The QCD Phase Transition with Domain Wall Fermions and Physical Pion Masses

31st International Symposium on Lattice Field Theory

July 30, 2013

Chris Schroeder (for the HotQCD/LLNL/RBC collaboration)

Lawrence Livermore National Laboratory

LLNL-PRES-641426

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

The Bottom Line

- Domain Wall Fermions
  - **chiral and $U(1)_A$ symmetries unbroken by discretization**
    → *can study both chiral and $U(1)_A$ symmetry breaking*
  - **3 pions** *(just like reality!)*

- Physical (and 200 MeV) pion (and kaon) masses
  - m_π = 200 MeV, N_τ = 8, N_σ = 32 (*and* 16 *and* 24) (LLNL/RBC)
  - **m_π = 135 MeV**, N_τ = 8, N_σ = 32 (*and* 64) (HotQCD)

The Bottom Line

- Chiral Symmetry Breaking
  - confirm staggered results for $T_{\chi SB}$ (quasi-critical temperature)
  - tension with staggered results for $\chi_{l,\mathrm{disc}}$ and m_π dependence

- $U(1)$ Axial Symmetry Breaking
  - $U(1)_A$ broken above $T_{\chi SB}$
  - confirm features of dilute instanton gas approximation

The Bottom Line

- Calculations not possible without state of the art HPC
  - algorithms: DSDR, Möbius
  - software: BAGEL (for BG/Q), CPS
  - machines: LLNL/IBM Sequoia/Vulcan Blue Gene/Q

Outline

- the QCD finite-temperature transition
- domain wall fermions
- chiral susceptibilities and chiral symmetry
- chiral susceptibilities and $U(1)_A$
- the Dirac spectrum and dilute instanton gas approximation
- a new and improved subtracted chiral condensate

The QCD Finite-T Transition

The spontaneous breaking of chiral symmetry

$$SU(2)_L \times SU(2)_R \rightarrow SU(2)_V$$

is a crucial aspect of the history and present state of our Universe

- studied intensely for over 30 years, experimentally and theoretically
- outstanding puzzle #1: role of anomalous $U(1)_A$ axial symmetry
- outstanding puzzle #2: role of light quark masses

The QCD Finite-T Transition

- $m_q = 0$:
  - $U(1)_A$ thought to be clearly broken at $T_{\chi SB}$
    → **4** light d.o.f. (σ, π), O(4)-class 2nd order criticality
  - Pisarski, Wilczek (1984):
    if $U(1)_A$ breaking at $T_{\chi SB}$ is mild, have **8** light d.o.f.
    → NOT O(4)-class – $SU(2)_L \times SU(2)_R / U(2)_V$?
    → maybe even 1st order

  → $U(1)_A$ of fundamental importance and NOT understood
- m_q physical:
  - transition appears to be analytic crossover
- 2+1 flavors and very light m_l:
  - nature of transition unknown

Domain Wall Fermions

- chiral fermions **expensive** but **essential**
- staggered fermions:
  - explicitly break $U(1)_A$ *and* 5/6 of $SU(2)_L$ x $SU(2)_R$
  - very costly continuum limit absolutely necessary
- domain wall fermions:
  - three, degenerate pions *and* exact anomalous current conservation *at finite lattice spacing* (for infinite L_s)
  - near-continuum results for sufficiently large L_s

Domain Wall Fermions

- Wilson, w/ chiralities separated in 5th dimension
- LH and RH fields localized on domain walls, x_s=0 and L_s, overlap in bulk for finite L_s
- Want "L_s~∞" – **expensive** but manageable

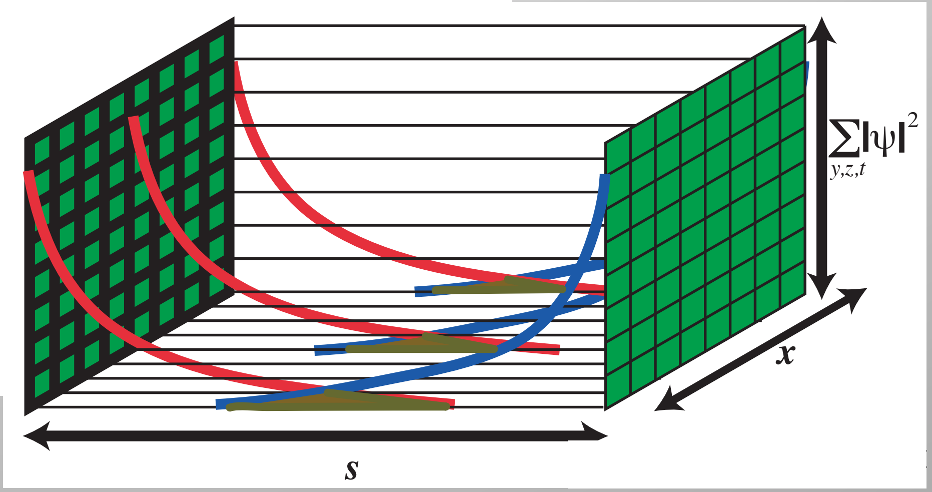
Then there are two chiral zeromode solutions $\Psi_0^{\pm}$ given by

$$\Psi_0^{\pm}(\vec{p}, z) = e^{i\vec{p}\cdot\vec{x}}\phi_{\pm}(s, \vec{p})u_{\pm}$$

where the transverse wavefunctions are given by

$$\phi_+(s, \vec{p}) = e^{-\mu_0|s|}$$

$$\phi_-(s, \vec{p}) = (-1)^{n_s}\phi_+(s, \vec{p}) \ .$$

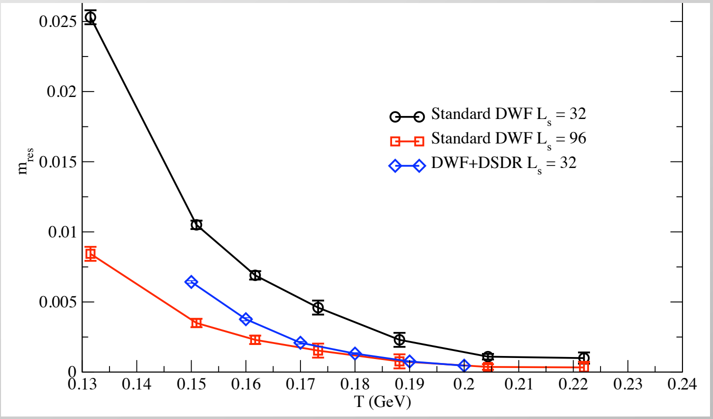


Domain Wall Fermions

- Substantial cost reductions:
  - Dislocation Suppressing Determinant Ratios (DSDR)
    - introduce ratio of Wilson fermions with negative unphysical mass
    - suppress "dislocations" - low modes due to O(*a*) effects – without freezing topology
    - achieve target m_{res} at reduced L_s
  - Möbius Formulation
    - generalize Shamir formulation with overall scaling factor
    - improve sign function approximation in low-mode, residual-χSB region
    - achieve target m_{res} at further reduced L_s

~3X faster for m_π~200 MeV

~10X faster for m_π~135 MeV

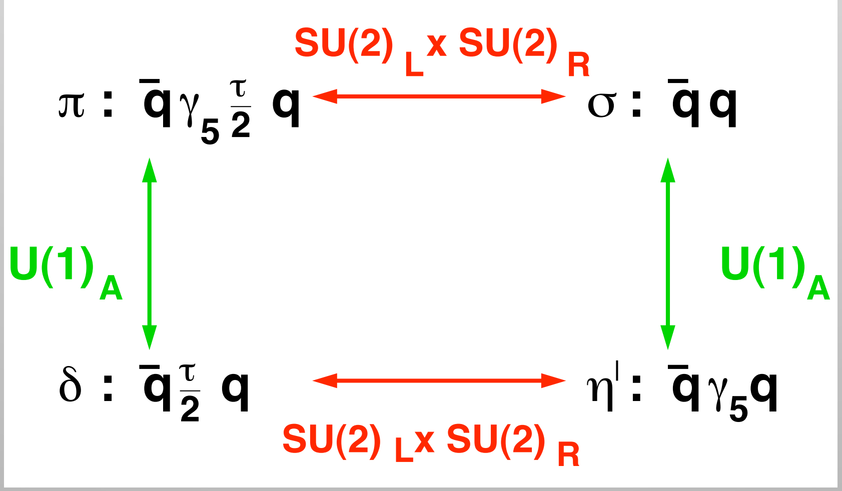


additional 2X faster for m_π~135 MeV

(not utilized for m_π~200 MeV)

Chiral Susceptibilities

- pseudo-/scalar, non-/singlet susceptibilities probe both chiral and $U(1)_A$ symmetries
  - more sensitive than condensate
  - independent probes of chiral and $U(1)_A$ symmetry breaking
  - precision boost from random Z_2 wall source
  - renormalized to $\overline{\mathrm{MS}}(\mu=2\ \mathrm{GeV})$ with $(Z_{m\to\overline{\mathrm{MS}}})^{-2}$



$\chi_{l,\text{disc}}$ *and* $T_{\chi SB}$ – m_π = 200 MeV

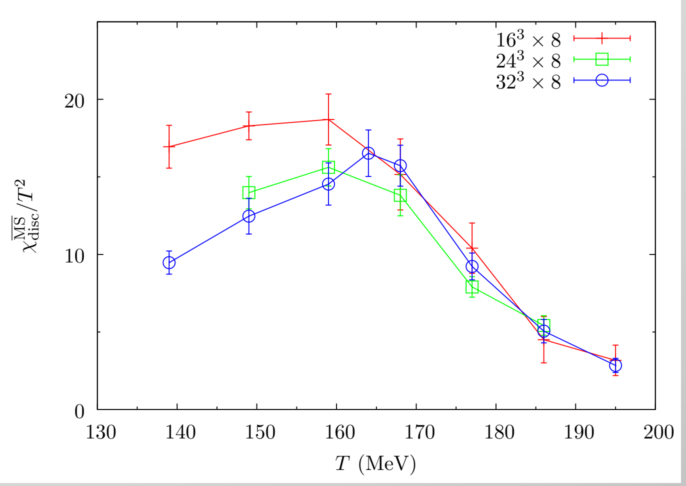
- Better probe of χSB: chiral susceptibility

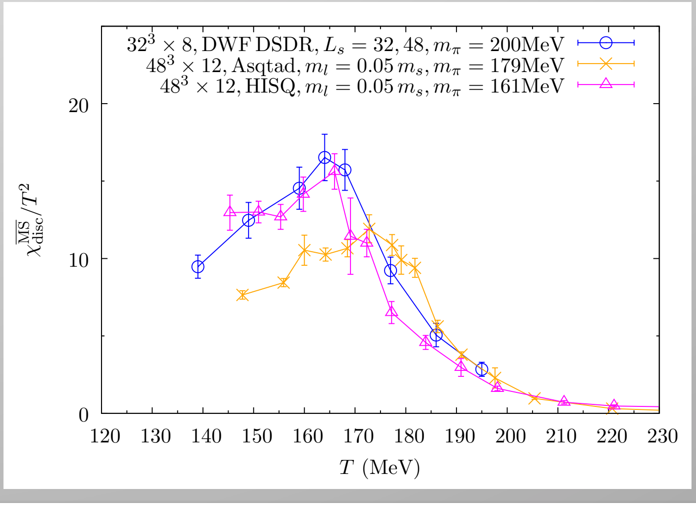
$$\chi_{l,\text{disc}} = \left(\frac{\partial}{\partial m_l}\langle\bar{\psi}\psi\rangle_l\right)_{\text{disc}} = \frac{1}{N_\sigma^3 N_\tau}\left\{\left\langle(\mathrm{Tr}M_l^{-1})^2\right\rangle - \left\langle\mathrm{Tr}M_l^{-1}\right\rangle^2\right\}$$

  - clearly peaked at $T_{\chi SB}$
  - UV divergence logarithmic and suppressed by m_l^3

$\chi_{l,disc}$ *and* $T_{\chi SB}$ – m_π = 200 MeV

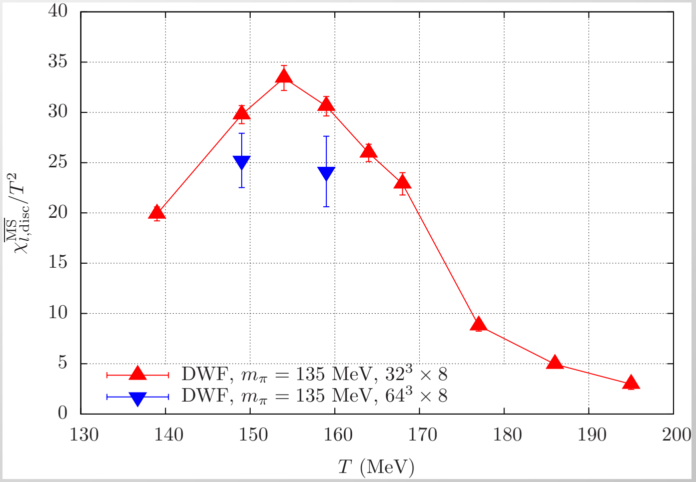
- $T_{\chi SB}$ ~ 165 MeV
- finite volume effects:
  - ~20% for L/a = 16, T < 160 MeV
  - very small for T > 160 MeV
  - < 5% for L/a = 24
- comparison with staggered
  - DWF w/ m_π = 200 MeV and N_τ=8 coincides remarkably well with HISQ w/ m_π = 160 MeV and N_τ=12
    - — taste breaking? other cutoff effects?
    - — need continuum limits
  - AsqTad w/ m_π = 180 MeV and N_τ=12 appears to be far from continuum for T < 180 MeV

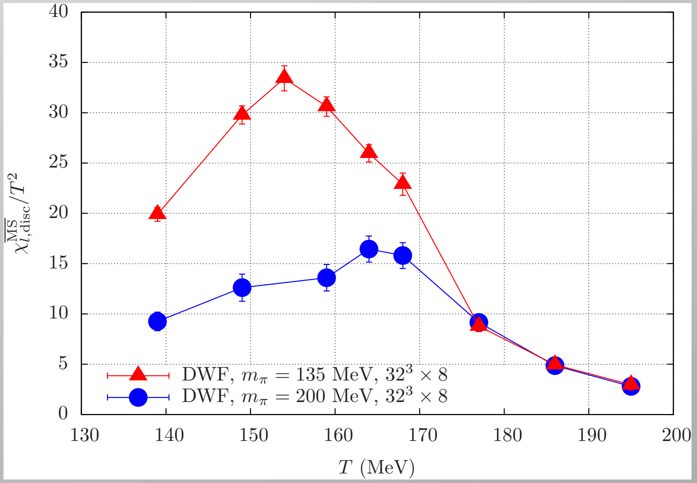




$\chi_{l,disc}$ and $T_{\chi SB}$ – m_π = 135 MeV

- $T_{\chi SB}$ ~ 155 MeV
  - good agreement with staggered
- finite volume effects:
  - ~20% for L/a = 32?
  - L ~ 4 N_τ insufficient?
  - need more stats for L/a = 64
- mass dependence
  - $T_{\chi SB}$ ~ 6% lower than for 200 MeV
  - peak ~ 2x higher than for 200 MeV
    - — compatible with O(4) scaling, $m_\pi^{-1.6}$
    - — finite volume?



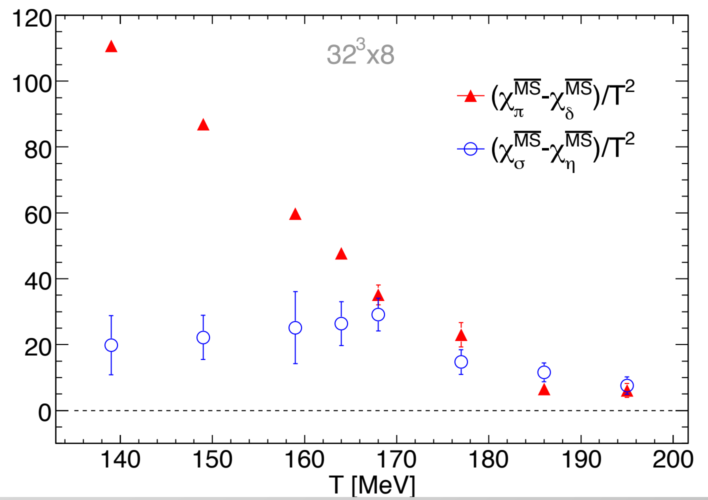


$U(1)_A$ near $T_{\chi SB}$

- $\chi_\pi - \chi_\delta = \chi_\sigma - \chi_\eta$

  → chiral symmetry restoration

  → $T_{\chi SB} \sim 170$ MeV

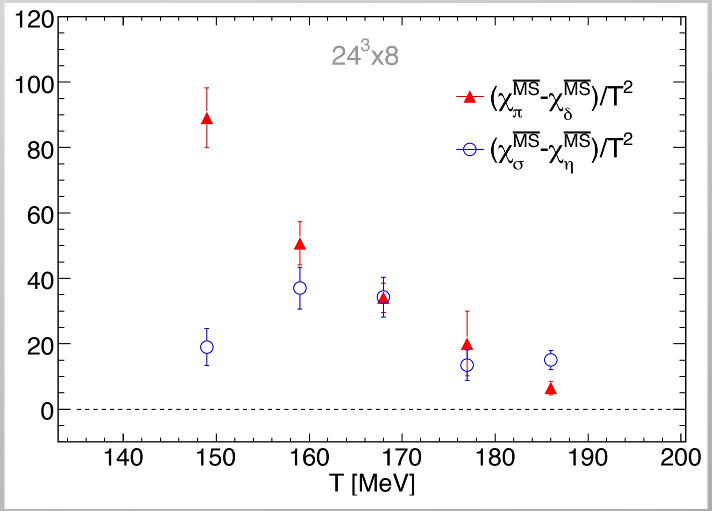


- $\chi_\pi - \chi_\delta,\ \chi_\sigma - \chi_\eta \neq 0$

  → $U(1)_A$ **not** restored

  - not explicit breaking:
    $(m_{res}/T)^2 \sim 10^{-3}$, negligible

  - not finite volume:
    same picture for L/a = 24 and 32



The Dirac Eigenvalue Spectrum

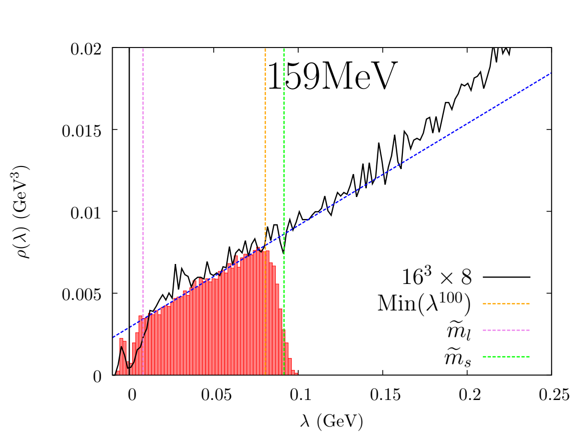
- zero intercept indicates chiral symmetry restoration above $T \sim 170$ MeV
- spectral form of $\chi_\pi - \chi_\delta$

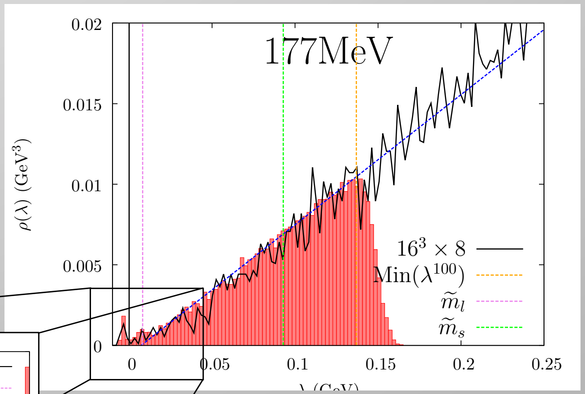
$$\Delta_{\pi-\delta} \equiv \chi_\pi - \chi_\delta = \int \mathrm{d}\lambda\ \rho(\lambda) \frac{4m_l^2}{\left(m_l^2 + \lambda^2\right)^2}$$

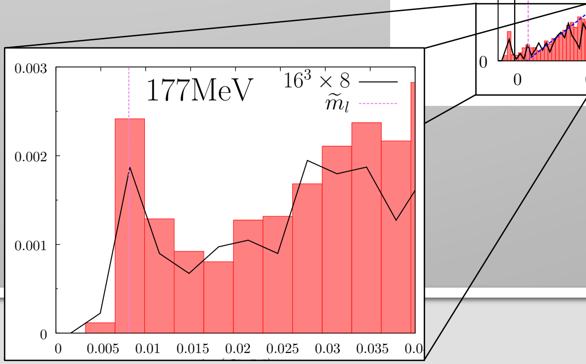
  - agrees with correlator sum

and

  - reveals $U(1)_A$ breaking is dominated by cluster of near-zero modes







The Dirac Eigenvalue Spectrum

- Dilute Instanton Gas vs. Topology
  - Volume dependence:

    topology: $\rho \propto 1/\sqrt{V}$

    DIGA: ρ independent of V

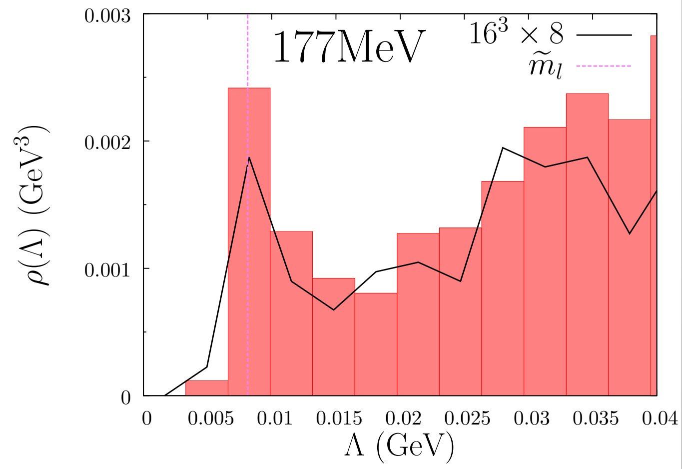
    Results support … DIGA
  - Distribution of chiralities:

    topology: bimodal (all the same for each cfg)

    DIGA: binomial (democratic)

    Results support … DIGA

→ Results support DIGA description of anomalous $U(1)_A$ breaking



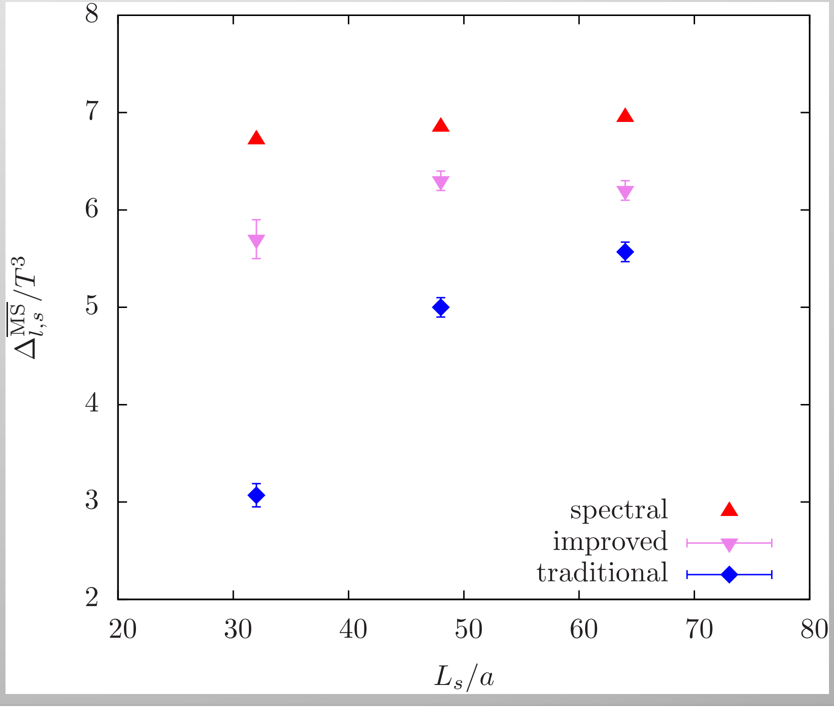
N_+	0	1	2	3	4	5
$N_0 = 1$	28	19	-	-	-	-
$N_0 = 2$	16	19	12	-	-	-
$N_0 = 3$	4	11	8	3	-	-
$N_0 = 4$	1	3	4	3	0	-
$N_0 = 5$	0	2	1	1	1	0

New and Improved Subtracted Chiral Condensate

- UV divergence in $\Sigma_l \equiv -\frac{1}{2}\langle\bar{\psi}\psi\rangle_l$ usually removed by subtracting $\frac{\widetilde{m}_l}{\widetilde{m}_s}\Sigma_s$
- Better: use DWF GMOR $m_l\chi_\pi + \frac{1}{4}\int d^4x\langle 0|T(iJ_{5q}(x)^a\pi^a(0))\rangle = \Sigma_l$
- Even better: use GMOR relation to define

$$\widetilde{\Delta}_{l,s} = \widetilde{m}_l\left(\chi_{\pi_l} - \chi_{\pi_s}\right)$$

  - identical continuum limit
  - no m_{res}/a^2 term → more physical
  - better for comparison with other actions (e.g. HISQ)



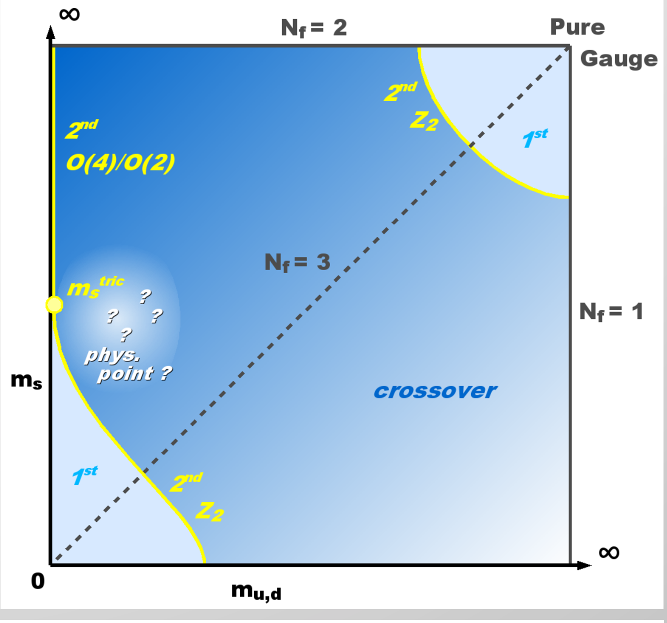
Much more to do for m_π *= 135 MeV*

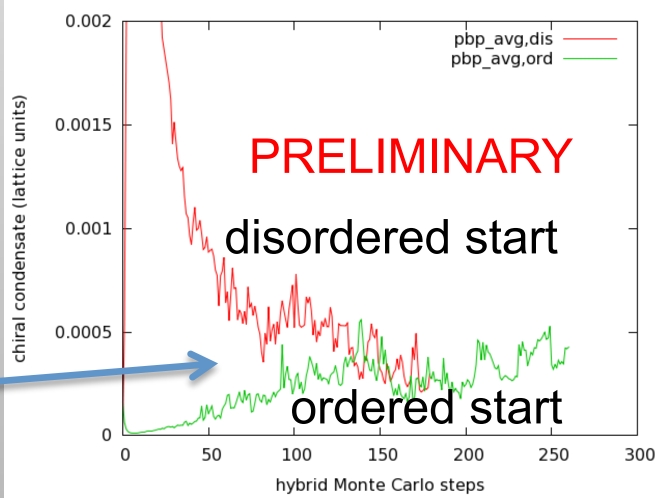
- $\delta/\eta/\pi/\sigma$ susceptibilities → $U(1)_A$ breaking
- Dirac spectrum → comparison with DIGA
- understand finite-volume effects
- confirm/improve scale setting
- …

m_π ~ 100 MeV

- 1^{st} order phase transition for small m_π?

- investigation underway with m_π = 100 MeV and 64^3x8 (but **slow**)





No sign of metastability at T=160 MeV
(T = 140 MeV in the queue)

The Bottom Line

- Domain Wall Fermions
  - **chiral and $U(1)_A$ symmetries unbroken by discretization**
    → *can study both chiral and $U(1)_A$ symmetry breaking*
  - **3 pions** *(just like reality!)*

- Physical (and 200 MeV) pion (and kaon) masses
  - m_π = 200 MeV, N_τ = 8, N_σ = 32 (*and* 16 *and* 24) (LLNL/RBC)
  - **m_π = 135 MeV**, N_τ = 8, N_σ = 32 (*and* 64) (HotQCD)

The Bottom Line

- Chiral Symmetry Breaking
  - confirm staggered results for $T_{\chi SB}$ (quasi-critical temperature)
  - tension with staggered results for $\chi_{l,\mathrm{disc}}$ and m_π dependence

- $U(1)$ Axial Symmetry Breaking
  - $U(1)_A$ broken above $T_{\chi SB}$
  - confirm features of dilute instanton gas approximation

The Bottom Line

- Calculations not possible without state of the art HPC
  - algorithms: DSDR, Möbius
  - software: BAGEL (for BG/Q), CPS
  - machines: LLNL/IBM Sequoia/Vulcan Blue Gene/Q

Thank you for your attention!

Thanks to the organizers for 15 minutes of fame.

Thanks to all my collaborators for their hard work.

A. Bazavov, T. Bhattacharya, M. Buchoff, **P. Boyle**, M. Cheng, **N. Christ**, C. DeTar, **H.-T. Ding**, S. Gottlieb, R. Gupta, P. Hedge, U.M. Heller, **C. Jung**, **F. Karsch**, E. Laermann, L. Levkova, **Z. Lin**, **R.D. Mahwinney**, S. Mukherjee, P. Petreczky, D. Renfrew, C. Schmidt, **C. Schroeder**, R.A. Soltz, C. Soeldner, R. Sugar, D. Toussaint, W. Unger, **P. Vranas**, H. Yin

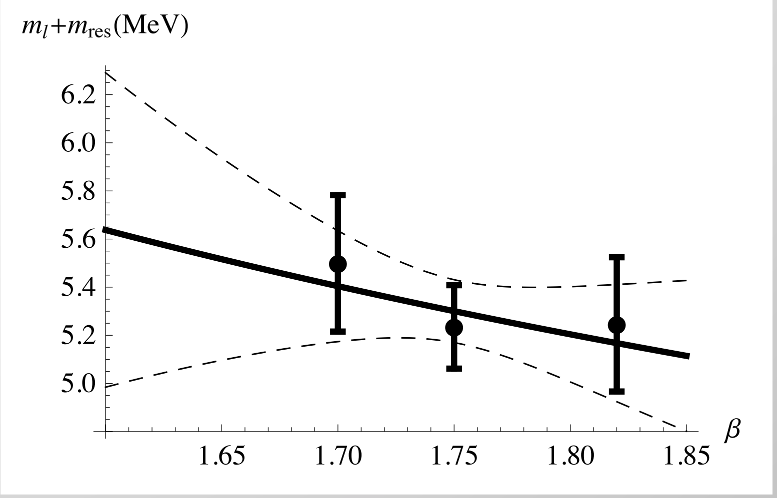
Thanks to LLNL and BNL for HPC resources and support.

Thanks to the DOE and NSF for funding this work.

additional material

Parameter Determination

- m_s and $m_{u,d}$ tuned to 5% level to obtain m_K= 495 MeV and m_π= 200 (or 135) MeV



- lattice spacing determined using Sommer method with RBC/UKQCD r_0, r_1 (using m_Ω at β=1.75)