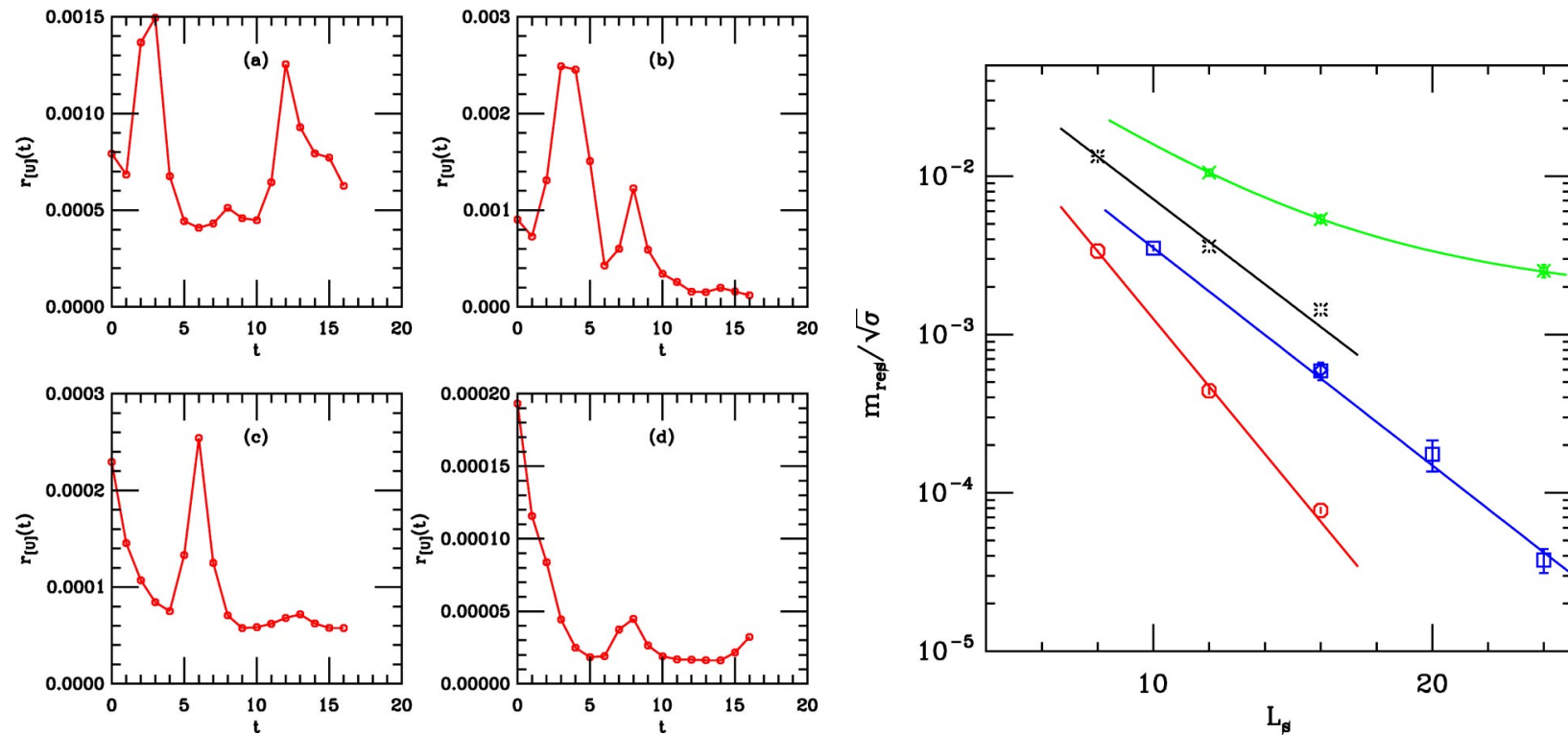
Iwasaki suppresses low modes in the gap. Gap is also larger.

At strong coupling gap closes: Aoki phase [Aoki (1980)]



Suppression of low modes: quenched case

“residual mass” on a typical Wilson, Symanzik, Iwasaki, and DBW2 gauge configuration (left). m_{res} (right)



Low modes localized around “spikes” and small regions of large topological charge density [Aoki, *et al.*, RBC Collab. (2004)]

Suppression of low modes: quenched case

Suppression is easy to understand. Modification of the gauge action of order $O(a^2/\rho^2)$ is positive for Iwasaki (and DBW2), so small instantons are suppressed. [Garcia Perez, Gonzalez-Arroyo, Snippe, van Baal (1994)].

Towards the continuum limit, tunneling of topological charge is suppressed, and it is worse for improved actions

Have to be careful: χ symmetry is better, but should not sacrifice correct average over topological sectors

In dynamical simulations, already use Iwasaki action, how can we suppress further?

Dislocation Suppressing Determinant Ratio

Add Wilson determinant(s) evaluated at $-M_5$ explicitly to (rational) hybrid monte-carlo evolution:

$$\det \frac{(\not{D}_W(-M_5) + i\epsilon_f \gamma_5) (\not{D}_W(-M_5) + i\epsilon_f \gamma_5)^\dagger}{(\not{D}_W(-M_5) + i\epsilon_b \gamma_5) (\not{D}_W(-M_5) + i\epsilon_b \gamma_5)^\dagger} = \prod \frac{\lambda^2 + \epsilon_f^2}{\lambda^2 + \epsilon_b^2}$$

$\det \not{D}_W(-M_5)$ - [Vranas (2000,2006) (GapDWF)]
suppresses zeroes at $-M_5$

$\det (\not{D}_W(-M_5) + i\epsilon_b \gamma_5)$ [JLQCD (2006) (fixed topology/overlap)]
Moderates the large shift in β caused by numerator

$\det (\not{D}_W(-M_5) + i\epsilon_f \gamma_5)$ [D. Renfrew, *et al.* (RBC) (2008)(unfix topology)]
allows for topology change

RBC/UKQCD I-DSDR Ensembles

After significant parameter searching, chose

$$\epsilon_f = 0.02$$

$$\epsilon_b = 0.50$$

$$\beta_I = 1.75$$

$$L_s = 32$$

and find $a^{-1} \approx 1.34$ GeV and $m_{\text{res}} \approx 0.0018$

Compare to 1.73 GeV and 0.003 (2 times reduction in m_{res} physical units)

RBC/UKQCD Gauge Ensembles (N. Christ's colloquium on 7/28)

Volume	$1/a$	L	m_π	Time units	$m_{\text{quark}}a$	Gauge Action
24³ x 64	1.73 GeV	2.7 fm	315 MeV	9000	0.005+0.0032	Iwasaki
			402 MeV	9000	0.01+0.0032	
32³ x 64	2.28 GeV	2.7 fm	290 MeV	7000	0.004+0.0006	
			350 MeV	8000	0.006+0.0006	
			410 MeV	6000	0.008+0.0006	
32³ x 64	1.4 GeV	4.5 fm	180 MeV	1000	0.001+0.0018	
			250 MeV	1800	0.004+0.0018	

Compare Iwasaki+DWF to I-DSDR+DWF
(latter is **preliminary**)

Topological Charge

Continuum:

$$Q = \frac{g^2}{16\pi^2} \int d^4x G_{\mu\nu}(x) \tilde{G}_{\mu\nu}(x) \quad \text{and} \quad \chi_Q = \langle Q^2 \rangle / V$$

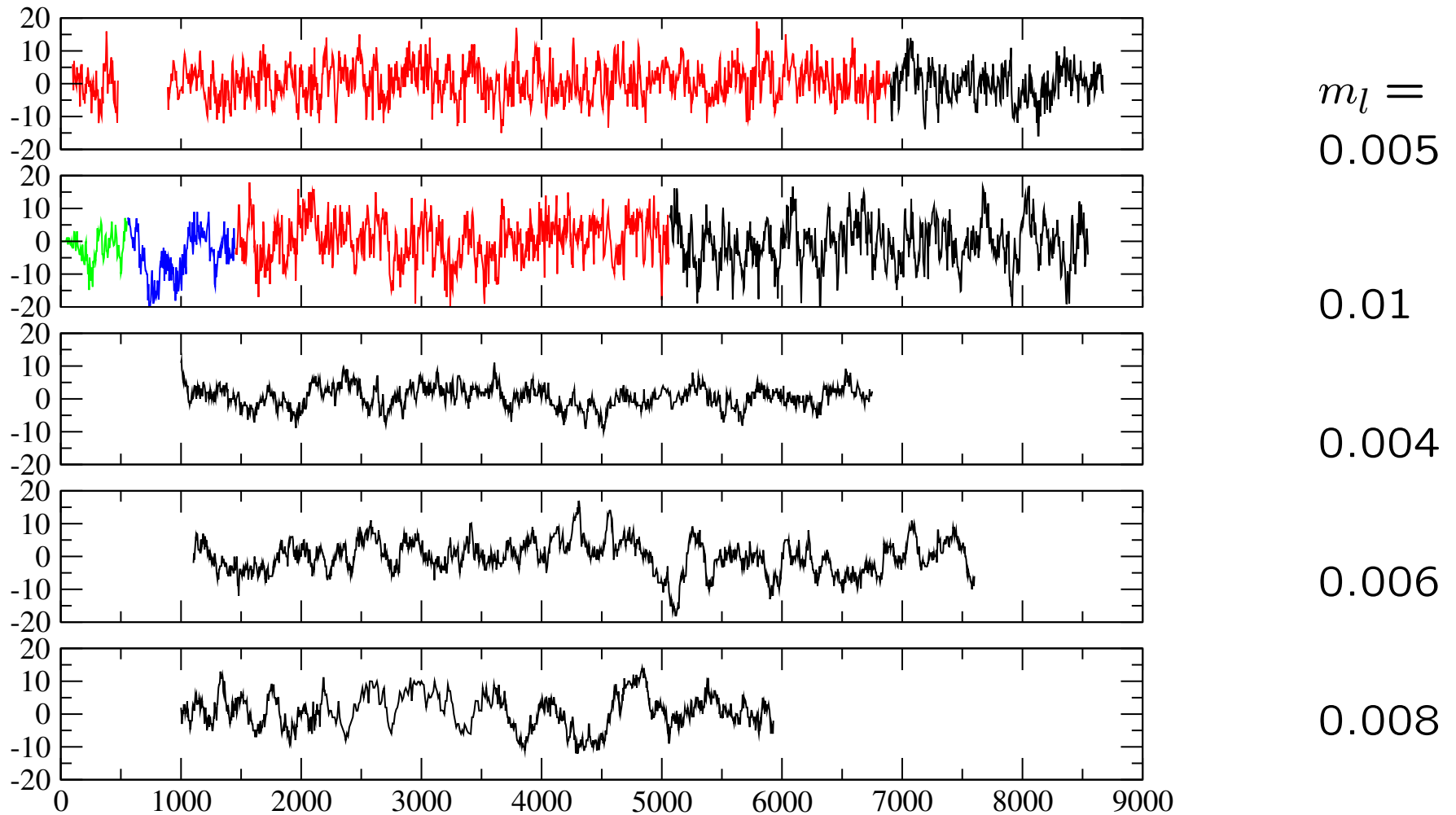
Define lattice Q using the “5 loop Improved” operator, linear combination of 5 loops: 1x1, 1x2, 1x3, 2x2, and 3x3.

[de Forcrand, *et al.* (1997)], after

APE smearing the links 60 times with $\alpha_{\text{smear}} = 0.45$

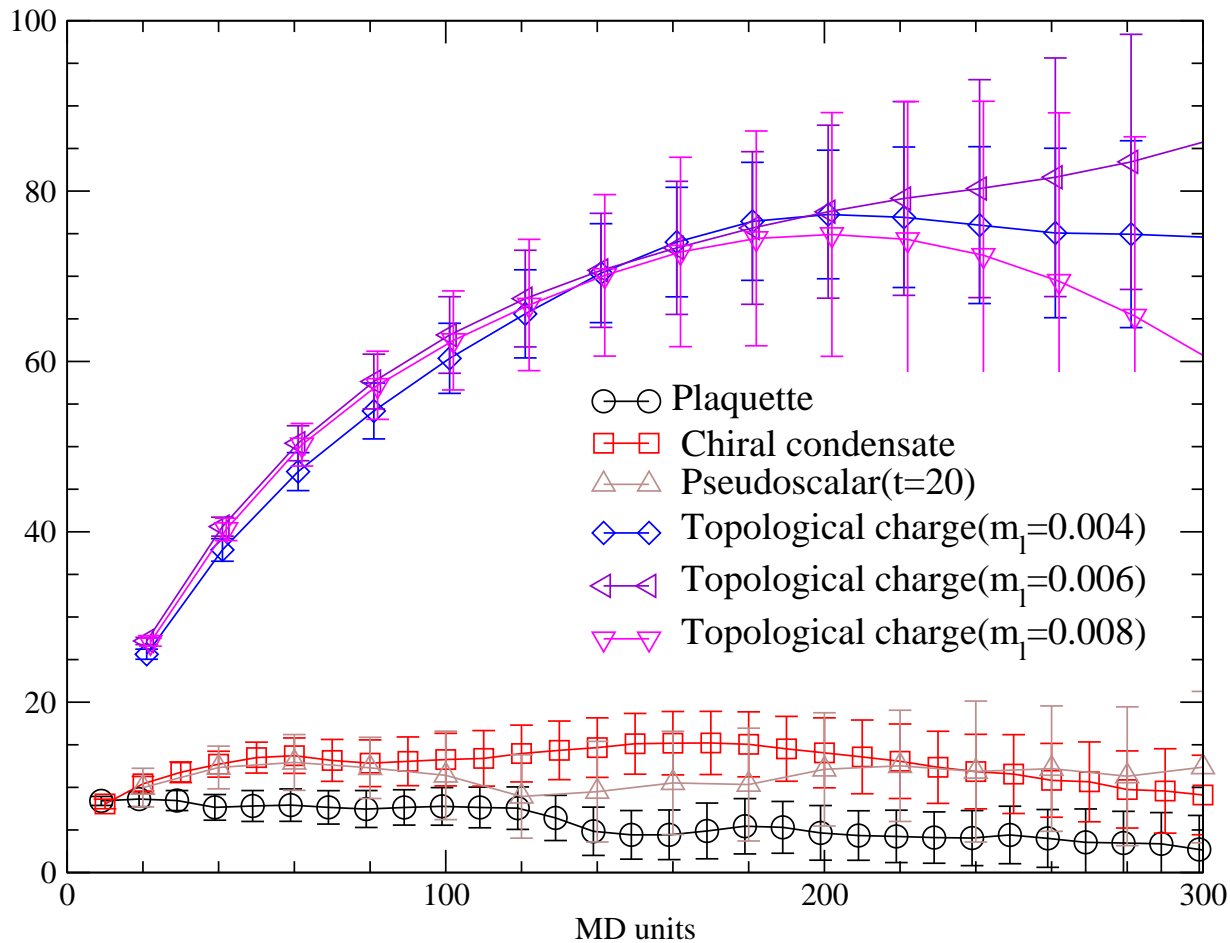
Topological Charge

Iwasaki gauge action, $a^{-1} = 1.73$ (upper) and 2.28 (lower)



Topological Charge

Integrated autocorrelations in Q (and plaq, $\bar{\psi}\psi$, m_{PS})
 $a^{-1} = 2.28$ GeV ensembles



Topological Charge (histograms)

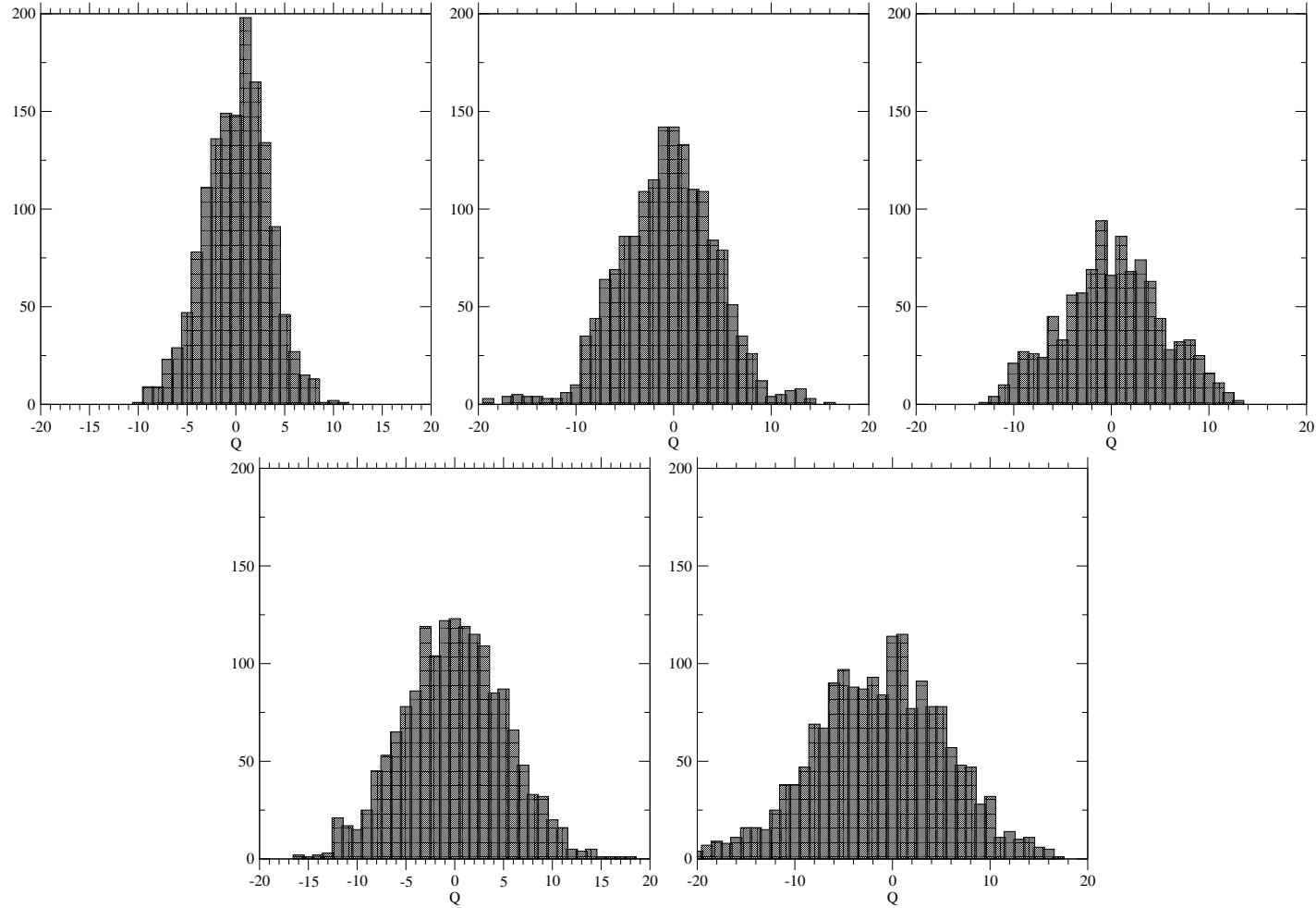
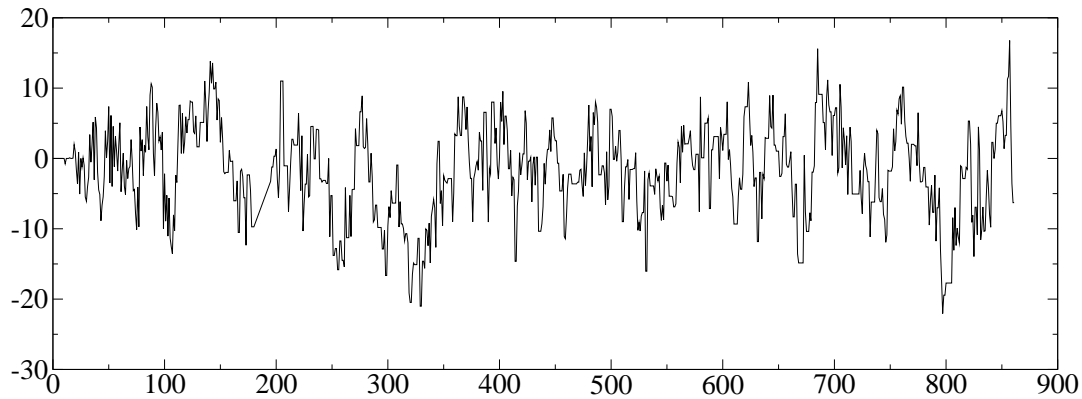


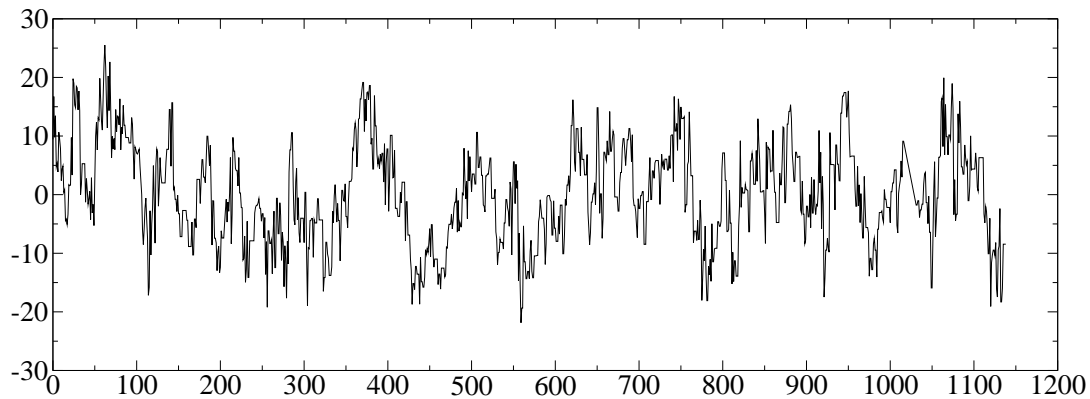
FIG. 52: Topological charge distributions. Top: 32^3 , $m_l = 0.004 - 0.008$, left to right. Bottom: 24^3 , $m_l = 0.005$ and 0.01 .

Topological Charge

I-DSDR gauge action, $m_l = 0.0042$ (upper) and 0.001 (lower)



$m_l =$
0.001



0.0042

Topological Susceptibility

Lowest order [DiVecchia, Veneziano (1980); Leutwyler, Smilga (1992)]

$$\chi_Q = \Sigma \left(\frac{1}{m_u} + \frac{1}{m_d} \right)^{-1} = \Sigma \frac{m_u m_d}{m_u + m_d},$$

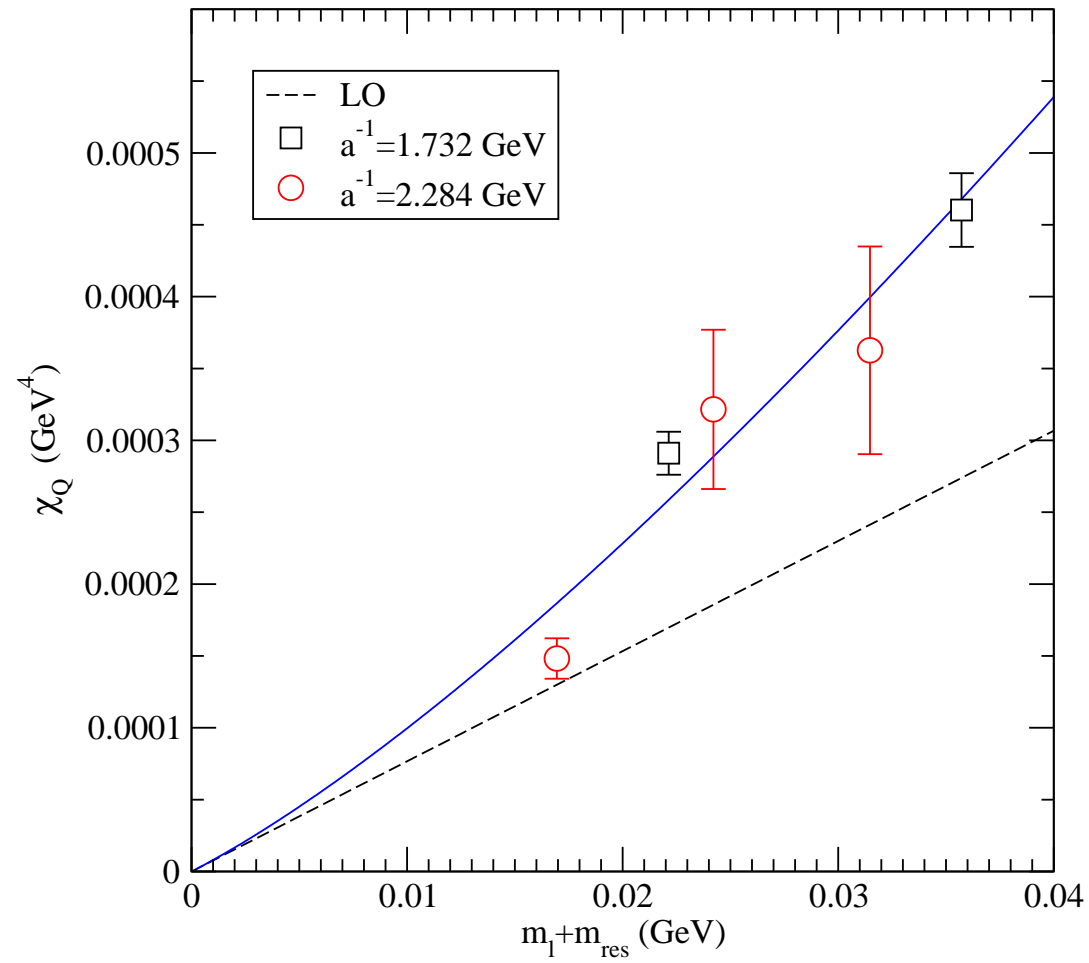
where $(\Sigma)^{1/3} = (Bf^2/2)^{1/3} = 251(4)(2)$ MeV.

At one-loop in chiral perturbation theory [Chiu and Mao (2009)],

$$\begin{aligned} \chi_Q &= \Sigma \left(\frac{1}{m_u} + \frac{1}{m_d} \right)^{-1} \times \\ &\quad \left(1 - \frac{3}{(4\pi f)^2} m_\pi^2 \log \frac{m_\pi^2}{\Lambda^2} + K_6(m_u + m_d) + 2(2K_7 + K_8) \frac{m_u m_d}{m_u + m_d} \right) \\ &= \Sigma \frac{m_l}{2} \left(1 - \frac{3}{(4\pi f)^2} m_{ll}^2 \log \frac{m_{ll}^2}{\Lambda^2} + (2K_6 + 2K_7 + K_8) m_l \right), \end{aligned}$$

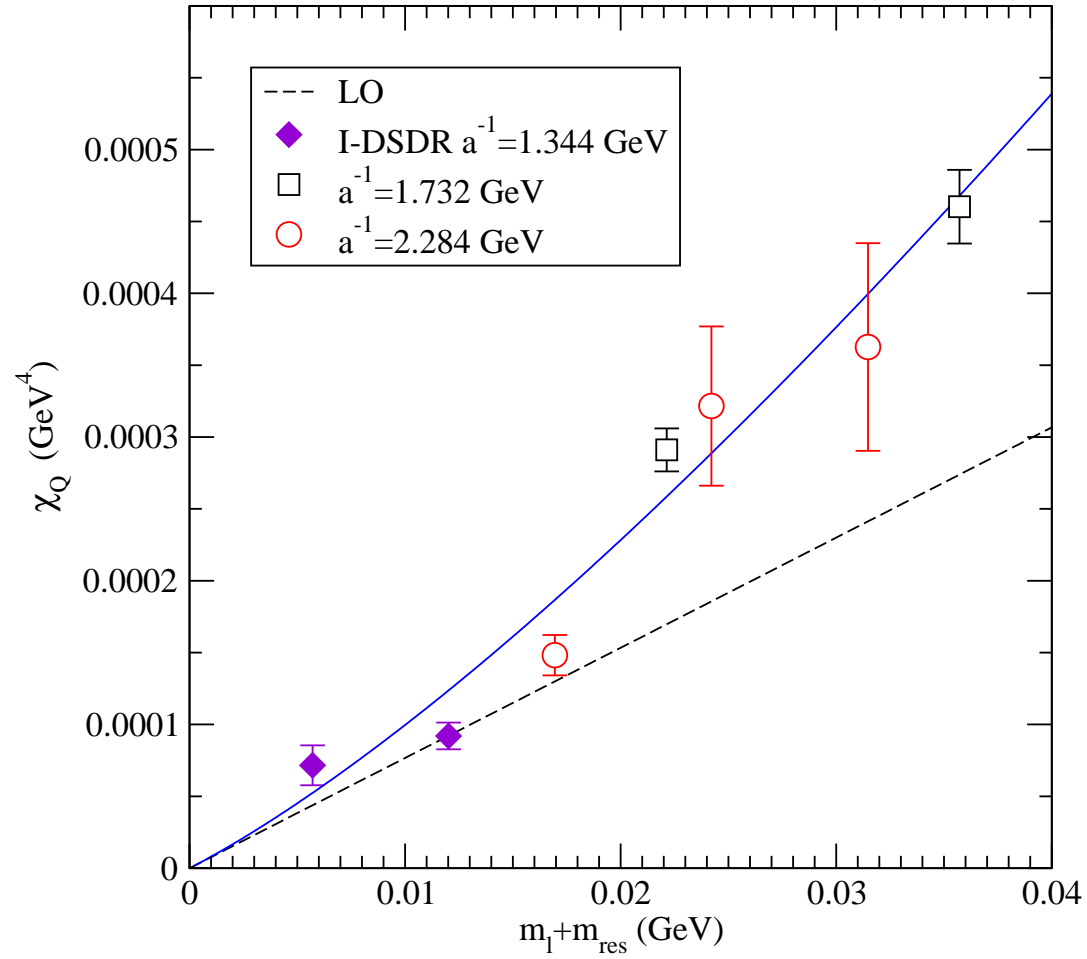
where $K_i = 128 \Sigma L_i / f^4$

Topological Susceptibility



Fit does not include $O(a^2)$ corrections

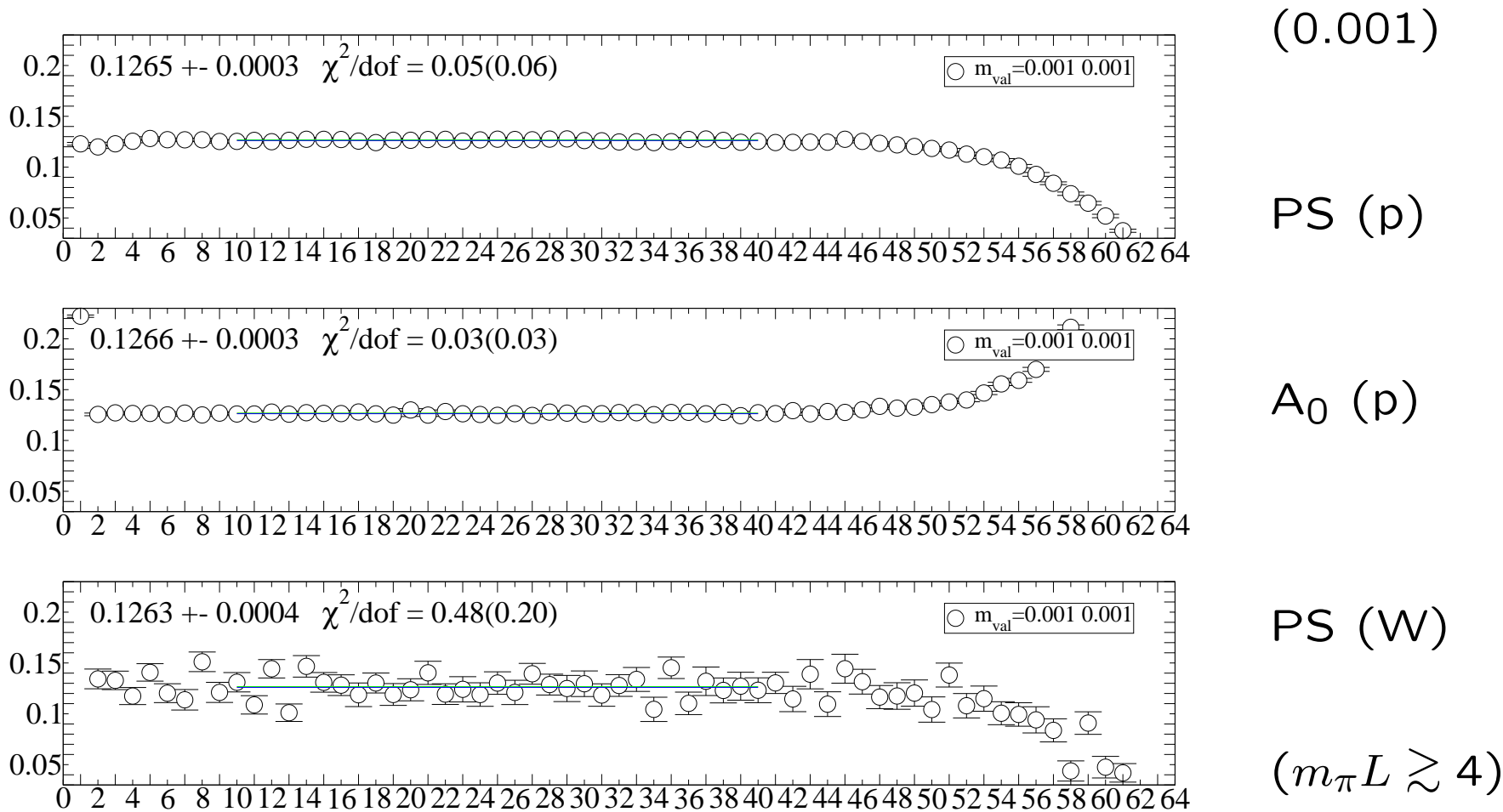
Topological Susceptibility



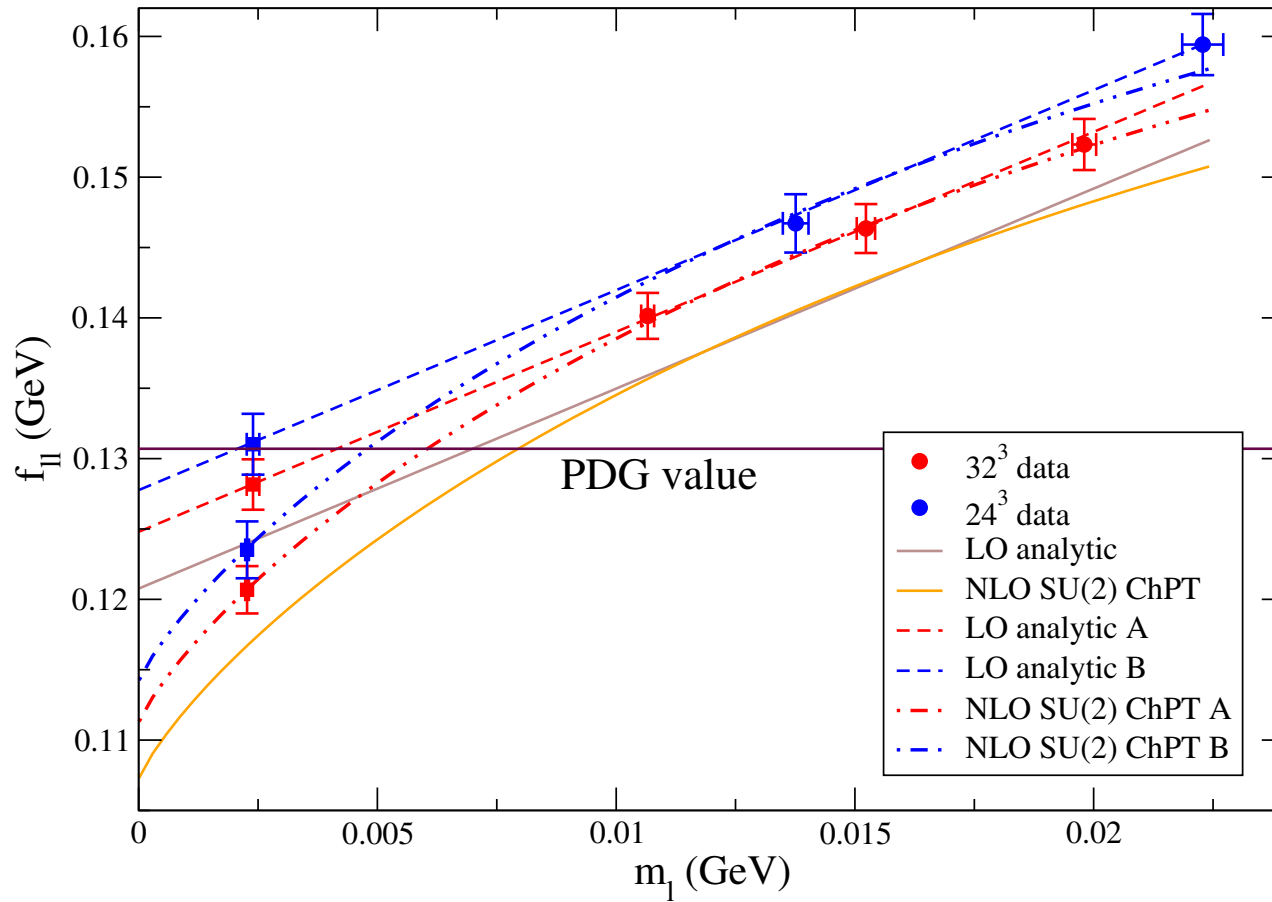
I-DSDR points preliminary (not included in fit)

Meson mass and decay constant fits (effective masses)

Simultaneously fit wall-point, wall-wall, PS and Axial Vector 2-pt functions: 1 mass, 3 amplitudes \rightarrow decay constants

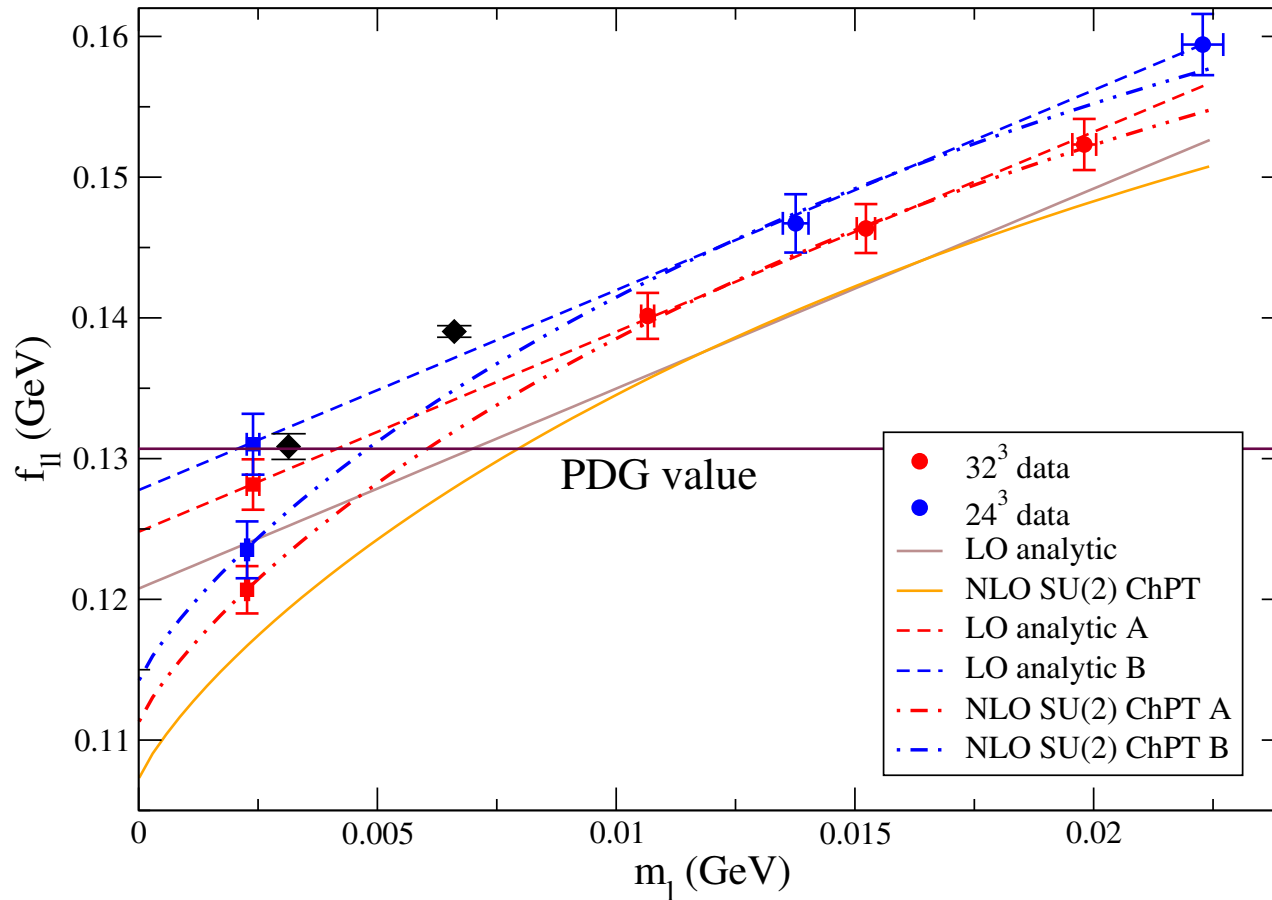


Pion Decay Constant Iwasaki+DWF



$f_{\pi} = 122(2)(5)$ MeV (average of NLO/FV and analytic fits)

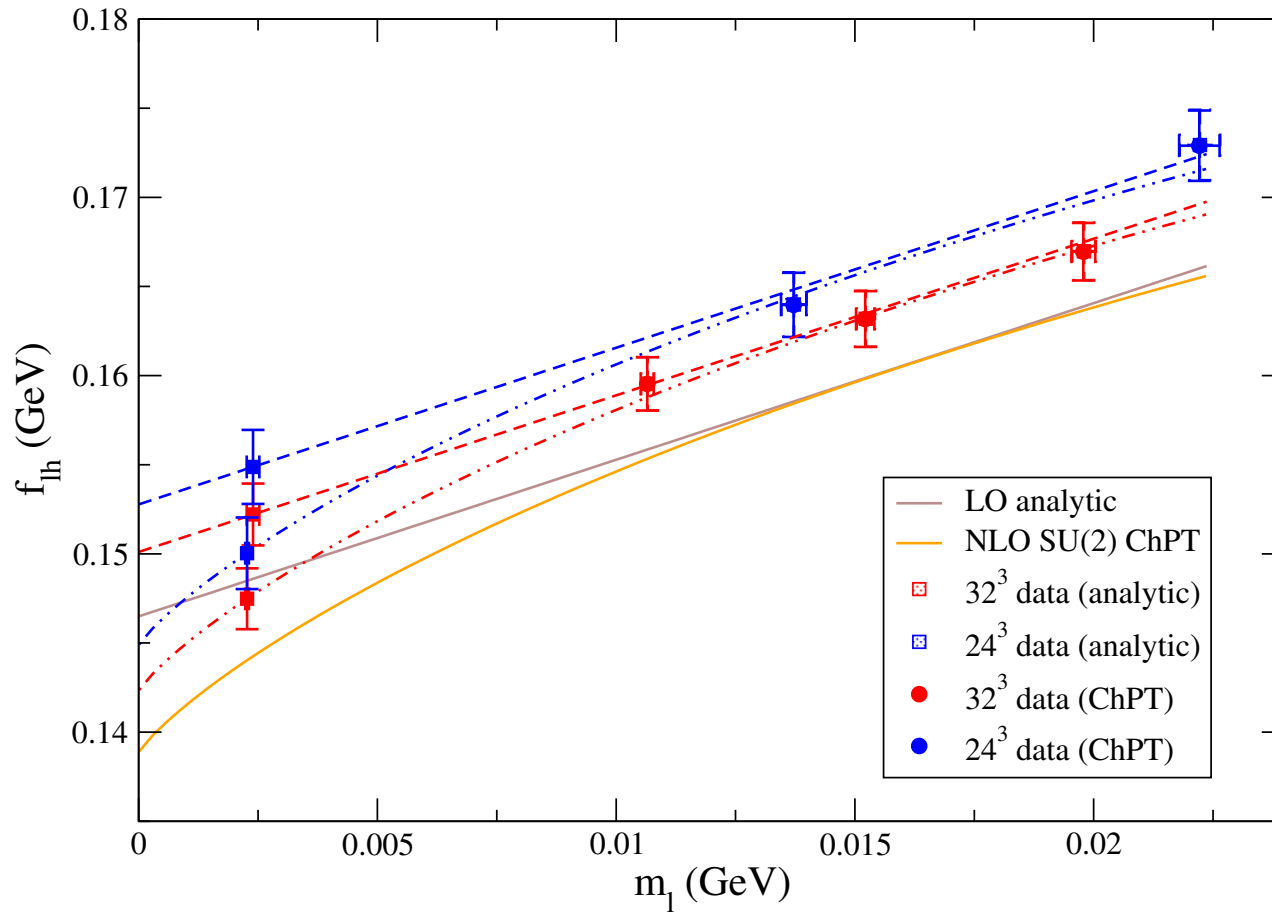
Pion Decay Constant Iwasaki+DWF, I-DSDR+DWF



$f_{\pi} = 122(2)(5)$ MeV (average of NLO/FV and analytic fits)

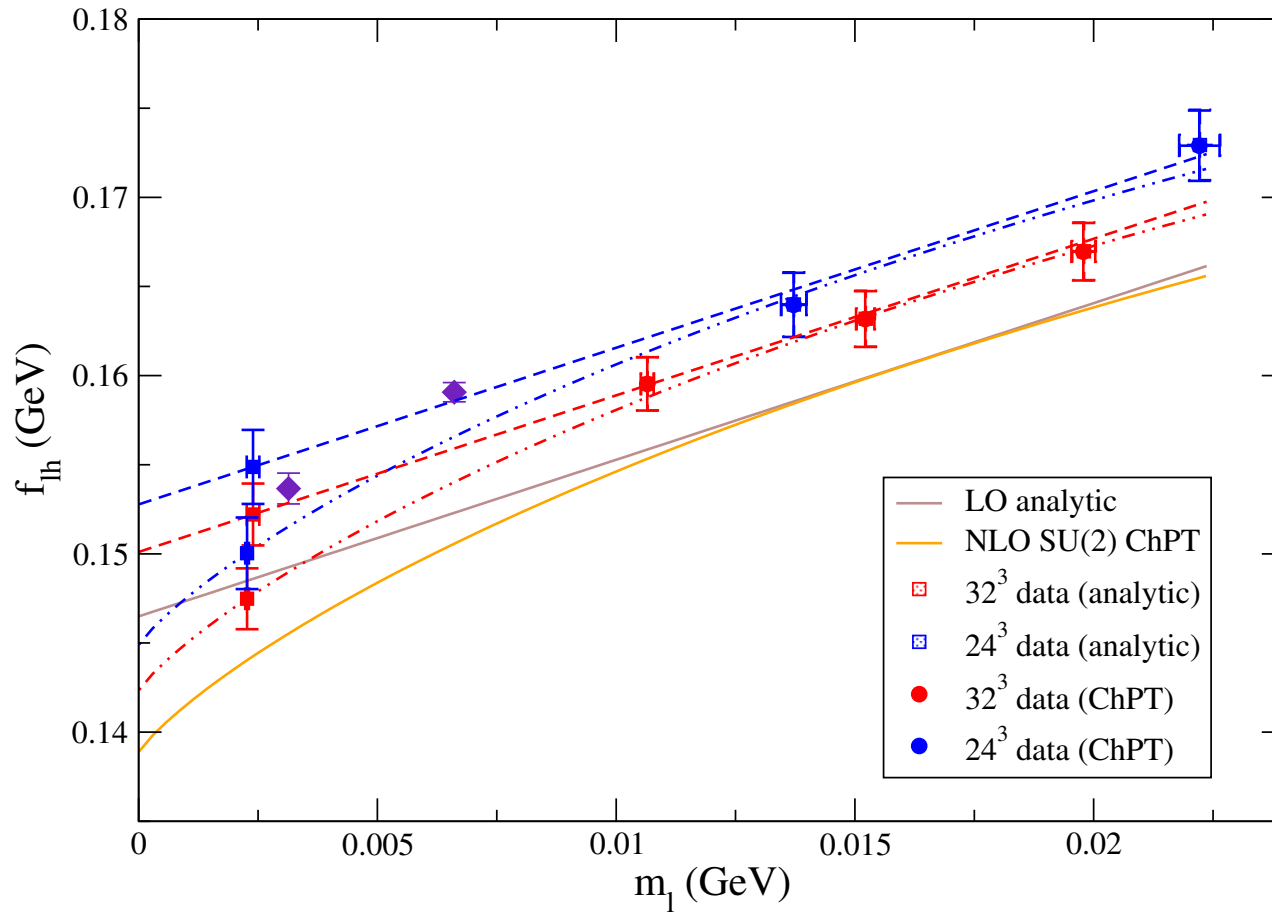
I-DSDR points are Preliminary

Kaon Decay Constant Iwasaki+DWF



$$f_K = 147(2)(4) \text{ MeV}$$

Kaon Decay Constant Iwasaki+DWF, I-DSDR+DWF

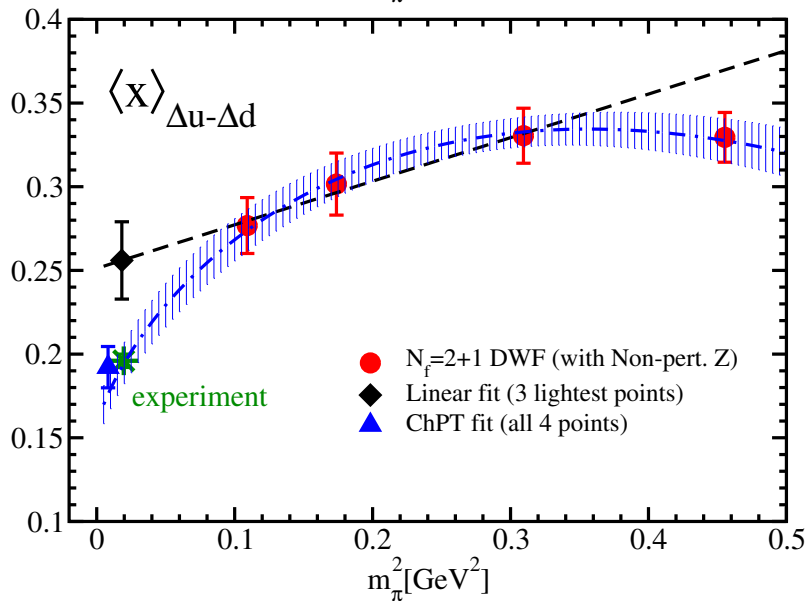
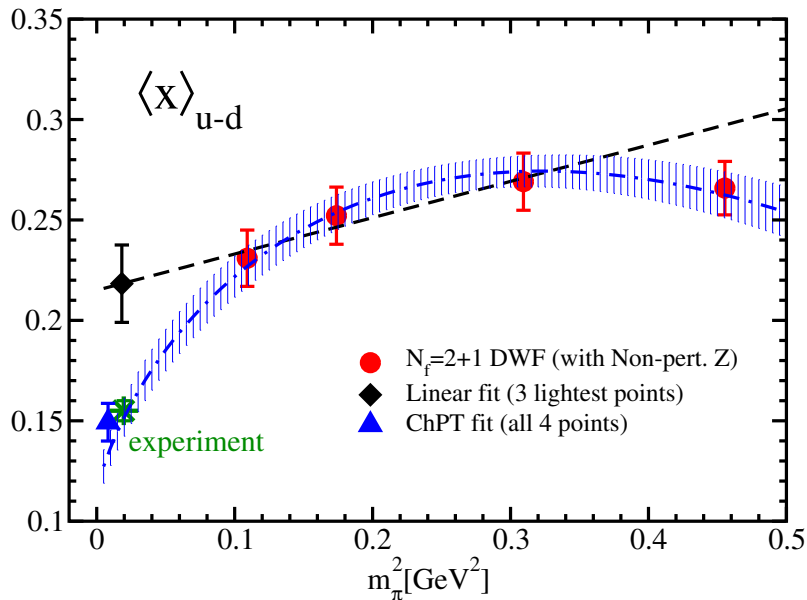


$f_K = 147(2)(4)$ MeV **I-DSDR points Preliminary**

Nucleon Structure ($\langle x \rangle_q$, $\langle x \rangle_{\Delta q}$, axial charge g_A)

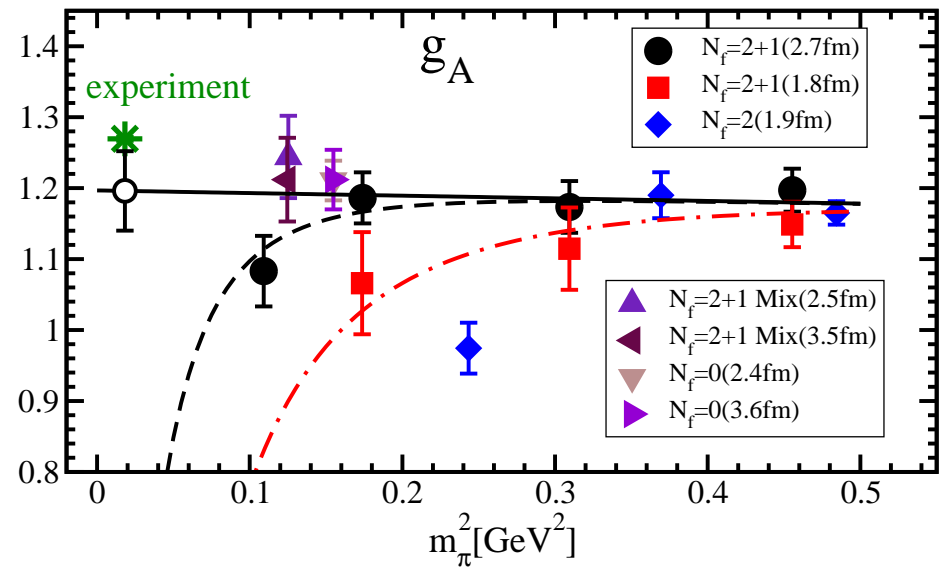
- Long standing “puzzles” (lack of agreement with exp.!)
- Heavy Baryon Chiral Perturbation Theory

$$\begin{aligned}\langle x \rangle_{u-d} &= C \left[1 - \frac{3g_A^2 + 1}{(4\pi F_\pi)^2} m_\pi^2 \ln \left(\frac{m_\pi^2}{\Lambda^2} \right) \right] + e(\Lambda^2) \frac{m_\pi^2}{(4\pi F_\pi)^2} \\ \langle x \rangle_{\Delta u - \Delta d} &= \tilde{C} \left[1 - \frac{2g_A^2 + 1}{(4\pi F_\pi)^2} m_\pi^2 \ln \left(\frac{m_\pi^2}{\Lambda^2} \right) \right] + \tilde{e}(\Lambda^2) \frac{m_\pi^2}{(4\pi F_\pi)^2}\end{aligned}$$



Iwasaki+DWF

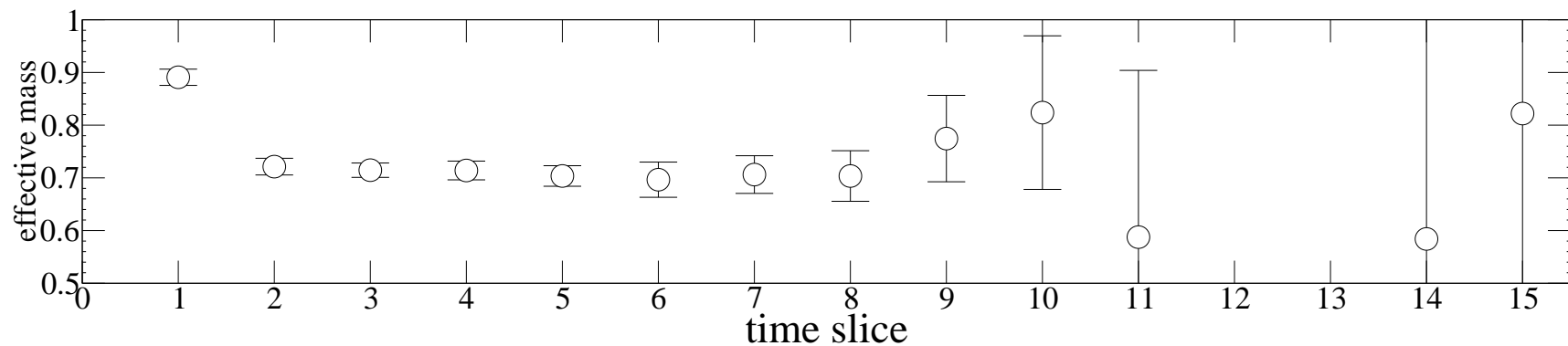
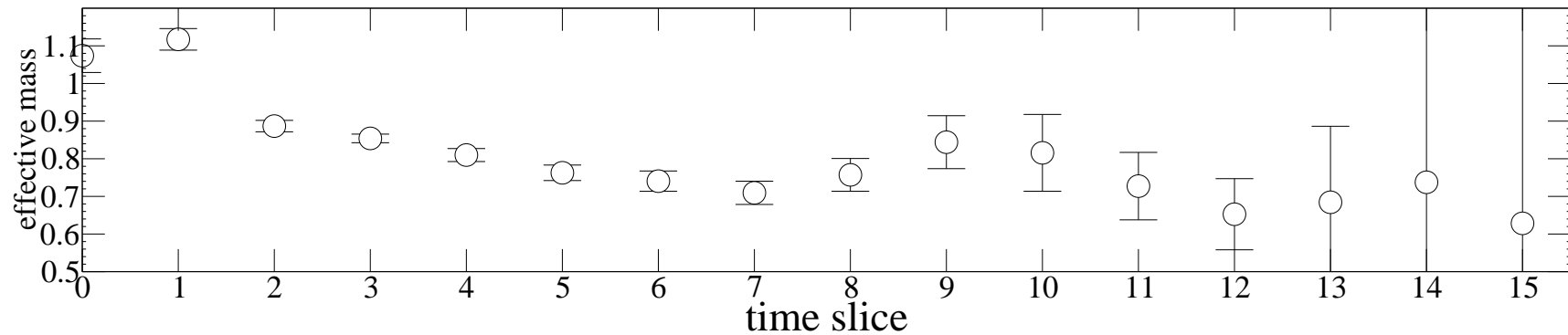
24^3 , 1.73 GeV ensembles



[Yamazaki, *et al.* (RBC/UKQCD) (2008)]

[Aoki, *et al.* (RBC/UKQCD) (2009)]

Nucleon effective masses tuning sources, I-DSDR ensembles

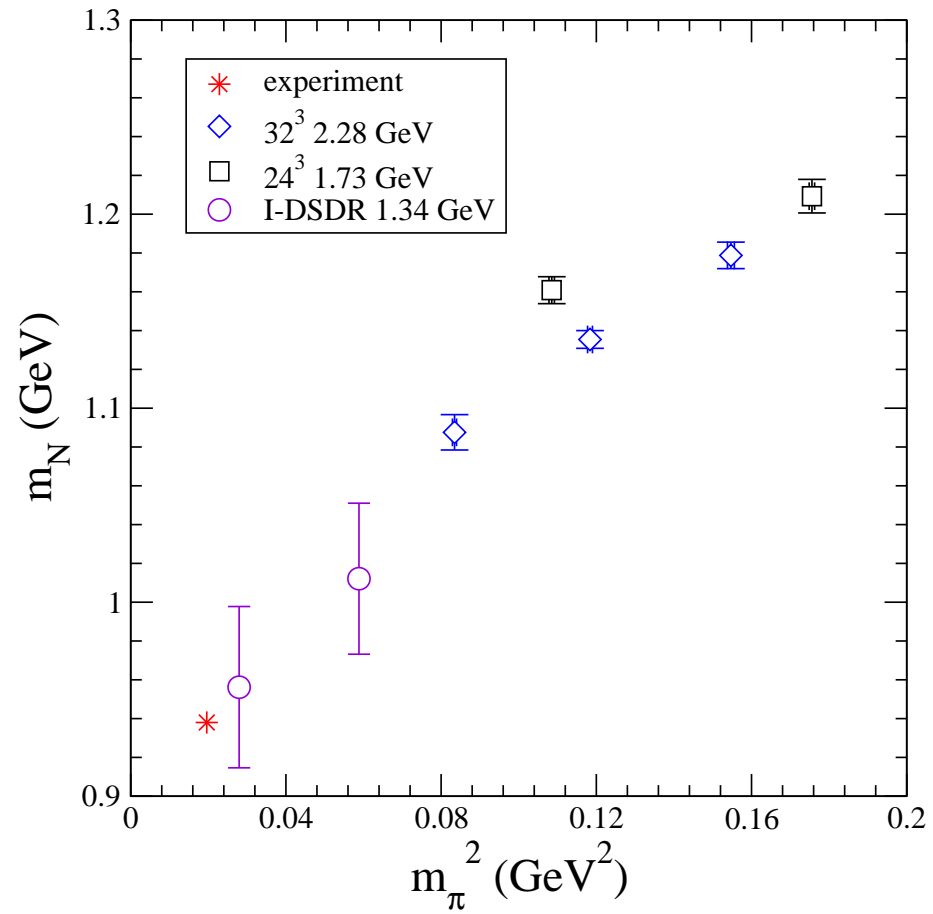


Gaussian and link smeared sources

($r/a=4.0$, 0.0042 upper and $r/a=6.0$, 0.001 lower)

only 26 and 49 configs but multiple sources

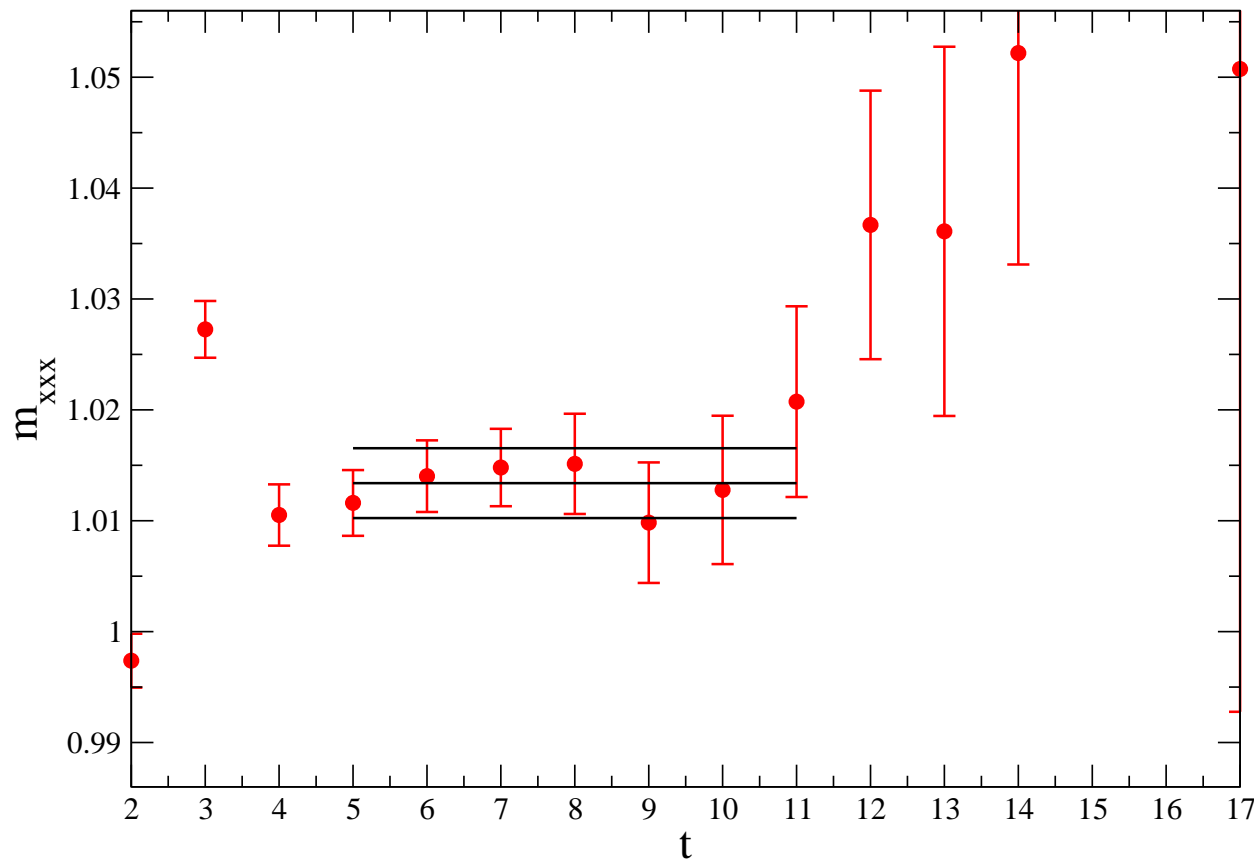
Nucleon Mass



I-DSDR points Preliminary

Scaling

We set the scale using the Ω baryon mass since it has simple chiral extrapolation [Toussaint and Davies (2005)] and can be obtained with good precision



24^3 , $m_l = 0.005$
“Box” source
($L_B = 16$)

Scaling: Iwasaki+DWF

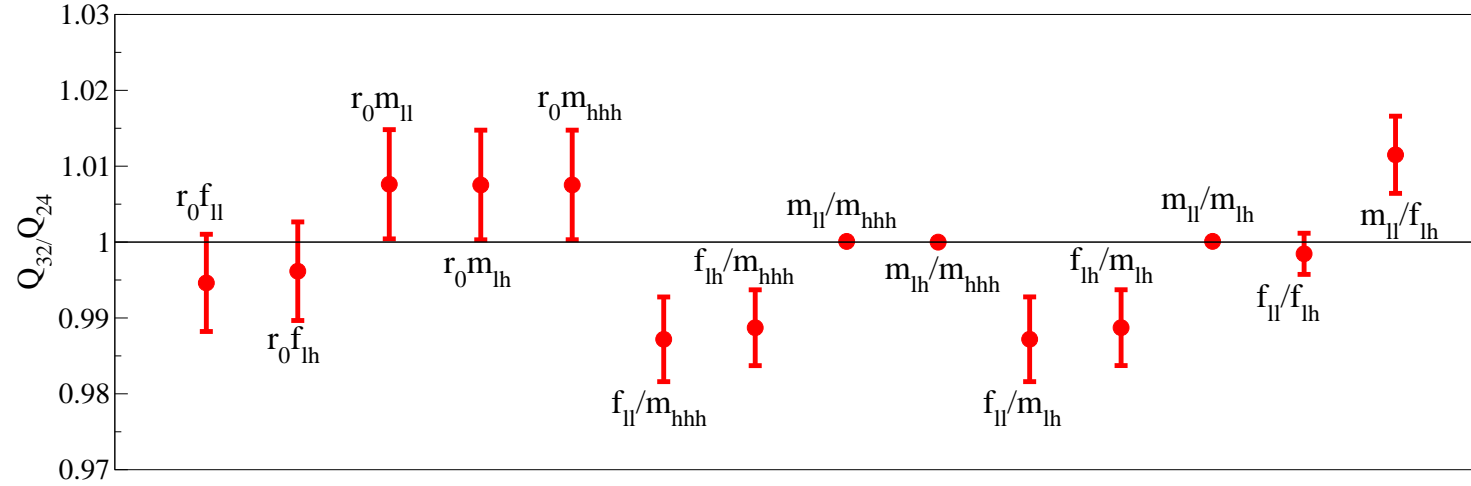


FIG. 1: Ratios of dimensionless combinations of lattice quantities Q (listed in the figure) between the 32^3 and 24^3 lattices at the match point corresponding to $m_l = 0.006$, $m_h = 0.03$ on the 32^3 lattice. A value of unity indicates perfect scaling. The ratios m_{ll}/m_{hhh} and m_{lh}/m_{hhh} (and consequently m_{ll}/m_{lh}) are defined to scale perfectly at these quark masses through our choice of scaling trajectory.

A wide range of *ratios* of physical observables scale very well between 1.73 and 2.28 GeV ensembles when matched at mass points where we have done simulations.

Scaling: I-DSDR+DWF

Only one lattice spacing so far

But, can still match at unphysical point with Iwasaki ensembles

Using 2.28 GeV ensemble, decay constants f_π and f_K scale within 3% and 2% respectively at the (0.001) match point

Both Iwasaki+DWF and I-DSDR+DWF appear to have modest lattice artifacts

Another I-DSDR at smaller a needed to confirm

Summary

- Simulation of new I-DSDR ensembles well underway
- residual χ SB small, even at large a ($m_{\text{res}} \approx 2.5$ MeV @ $a = 0.14$ fm)
- Unitary pion masses roughly 170 and 240 MeV
- Partially quenched physical pion/kaon masses (*c.f.*, $K \rightarrow \pi\pi(I = 2)$)
- Large volume $\gtrsim 4.5$ fm
- Scaling errors appear modest
- Physics prospects look bright ($K \rightarrow \pi\pi$, Nucleons, chiral pt, ...)

Calculations done on [NY Blue](#) and [QCDOC](#) supercomputers at Brookhaven National Lab, Argonne National Lab [Bluegene P](#), and the [RICC cluster](#) at RIKEN. Thanks to [BNL](#), [RBRC](#), [RIKEN](#), and [USQCD](#) for computational resources.

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Ciao.