2+1 flavor DWF QCD: Zero and finite temperature ensembles and $\Delta S = 1$ physics

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DWF @ 10
Brookhaven National Laboratory
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25,000 nodes at Brookhaven
RBRC and USDOE machines

14,000 nodes at the University of Edinburgh

Collaboration Members

RBC members:

Y. Aoki, C. Aubin, T. Blum, M. Cheng, N. Christ, S. Cohen, C. Dawson, T. Doi, K. Hashimoto, T. Ishikawa, T. Izubuchi, C. Jung, M. Li, S. Li, M. Lightman, H. Lin, M. Lin, O. Loktik, R. Mawhinney, S. Ohta, S. Sasaki, E. Scholz, A. Soni, T. Yamazaki

UKQCD members:

C. Allton, D. Antonio, K. Bowler, P. Boyle, M. Clark, J. Flynn, A. Hart, B. Joo, A. Juettner, A. Kennedy, R. Kenway, C. Kim, C. Maynard, J. Noaki, B. Pendleton, C. Sachrajda, A. Trivini, R. Tweedie, J. Wennekers, A. Yamaguchi, J. Zanotti

Progress in DWF simulations

- Last 10 years have seen quenched, 2 flavor and now 2+1 flavor DWF simulations of QCD.

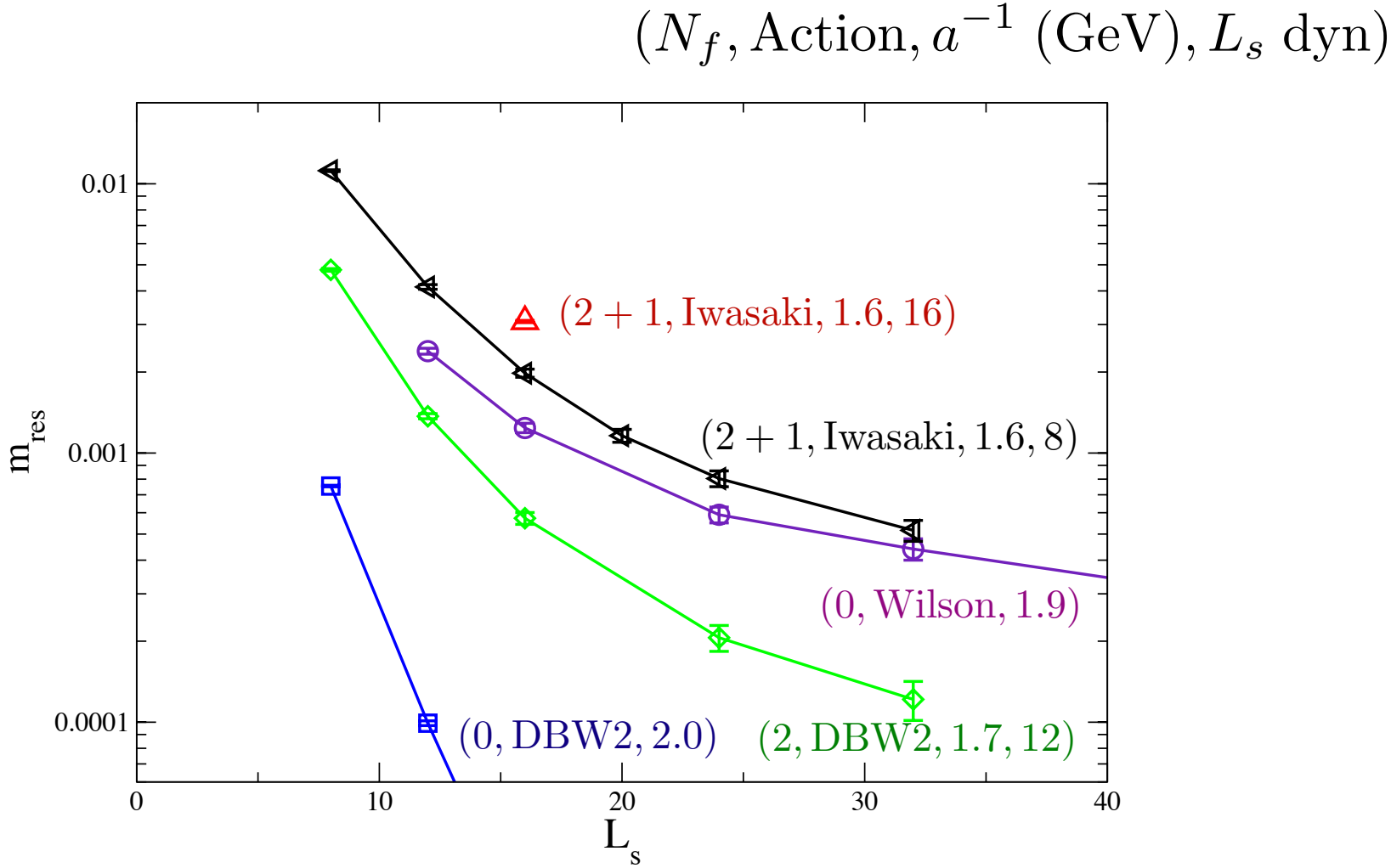
- Residual mass (m_{res}) markedly improved for quenched simulations by changing gauge action from Wilson to Iwasaki to DBW2.

- These actions smooth the gauge field at the scale of the lattice spacing, suppressing small topology-changing dislocations and reducing perturbative contributions.

$$m_{\text{res}} \sim \rho(0)/L_s + \exp(-\alpha L_s)/L_s$$

- Adding fermions, while keeping lattice spacing fixed, makes gauge fields rougher at the lattice scale, since β becomes smaller, and m_{res} increases.

Residual Mass



Zero Temperature Ensembles

Volume	a^{-1} (GeV)	(m_l m_s)	m_{res}	MD time units
$16^3 \times 32 \times 12$	1.69(5)	(0.02,∞) (0.03,∞) (0.04,∞)	0.00137(5)	2680.5 3097.5 3252.5
$16^3 \times 32 \times 8$	1.8(1)	(0.02, 0.04) (0.04, 0.04)	0.0107(1)	1797.5 1797.5
$16^3 \times 32 \times 16$	1.62(4)	(0.01, 0.04) (0.02, 0.04) (0.03,0.04)	0.00308(4)	4015 4045 4020+3580
$24^3 \times 64 \times 16$	1.6-1.7	(0.005,0.04) (0.01,0.04) (0.02,0.04) (0.03,0.04)	0.0031	4500 3785 2850 2813
$32^3 \times 64 \times 16$	2.1-2.2	(0.004, 0.03) (0.006, 0.03)	≈ 0.0005	500 892

First row is with DBW2 gauge action, all others use the Iwasaki action.

RHMC

$$\det \mathcal{M} = \int D\bar{\phi} D\phi \exp(-\bar{\phi}\mathcal{M}^{-\alpha}\phi)$$

$$= \int D\bar{\phi} D\phi \, \exp(-\bar{\phi}\, r^2(\mathcal{M})\phi)$$

with $\quad r(x) \approx x^{-\alpha/2}$

and $\quad r(x) = \sum_{k=1}^{n} \frac{\alpha_k}{x + \beta_k}$

Mike Clark, PhD Thesis, U. Edinburgh, 2005

Clark, de Forcrand, Kennedy, hep-lat/0510004

Omelyan Integrator

Omelyan, Mryglod, Folk, 2003. Takaishi, de Forcrand, hep-lat/0505020

Symmetric, symplectic, second order integrator

λ controls coefficient of higher order terms

$$\hat{U}_{\mathrm{QPQPQ}}(\delta\tau) = e^{\lambda\delta\tau Q}\, e^{\delta\tau P/2}\, e^{(1-2\lambda)\delta\tau Q}\, e^{\delta\tau P/2}\, e^{\lambda\delta\tau Q},$$

Expected to be 50% better than leapfrog

Some RHMC Implementation Options

- Choose Hasenbush preconditioning mass(es)
- Omelyan integrator parameter
- Number of different integration levels
- Relax stopping condition during evolution
- Optimize n since RHMC allows n version of 1/n power
- Split poles to different integrator time scales
- Chronological forecasting

More than 6x speed up and milder light quark limit

Different RHMC Decompositions

Let $\mathcal{D}(m_i) \equiv D^\dagger_{\mathrm{DWF}}(M_5, m_i) D_{\mathrm{DWF}}(M_5, m_i)$

RHMC I: 4 RHMC, 1 HMC and leapfrog integrator

$$\frac{\det\left[\mathcal{D}(m_l)\right]^{1/2} \det\left[\mathcal{D}(m_l)\right]^{1/2} \det\left[\mathcal{D}(m_s)\right]^{1/2}}{\det\left[\mathcal{D}(1.0)\right]^{1/2} \det\left[\mathcal{D}(1.0)\right]}$$

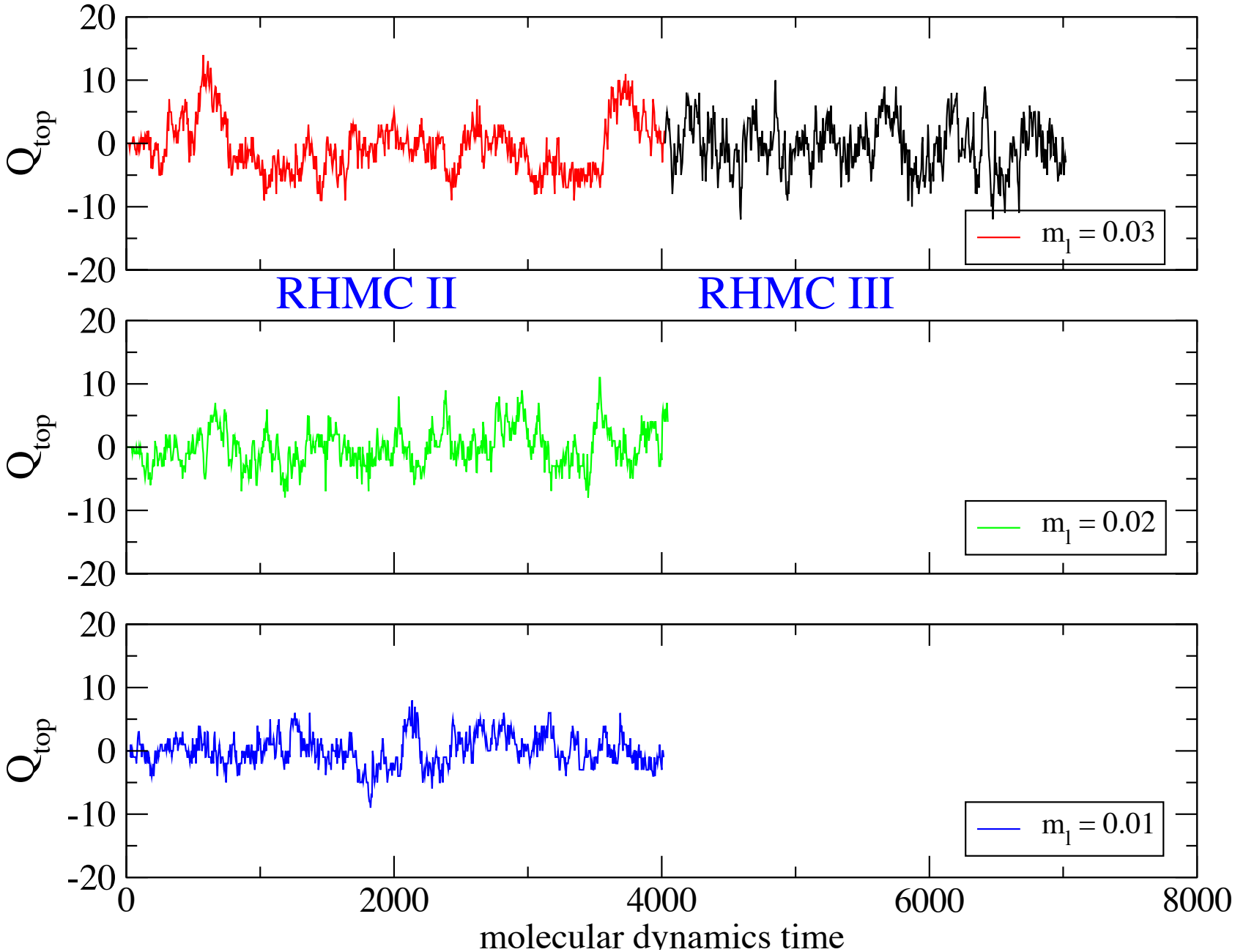
RHMC II: 4 RHMC, 1 HMC, multi-timescale Omelyan integrator with light poles coarser than heavy

$$\frac{\overset{\substack{0 \to 3 \\ 4 \to 10}}{\det\left[\mathcal{D}(m_l)\right]^{1/2}} \overset{\substack{0 \to 3 \\ 4 \to 10}}{\det\left[\mathcal{D}(m_l)\right]^{1/2}} \overset{\substack{0 \to 2 \\ 3 \to 10}}{\det\left[\mathcal{D}(m_s)\right]^{1/2}}}{\det\left[\mathcal{D}(1.0)\right]^{1/2} \underset{\substack{0 \\ 1 \to 6}}{\det\left[\mathcal{D}(1.0)\right]}}$$

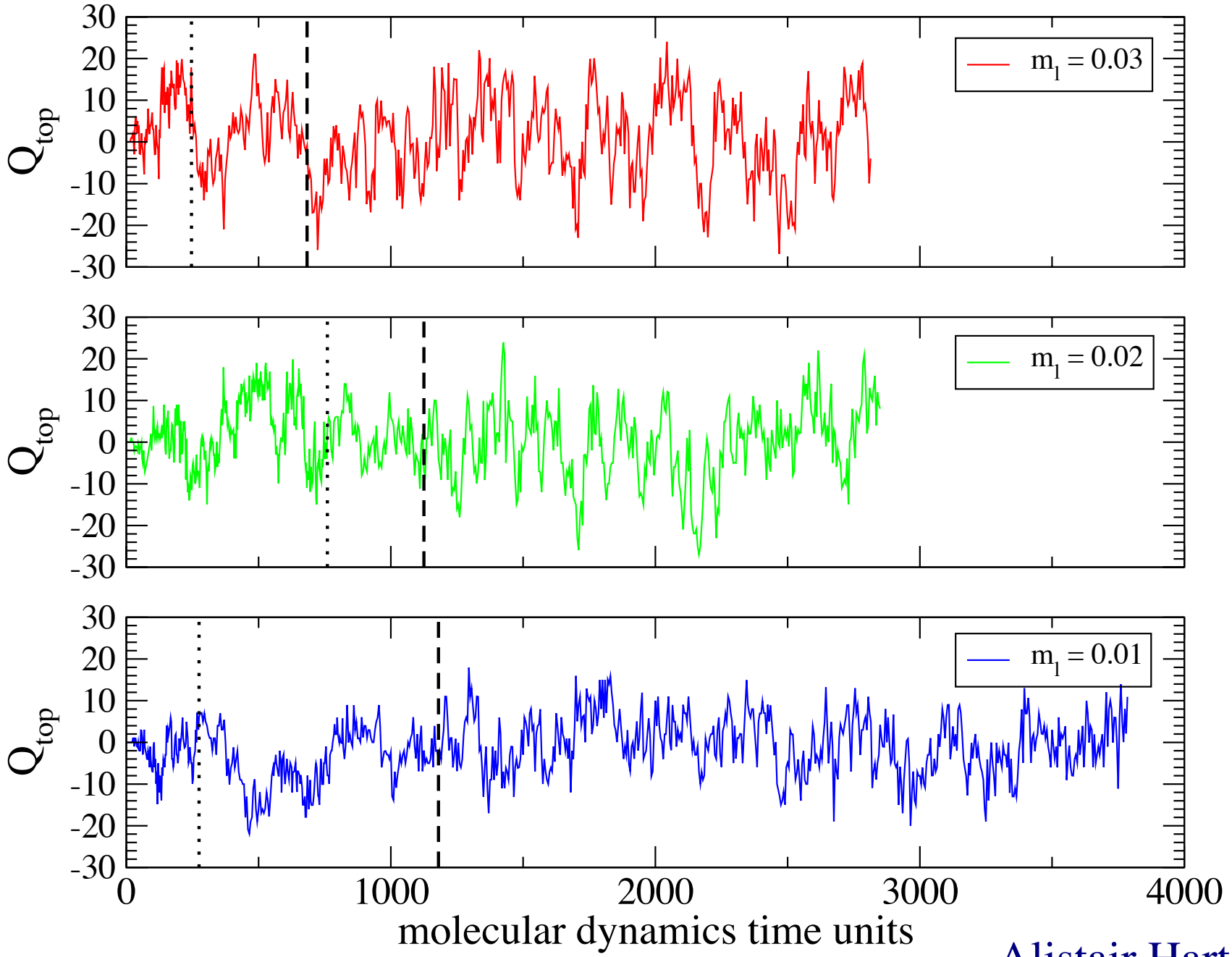
RHMC III: 3 RHMC, 1 HMC, quotient force term, Hasenbush preconditioning and 3 scale Omelyan integrator (HMC, RHMC, gauge)

$$\det\left[\frac{\mathcal{D}(m_l)}{\mathcal{D}(m_s)}\right] \det\left[\frac{\mathcal{D}(m_s)}{\mathcal{D}(1.0)}\right]^{1/2} \det\left[\frac{\mathcal{D}(m_s)}{\mathcal{D}(1.0)}\right]^{1/2} \det\left[\frac{\mathcal{D}(m_s)}{\mathcal{D}(1.0)}\right]^{1/2}$$

$16^3 \times 32 \times 16, 2+1$ Flavor Topology Evolutions

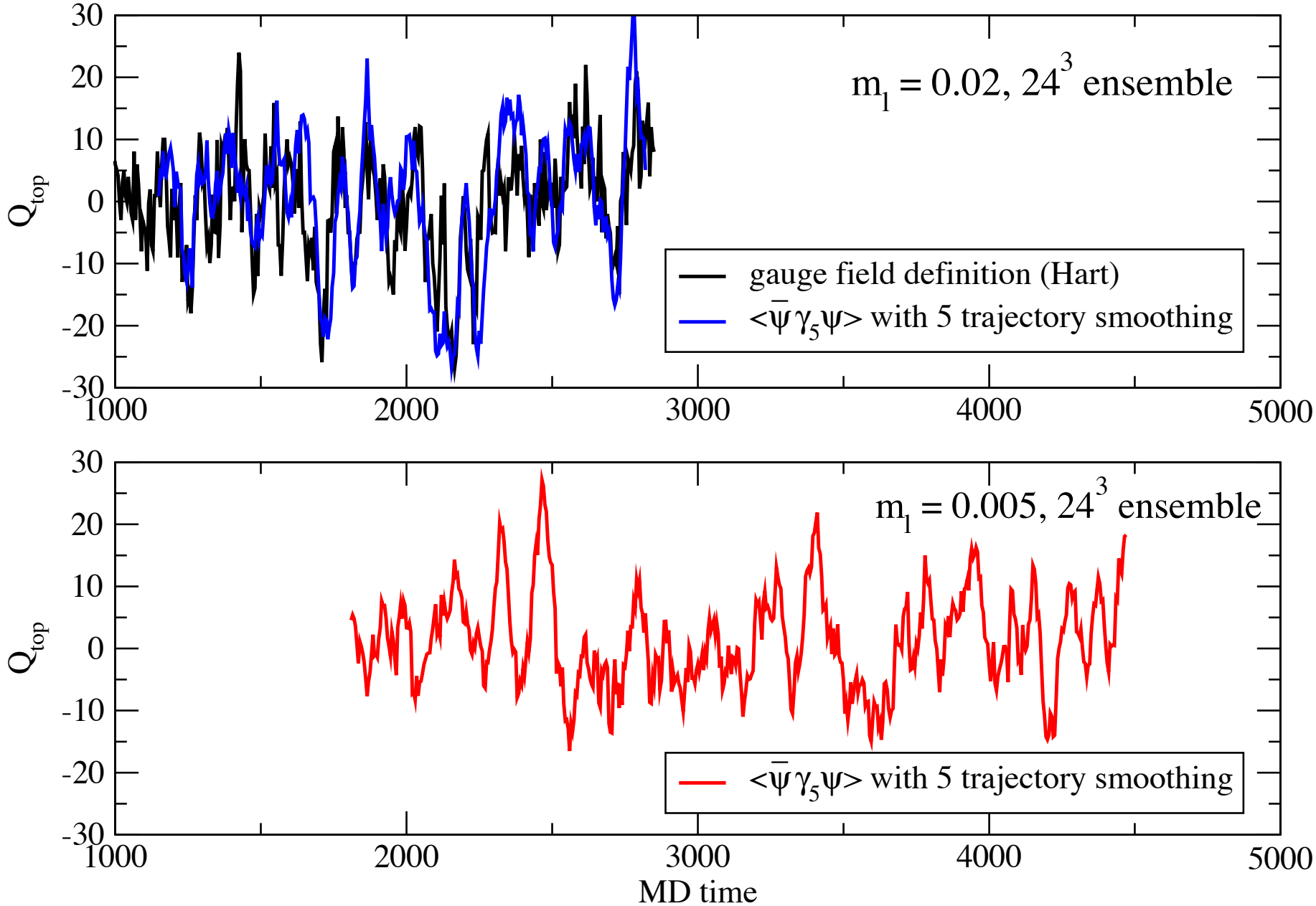


$24^3 \times 64 \times 16, 2+1$ Flavor Topology Evolutions



Alistair Hart

Q from gauge links compared to $\langle \overline{\psi}\gamma_5\psi \rangle$

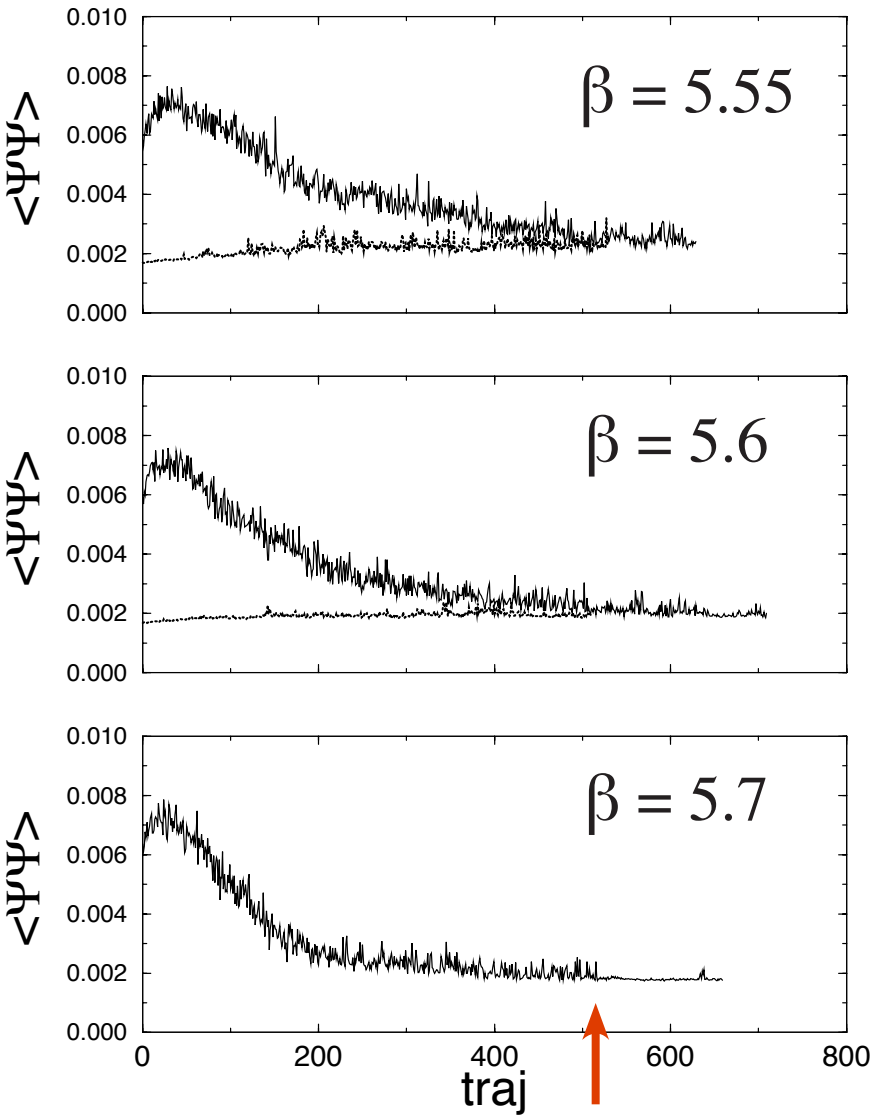


DWF Thermodynamics

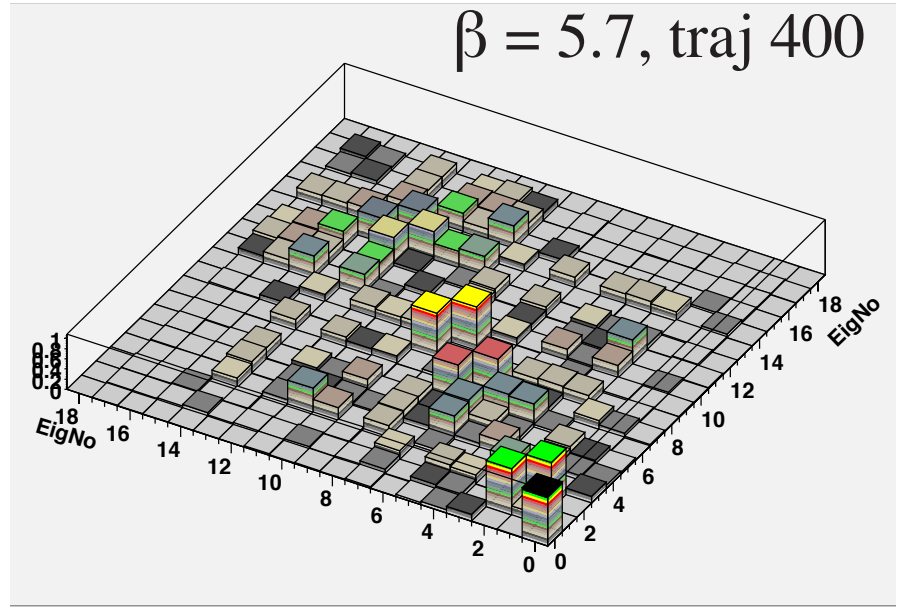
- Focus of considerable early activity with DWF
- Coarse lattices needed for $N_t = 4$, lead to large m_{res}
- U(1) axial symmetry breaking studied and topology seen in evolutions

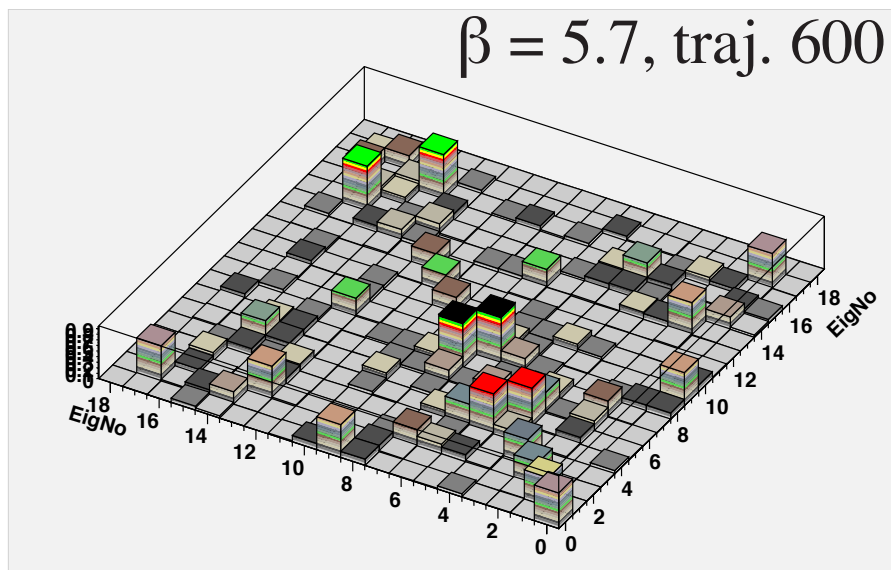
$N_t = 6$ DWF Thermodynamics

$16^3 \times 6 \times 32$, 2 flavors, $m_l = 0.02$. (Christ and Wu, Lattice 2001)



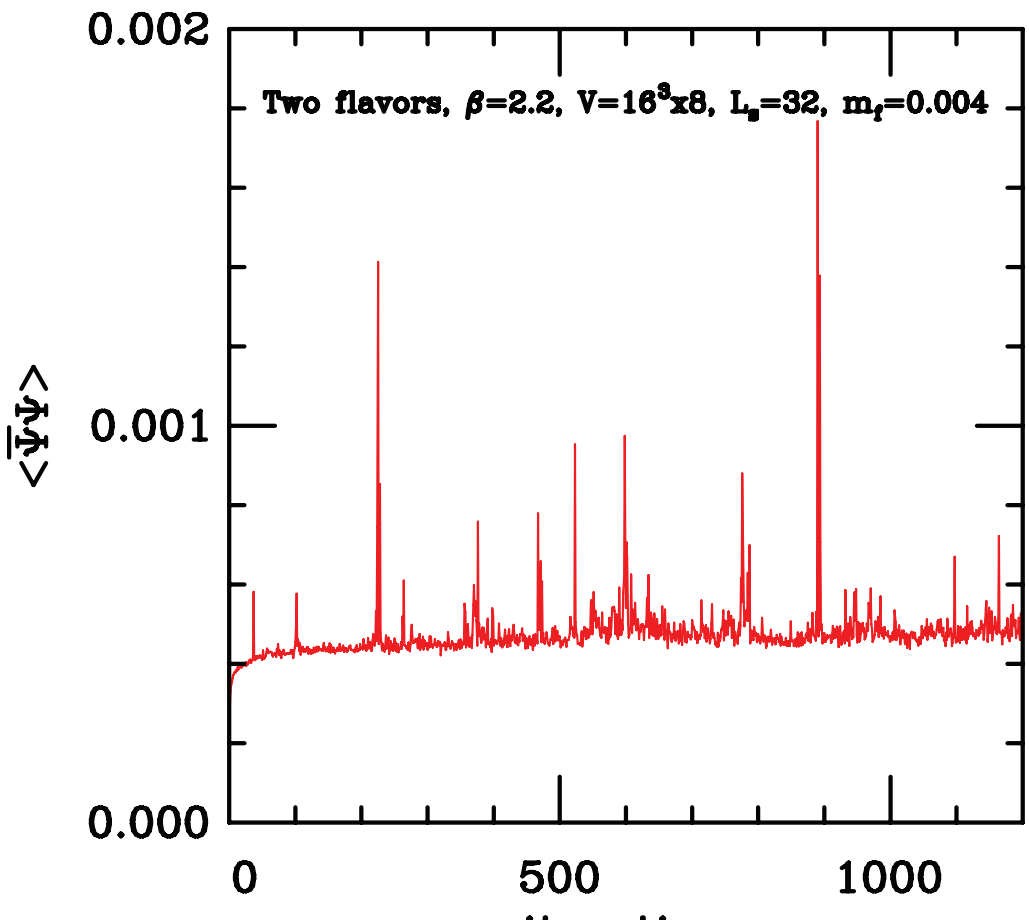
Topology changes





$N_t = 8$ DWF Thermodynamics

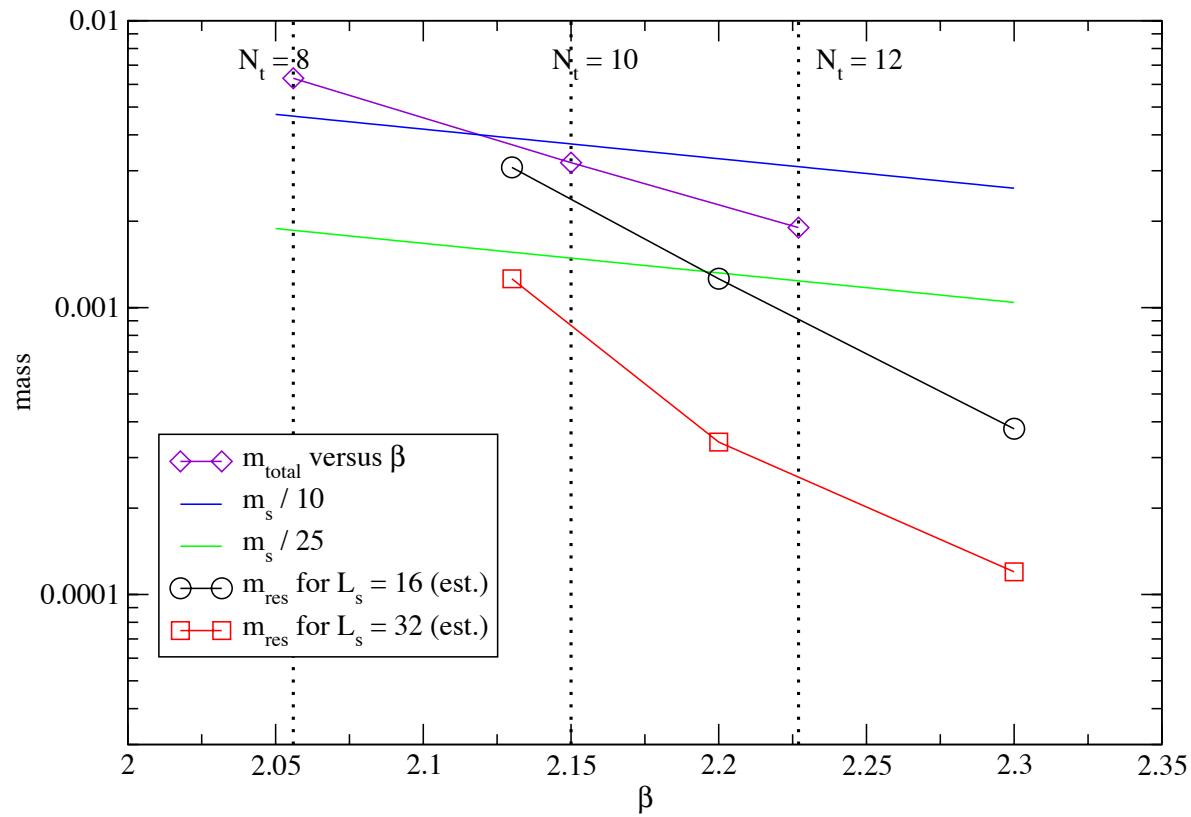
- Preliminary simulations underway on BGLs at Yorktown Heights, Livermore and on QCDOC at CU.
- Considerable coding effort by Jung, Vranas and Cheng.
- Vranas has scanned the transition for 2 flavors and sees features in $<\bar{\psi}\psi>$ just above T_c
- 2+1 flavor paramters estimated from T=0 results - simulations underway by Cheng and Renfrew.



DWF Thermodynamics Estimates

$$\langle \overline{\psi}\psi \rangle = v + \frac{c_1}{a^2} m_f + \frac{c_1'}{a^2} m_{\rm res} + \cdots$$

- Estimate v from $N_t = 4$
- Estimate c_1 from $N_t = 4$
- Use scales from 2+1 flavor T = 0 results
- Estimate m_{res} from valence L_s results
- Keep UV contribution from $m_{res} \approx v$



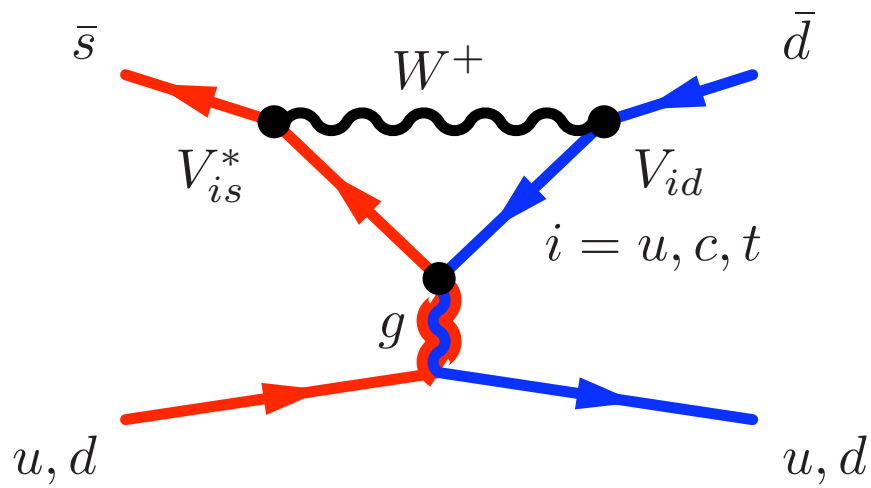
CP Violation in the Standard Model

Imaginary part for $K \to \pi\pi$ amplitudes comes from Cabbibo-Kobayashi-Maskawa (CKM) matrix, which relates quark electroweak eigenstates and quark mass eigenstates

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$$

V_{us} is essentially $\sin\theta_C$, where θ_C is the Cabbibo angle.

V_{ub} and V_{td} are complex. V_{td} effects $K \to \pi\pi$ through "penguin" diagrams.



CP Violation in the Kaon System

- Two amplitudes determine ϵ and ϵ'

$$\eta_{+-} = \frac{A(K_L^0 \to \pi^+\pi^-)}{A(K_S^0 \to \pi^+\pi^-)} = \epsilon + \epsilon' \qquad \eta_{00} = \frac{A(K_L^0 \to \pi^0\pi^0)}{A(K_S^0 \to \pi^0\pi^0)} = \epsilon - 2\epsilon'$$

- SM: $\overline{K}^0 - K^0$ mixing via $Q^{(\Delta S=2)} = (\bar{s}_\alpha d_\alpha)_{V-A}\,(\bar{s}_\beta d_\beta)_{V-A}$ defines B_K as;

$$\langle \overline{K}^0 | Q^{(\Delta S=2)}(\mu) | K^0 | \rangle \equiv \frac{8}{3} B_K(\mu) f_K^2 m_K^2$$

- RGI parameter $\hat{B}_K \equiv B_K(\mu)\left[\alpha_s^{(3)}(\mu)\right]^{-2/9}\left[1 + \frac{\alpha_s^{(3)}(\mu)}{4\pi} J_3\right]$ relates SM and ϵ

$$\epsilon = \hat{B}_K\, \mathrm{Im}\lambda_t\, \frac{G_F^2 f_K^2 m_K M_W^2}{12\sqrt{2}\pi^2 \Delta M_K} \left\{\mathrm{Re}\lambda_c\left[\eta_1 S_0(x_c) - \eta_3 S_0(x_c, x_t)\right] - \mathrm{Re}\lambda_t\, \eta_2 S_0(x_t)\right\} \exp(i\pi/4)$$

- Defining $A(K^0 \to \pi\pi(I)) \equiv A_I e^{(i\delta_I)}$, $P_2 \equiv \mathrm{Im}A_2/\mathrm{ReA}_2$, $P_0 \equiv \mathrm{Im}A_0/\mathrm{ReA}_0$:

$$\epsilon' = \frac{i e^{i(\delta_2 - \delta_0)}}{\sqrt{2}} \left(\frac{\mathrm{Re}\, A_2}{\mathrm{Re}\, A_0}\right)\left(\frac{\mathrm{Im}\, A_2}{\mathrm{Re}\, A_2} - \frac{\mathrm{Im}\, A_0}{\mathrm{Re}\, A_0}\right) \qquad w \equiv \frac{\mathrm{Re}\, A_0}{\mathrm{Re}\, A_2} \approx 22$$

$K \to \pi\pi$ in 3-flavor Effective Theory

- Hamiltonian for 3-flavor effective theory

$$\mathcal{H}^{(\Delta S=1)} = \frac{G_F}{\sqrt{2}} V_{ud} V_{us}^* \left\{ \sum_{i=1}^{10} \left[z_i(\mu) + \tau y_i(\mu) \right] Q_i \right\}$$

- Ten four-quark operators Q_i, only 7 independent.
  $K \to \pi\pi$ from lattice calculations and chiral perturbation theory.

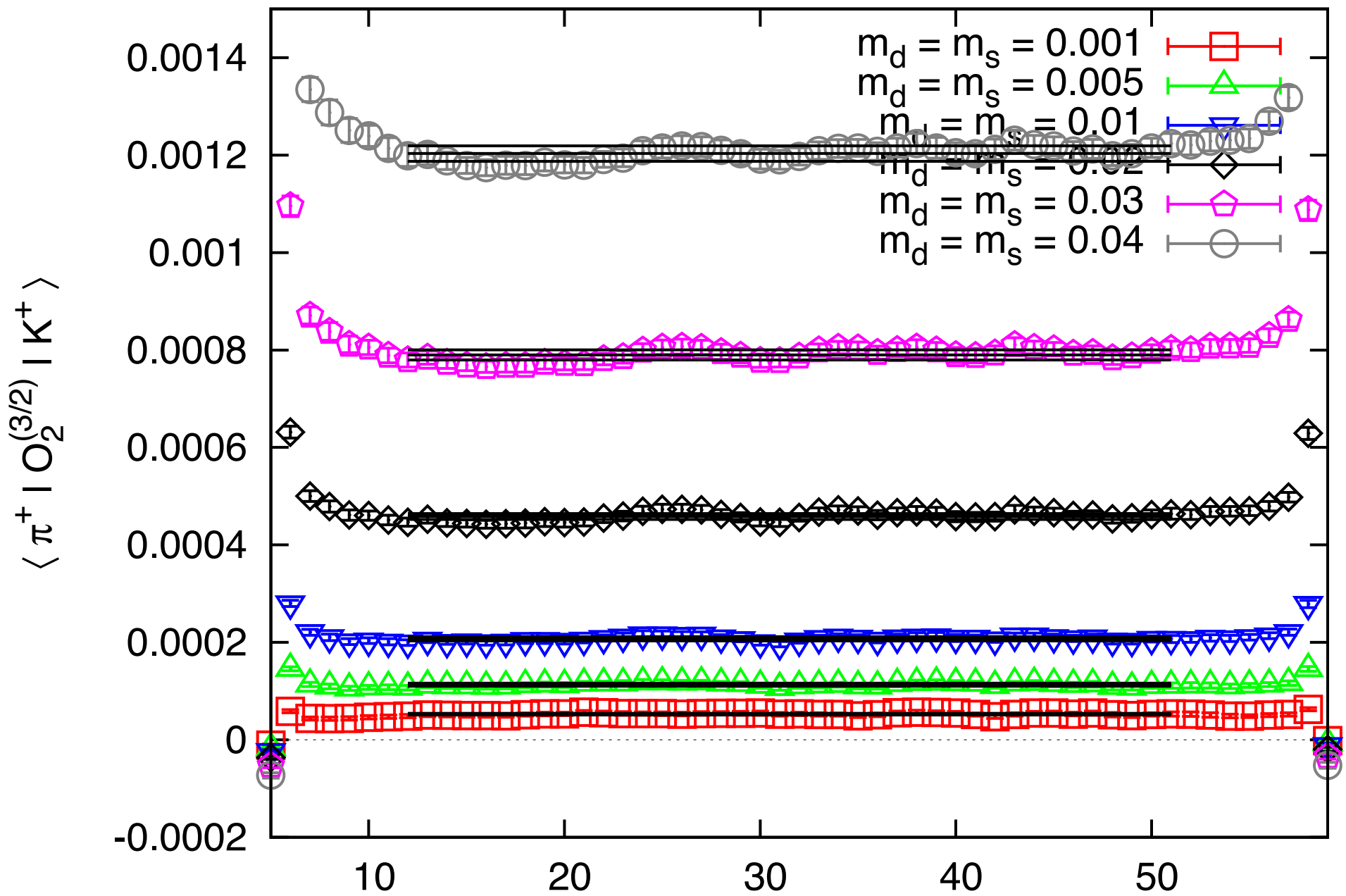
Irrep	Number	Isospin	$K^+ \to \pi^+$	$K^0 \to \pi^+\pi^-$
(27,1)	1	1/2, 3/2	$-\frac{4m_M^2}{f^2}\alpha^{(27,1)}$	$-\frac{4i}{f^3}m_{K^0}^2\alpha^{(27,1)}$
(8,1)	4	1/2	$\frac{4m_M^2}{f^2}(\alpha_1^{(8,1)} - \alpha_2^{(8,1)})$	$\frac{4i}{f^3}m_{K^0}^2\alpha_1^{(8,1)}$
(8,8)	2	1/2, 3/2	$-\frac{12}{f^2}\alpha^{(8,8)}$	$-\frac{12i}{f^3}\alpha^{(8,8)}$

- (8,1) requires determining $\alpha_2^{(8,1)}$ from $K \to |0\rangle$

$\Delta S = 1$ Measurements on 2+1 flavor, 24^3 ensembles

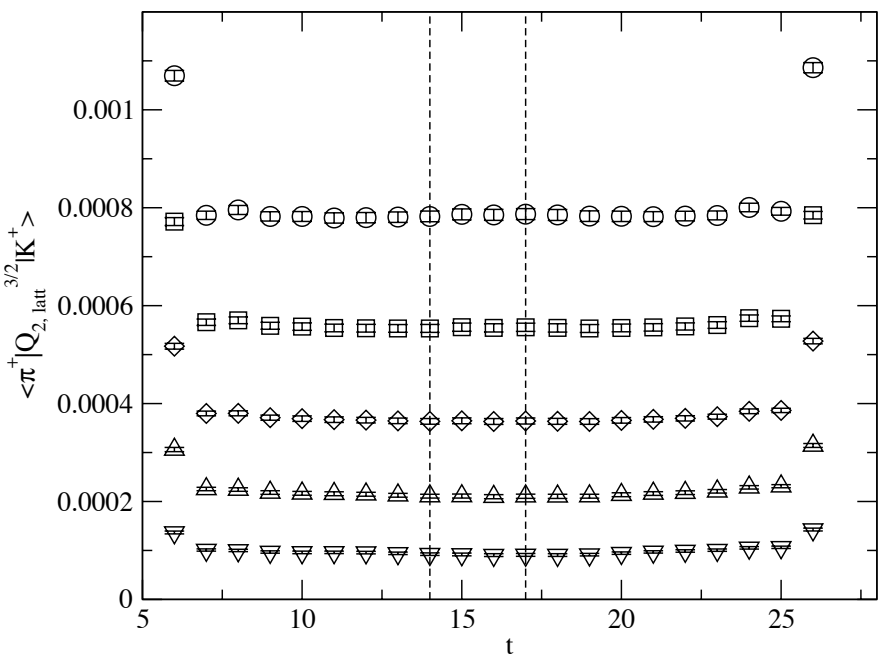
- Valence masses 0.001, 0.005, 0.01, 0.02, 0.03, 0.04
- Concentrating on 0.005/0.04 and 0.01/0.04 ensembles
- Large contributions by Tom Blum, Saul Cohen, Sam Li.
- 0.005/0.04 ensemble: 40 configurations separated by 80 MD time units
  0.01/0.04 ensemble: 30 configurations separated by 80 MD time units
- Concentrating on lighter quark masses where NLO chiral perturbation theory should be reasonable.
- Coulomb gauge fixed wall sources at t = 5 and 59
- Random noise source of length 40 for pupil calculations

ΔI = 3/2 Plateau

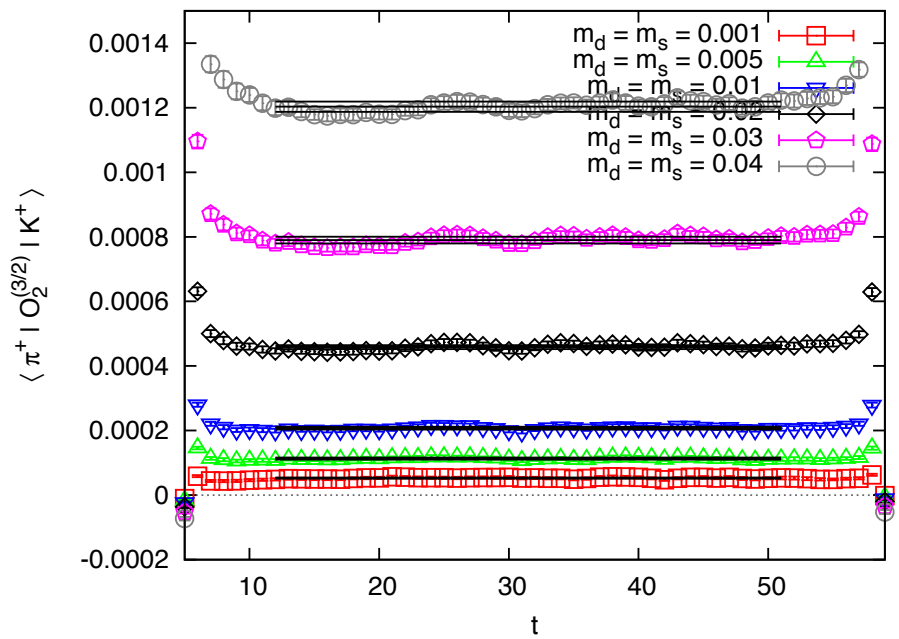


ΔI = 3/2 Plateau Comparisons

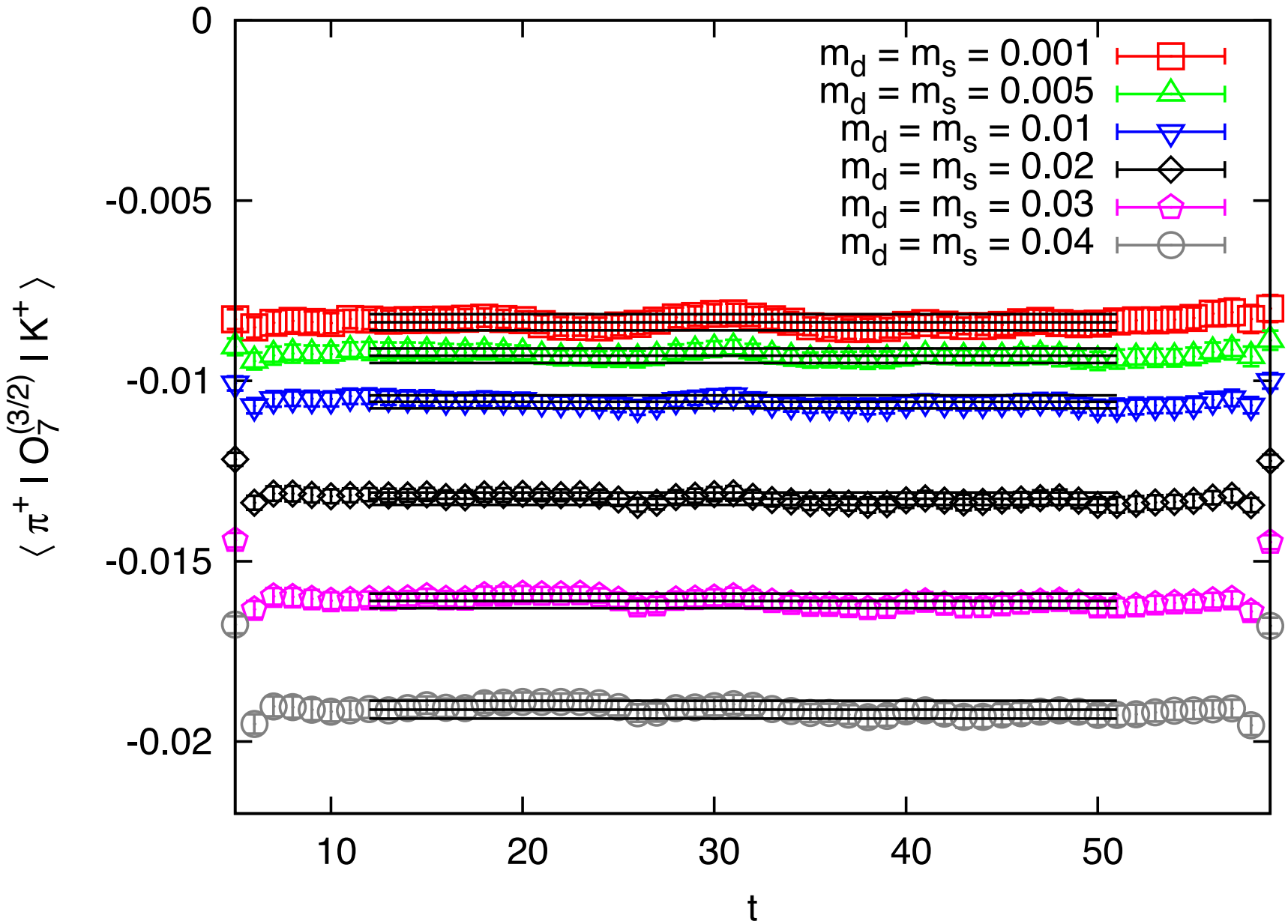
Previous Quenched



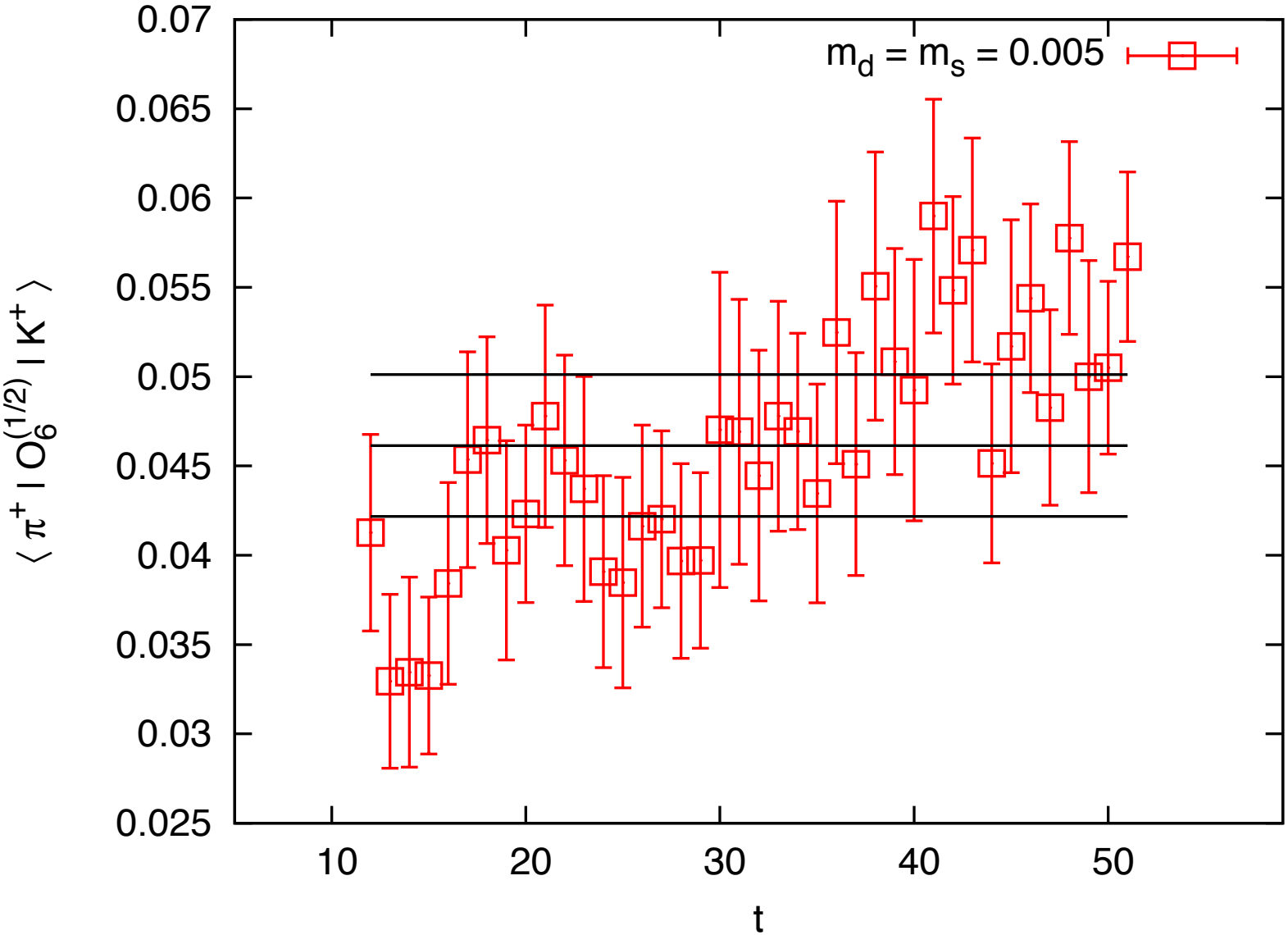
New 2+1 Flavor



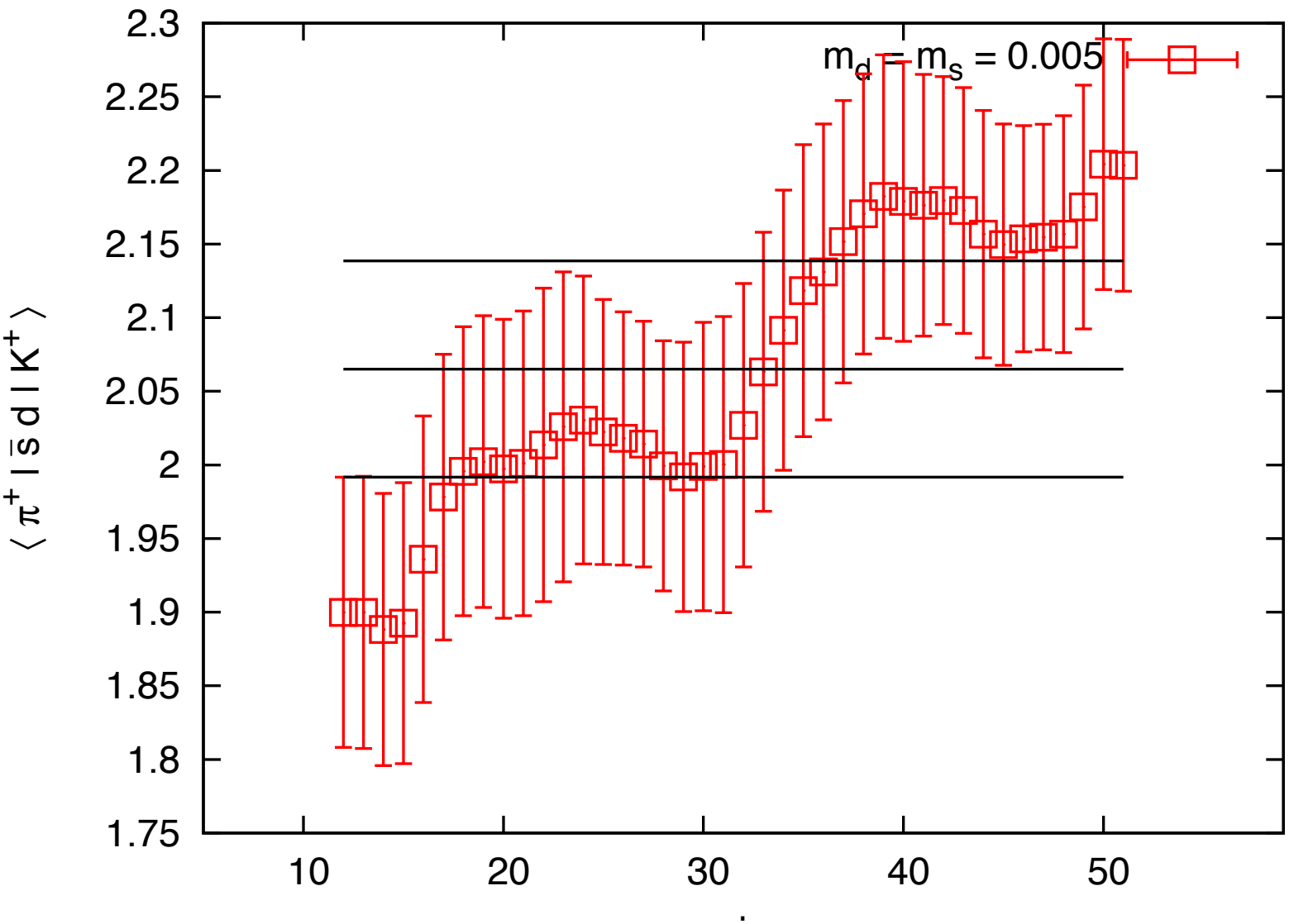
ΔI = 3/2 Plateau



$\Delta I = 1/2$ Plateau - unsubtracted Q_6

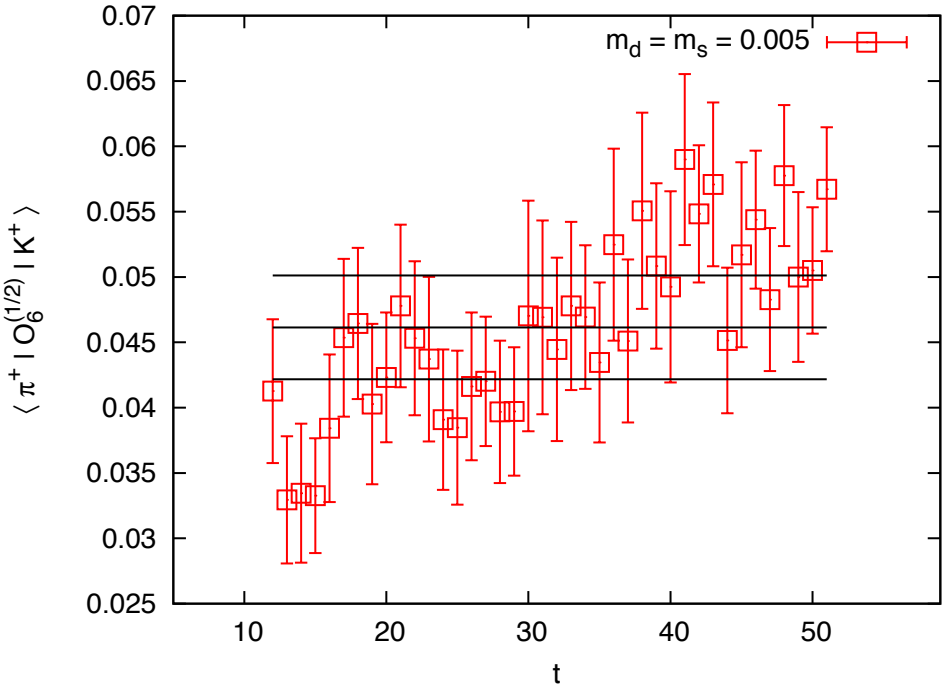


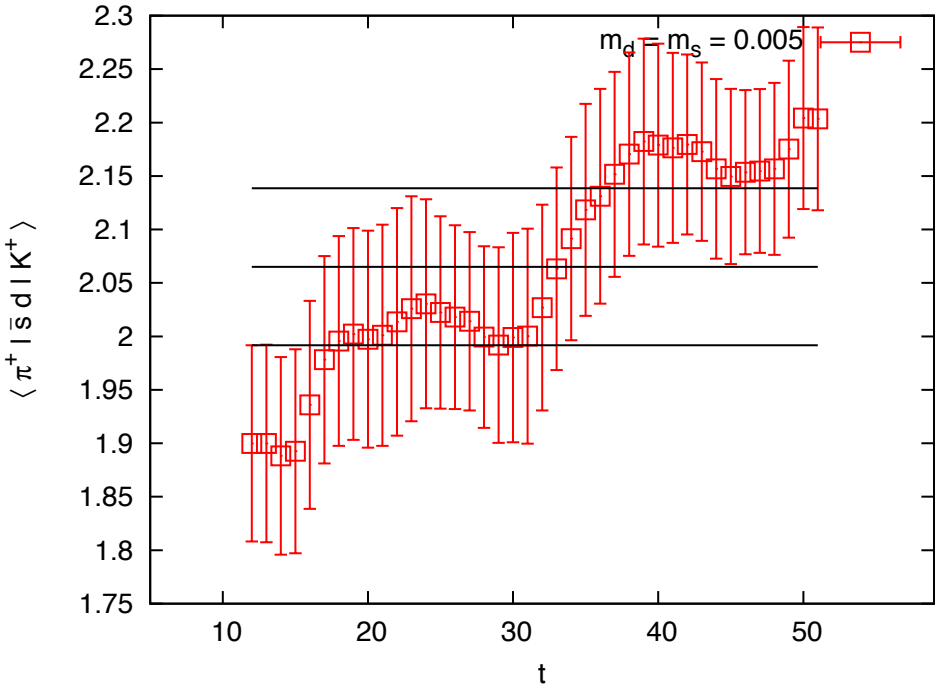
$\Delta I = 1/2$ Plateau - $\bar{s}d$



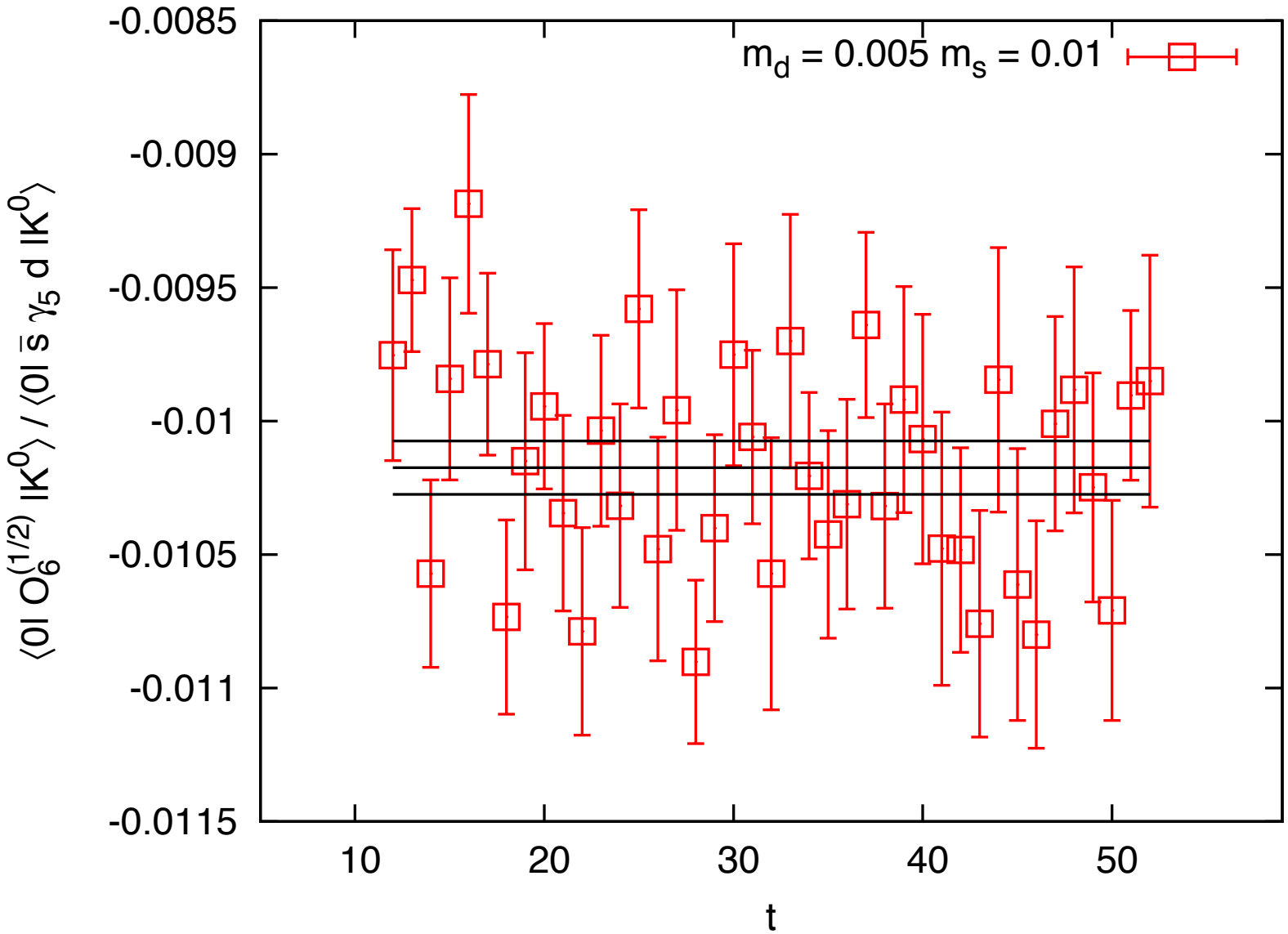
Comparing $\Delta I = 1/2$ Plateau

Common fluctuations in Q_6 and $\bar{s}d$





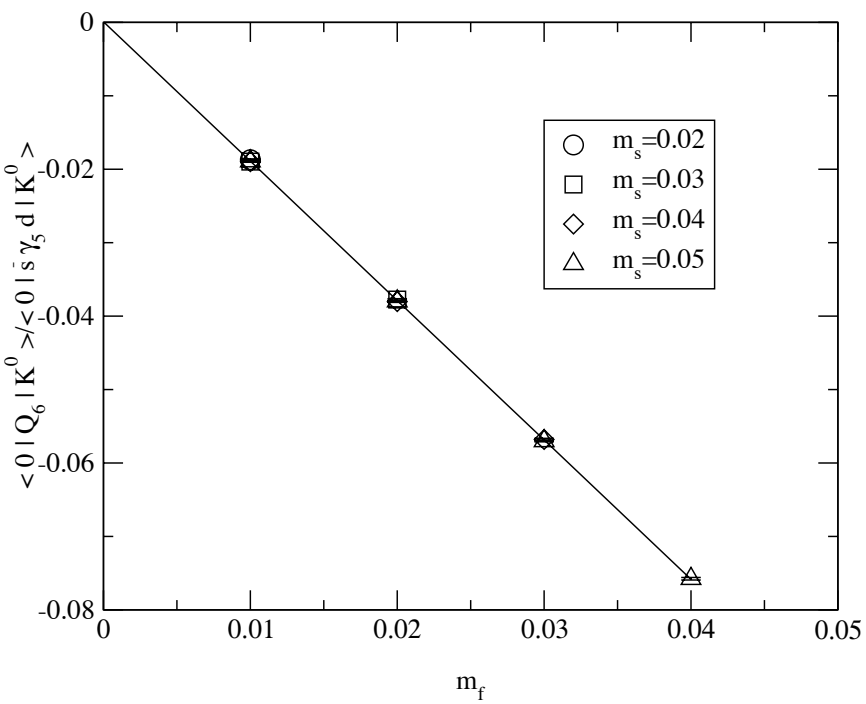
ΔI = 1/2 Subtraction



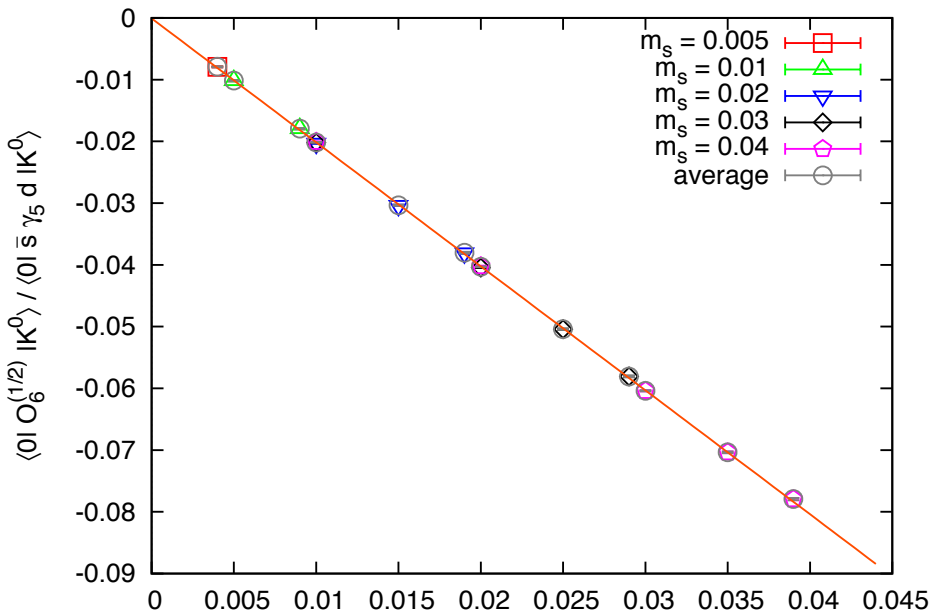
ΔI = 1/2 Subtraction Coefficient Comparisons

$$\frac{\langle 0|Q_{i,\mathrm{lat}}|K^0\rangle}{\langle 0|(\bar{s}\gamma_5 d)_{\mathrm{lat}}|K^0\rangle} = \eta_{0,i} + \eta_{1,i}\,(m_s - m_d)$$

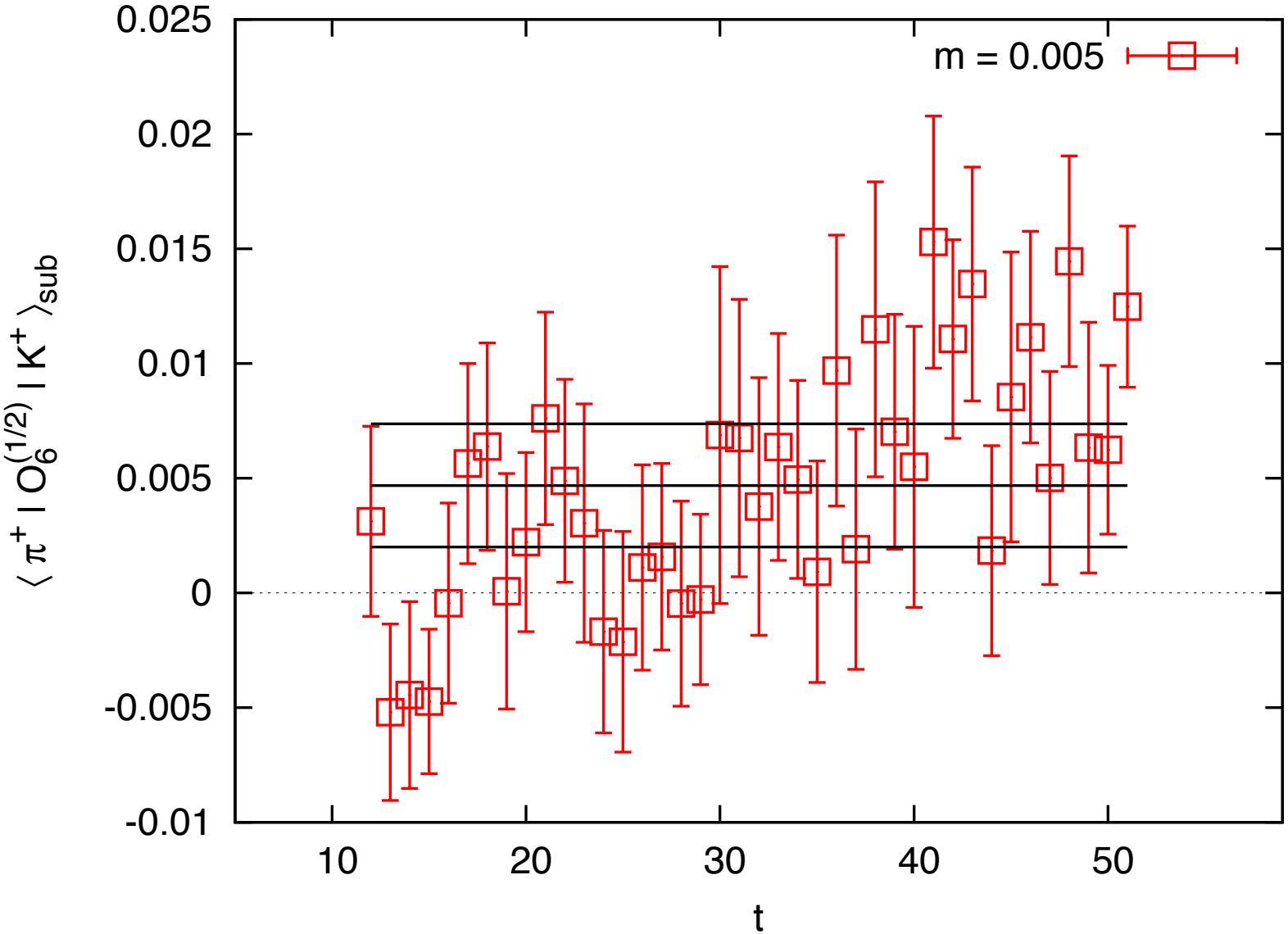
Previous Quenched



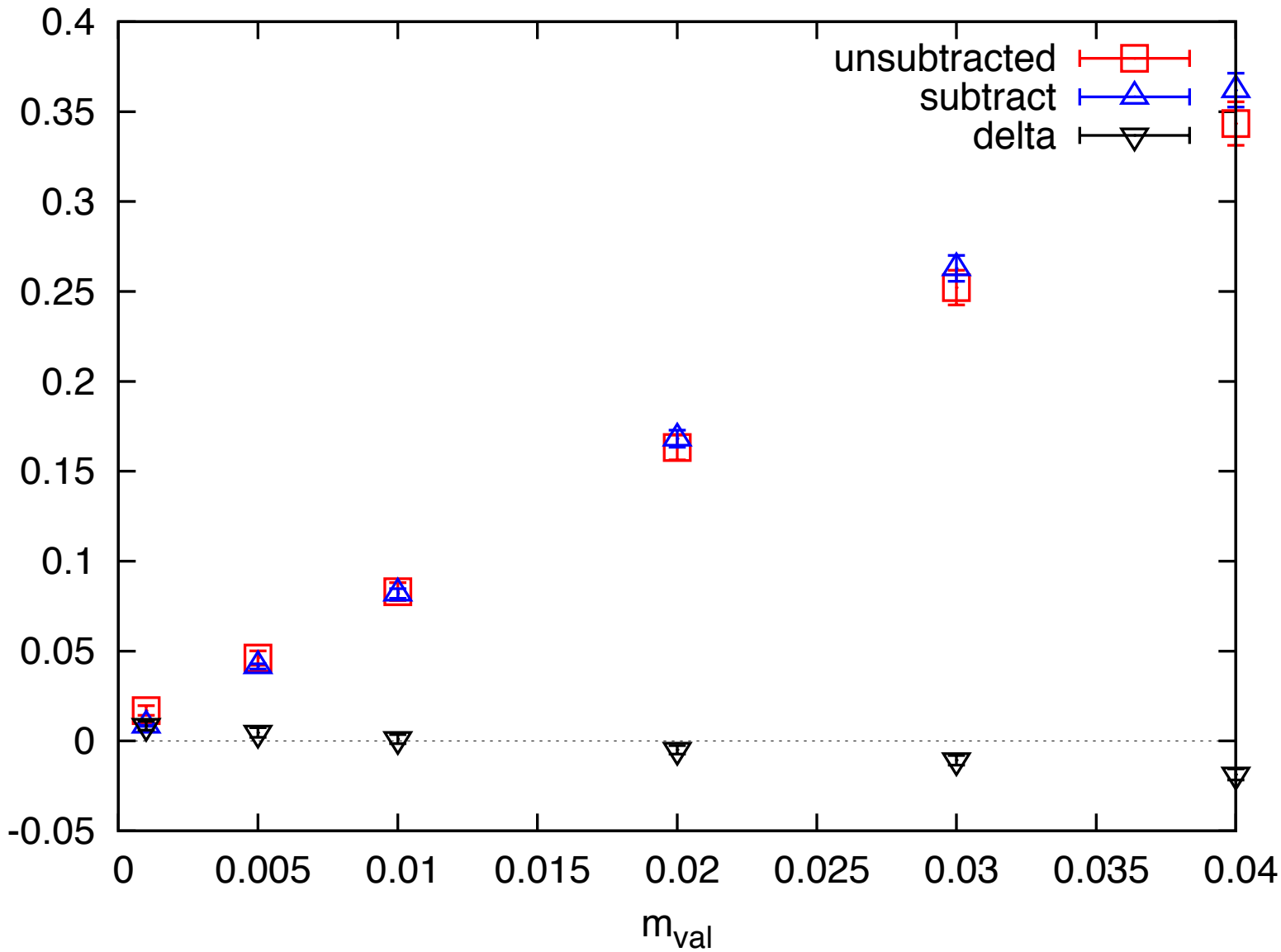
New 2+1 Flavor



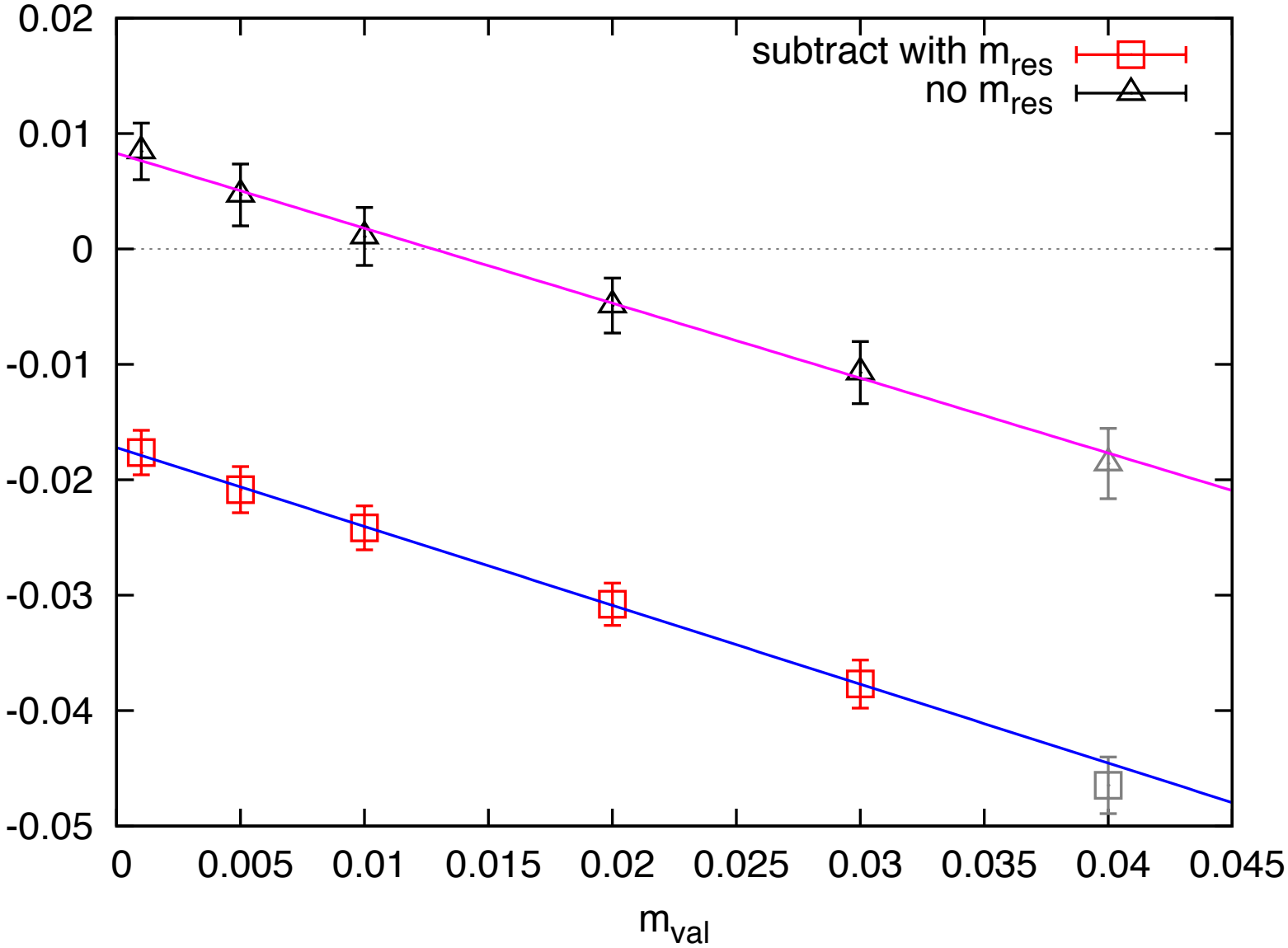
Subtracting Q_6



Subtracting Q_6



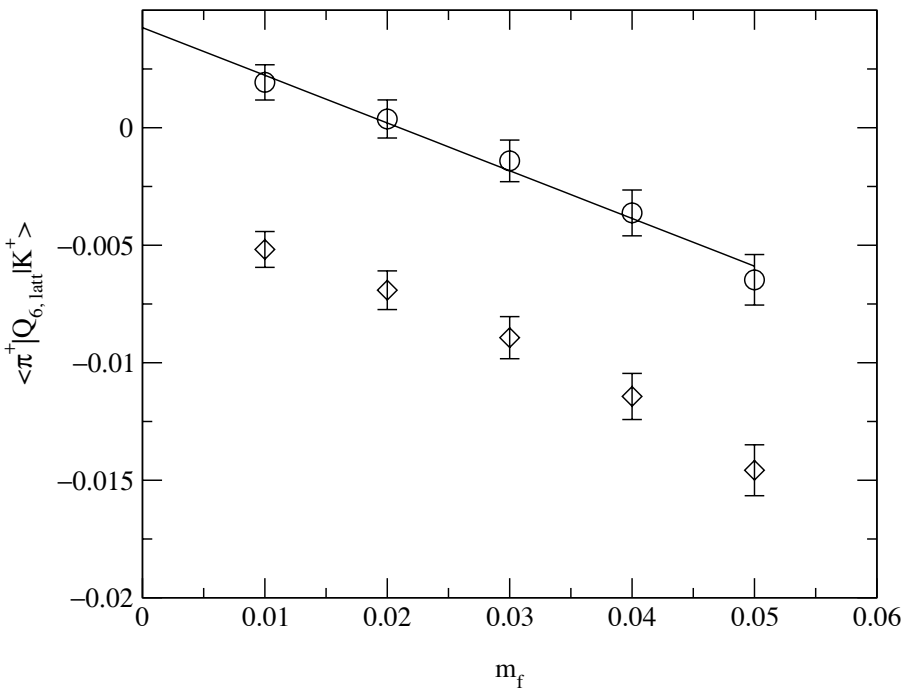
Subtracted Q_6



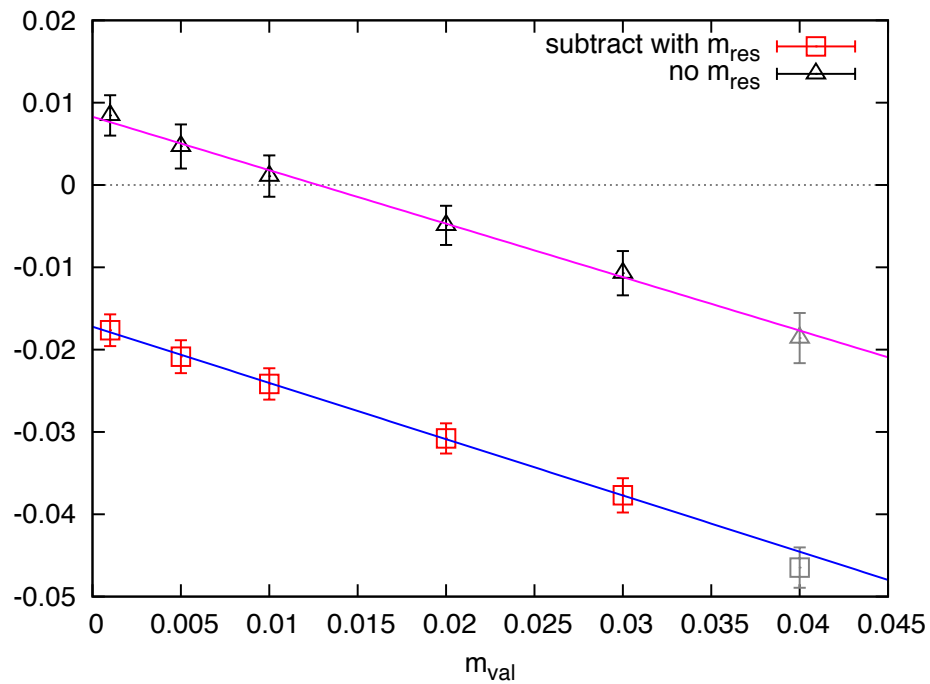
Subtracted Q_6 Comparison

$$\langle \pi^+ | Q^{(1/2)}_{i,\mathrm{lat}} | K^+ \rangle + \eta_{1,i}(m_s + m_d) \langle \pi^+ | (\bar{s}d)_{\mathrm{lat}} | K^+ \rangle$$

Previous Quenched



New 2+1 Flavor



Conclusions

- 2+1 flavor DWF QCD simulations well underway
  $(3\ \mathrm{fm})^3$ volumes at two lattice scales
  $m_l = m_s / 5$ on $a^{-1} = 1.6$ GeV lattices
  $m_l = m_s / 7$ on $a^{-1} = 2.1$ GeV lattices

- Wide range of physics topics being pursued by RBC and UKQCD collaborations: chiral limit, nucleons, weak matrix elements, Kl3, pion distribution amplitudes, nucleon EDM, E&M splittings,...

- Finite temperature simulations with $N_t = 8$ are underway with 2+1 flavors of DWF and the exact RHMC algorithm

- $\Delta S = 1$ matrix elements appear to be benefitting from large spatial volume, giving reduced statistical errors.

- Much more to come