

## Yasumichi Aoki

Field Theory Research Team RIKEN Center for Computational Science





### Acknowledgements



### Codes used:

• Grid (HMC)

BQCD (Measurements)

Bridge++ (Measurements)

Hadrons (Measurements)

#### **Grants:**

- KAKANHI (FY2020-2024) QCD phase diagram explored by chiral fermions 20H01907
- MEXT Program for Promoting Researches on the Supercomputer **Fugaku** (PPR-Fugaku)
  - (FY2020-2022) Simulation for basic science: from fundamental laws of particles to creation of nuclei JPMXP1020200105
  - (FY2023-2025) Simulation for basic science: approaching the new quantum era JPMXP1020230411

### **Computers:**

- RIKEN Hokusai BW
- Ito at Kyushu University (hp190124, hp200050)
- Polaire and Grand Chariot at Hokkaido University (hp200130)
- supercomputer Fugaku at R-CCS (ra000001; hp210032,hp220108,hp220233; hp200130, hp230207)



### **Projects**



### **Nf=2**:

- DWF → Overlap; high T:
  - chiral symmetry, fate of U(1)A, topology
- DWF
  - spectrum (see Lattice 2024 talk by David Ward)

### common set-up for:

- JLQCD type domain wall fermion (DWF)
  - Gauge: tree-level Symanzik
  - Fermions: Möbius DWF (scale factor=2 Shamir) with stout smeared links
- good knowledge of T=0 fine lattices for flavor physics
  - calibration for finite temperature needs only small effort (computational)

### Nf=2+1:

- DWF → Overlap for high T (led by Hidenori Fukaya)
- DWF: LCP analysis near and on the physical point
  - transition / crossover; topology
  - charge fluctuation (see talk by Jishnu Goswami)

### Nf=3:

DWF: phase hunting near three-flavor degenerate chiral limit (see talk by Yu Zhang)



### Members involved in the main topics of this talk















 $YA^{(1)}$ ,

H. Fukaya<sup>(2)</sup>, J. Goswami<sup>(1)</sup>, S. Hashimoto<sup>(3)(4)</sup>, I. Kanamori<sup>(1)</sup>, T. Kaneko<sup>(3)(4)(5)</sup>,





Y. Nakamura<sup>(1)</sup>, Y. Zhang<sup>(6)</sup>,,,,

- (1): RIKEN Center for Computational Science
- (2): Osaka University
- (3): KEK
- (4): SOKENDAI
- (5): Kobayashi-Maskawa Institute, Nagoya Univ.
- (6): Bielefeld University



## QCD phase transition near and on the physical point



- $N_f=2+1$ , 2 fine lattice DWF simulation and reweighting to overlap [PRD(2021), PTEP(2022)]
  - Profound relation among: chiral symmetry, axial anomaly and topological susceptibility
- R & D for the  $N_f=2+1$  thermodynamics with Line of Constant Physics (LCP)
  - Codes: Grid, Hadrons, Bridge++
  - LCP / Reweighting
  - Chiral order parameter and renormalization
  - Quark number susceptibility







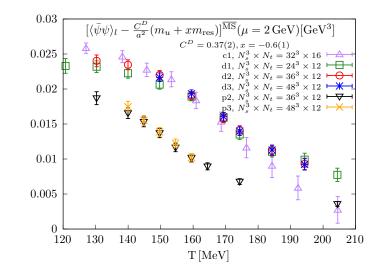


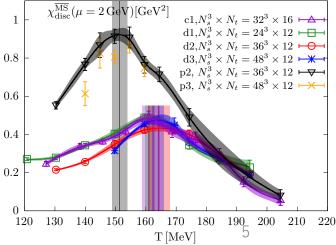






- $N_f=2+1$  thermodynamics with LCP (mass = ms/10 = about 3 x physical ud quark mass)
  - 2 step renormalization for chiral condensate (power and log divergence) with an  $xm_{res}$  correction
  - 2 lattice spacings  $N_t=12$ , 16
  - 3 volumes  $N_s/N_t=2$ , 3, 4
  - No phase transition!
  - $T_{pc}$  determined  $T_{pc} = 165(2)$  MeV
  - PPR-Fugaku FY2020-2022
  - [PoS Lattice 2021, 2022]
- Physical point study
  - PPR-Fugaku 2023- preliminary results →

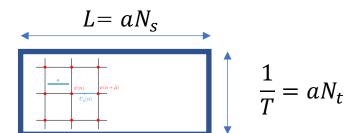


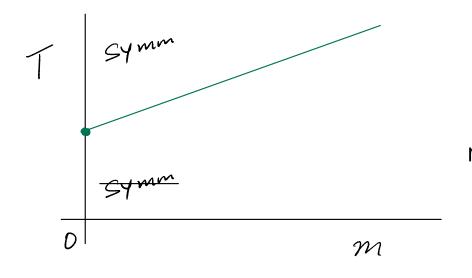


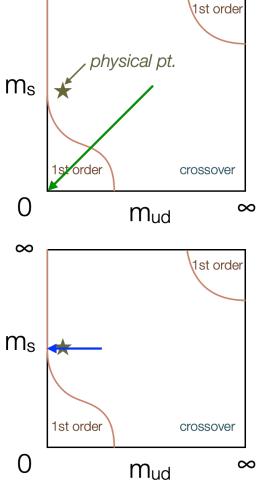
## Modes of Simulations

### to locate phase transition

- tune parameters near transition
- > T: fixed, change m
- > m: fixed, change T





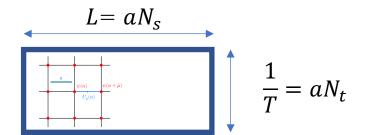


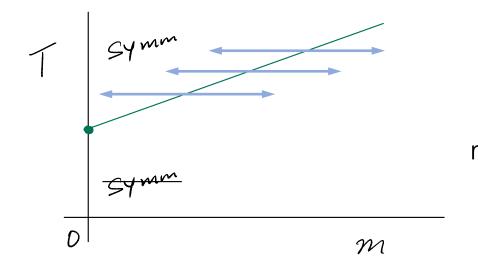
 $\infty$ 

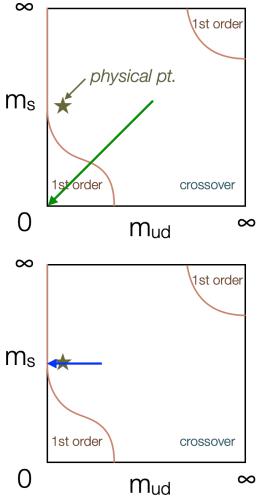
## Modes of Simulations

### to locate phase transition

- tune parameters near transition
- > T: fixed, change m
- > m: fixed, change T



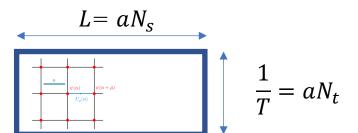




## Modes of Simulations

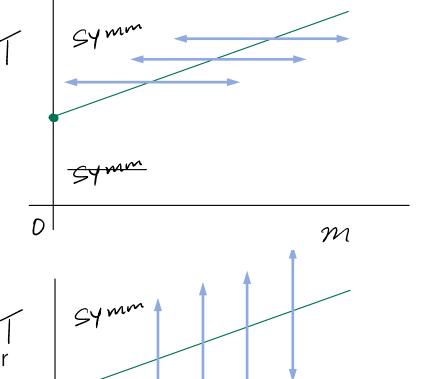
### to locate phase transition

- tune parameters near transition
- > T: fixed, change m
- > m: fixed, change T



Fixing / changing the controlling parameter

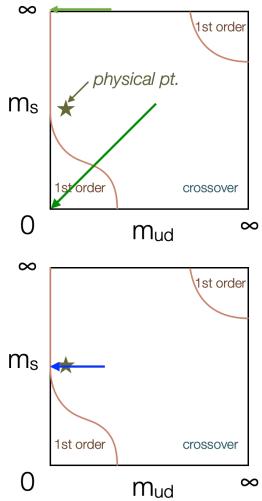
- T: controled by
  - $a(\beta)$ : controlled by  $\beta$
  - $N_t$  : discrete
- *m*: controlled by
  - input quark mass
  - $m(\beta) \leftarrow$  matching with hadronic scale:  $M_H(\beta, m)$



M

Nf=2: Ward (Lattice 2024)





## $N_f$ =2+1 Möbius DWF LCP for 2023-

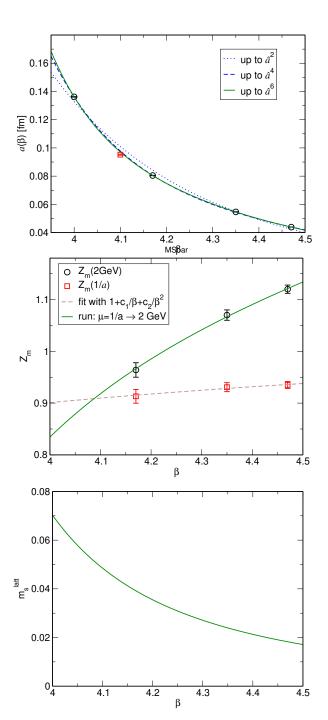
For the Line of Constant Physics:  $am_s(\beta)$  with  $a(\beta)$ 

- Step 1: determine  $a(\beta)$  [fm] with  $t_0$  (BMW) input
  - at  $\beta = 4.0, 4.1^*, 4.17, 4.35, 4.47$ 
    - \*  $\beta$ =4.0 new data, to add support at small  $\beta$
    - \*  $\beta$ =4.1 old pilot study data, removed small volume and statistics
- Step 2: determine  $Z_m(\beta)$  using Non-Perturbative Renormalization results
  - at  $\beta = 4.17, 4.35, 4.47$ ;  $Z_m$  with  $\overline{MS}$  2 GeV are available
  - NNNLO running:  $\mu = 2 \ GeV \rightarrow 1/a \ \& \beta$  polynomial fit & running back
  - use  $Z_m(\beta)$  so obtained for  $\beta \ge 4.0$ :  $\beta < 4.17$  region is extrapolation
  - $1/Z_m(\beta)$  will be used to renormalize scalar operator, **chiral condensate**
- Step 3: solve  $am_s(\beta)$  with input (quark mass input):
  - $m_s^R = Z_m \cdot a m_s^{latt} \cdot a^{-1} = 92 \text{ MeV}$
  - $\frac{m_s}{m_{ud}} = 27.4$  (See for example FLAG 2019)
- See for details in Lattice 2021 proc by S.Aoki et al.

#### Do simulation

Step 4: proper tuning of input mass: correct m<sub>res</sub>

Do simulation 2<sup>nd</sup> round / correction with reweighting + valence meas.



# Simulation plan: $2^{\rm nd}$ round w/ treatment of $m_{res}$ effect

 $L_s = 12$  fixed throughout this study

• 
$$N_t = 12$$

• 
$$m_l = 0.1 m_s$$

• 
$$m_q^{input} = m_q^{LCP} - m_{res}$$

• 
$$V_s = 24^3, 36^3$$

• 
$$N_t = 16$$

• 
$$m_l = 0.1 m_s$$

•  $m_{res}$  shift by reweighting

• 
$$V_s = 32^3$$

• 
$$N_t = 12$$

• 
$$m_l = m_{ud}$$

• 
$$m_q^{input} = m_q^{LCP} - m_{res}$$

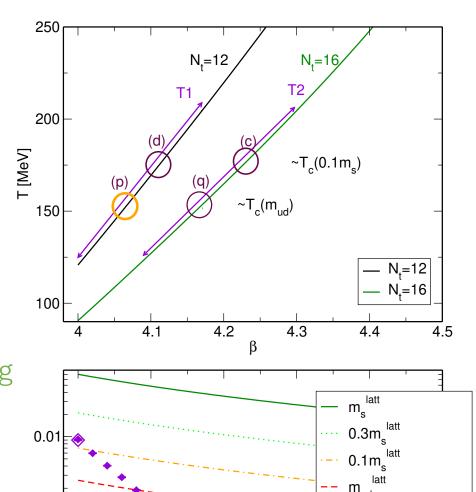
• 
$$V_{\rm s} = 36^3, 48^3$$

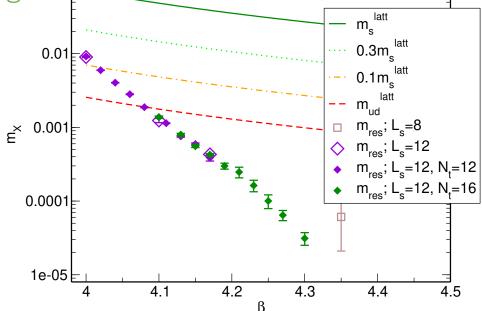
• 
$$N_t = 16$$

• 
$$m_l = m_{ud}$$

• 
$$m_q^{input} = m_q^{LCP} - m_{res}$$

• 
$$V_s = 48^3$$

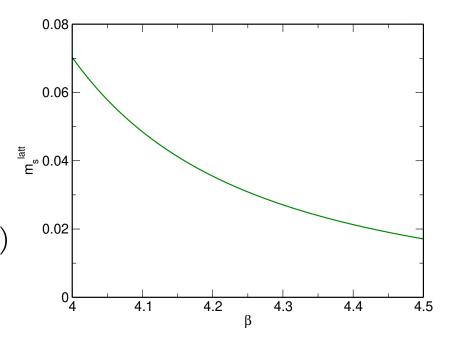




## LCP remarks for FT2023-

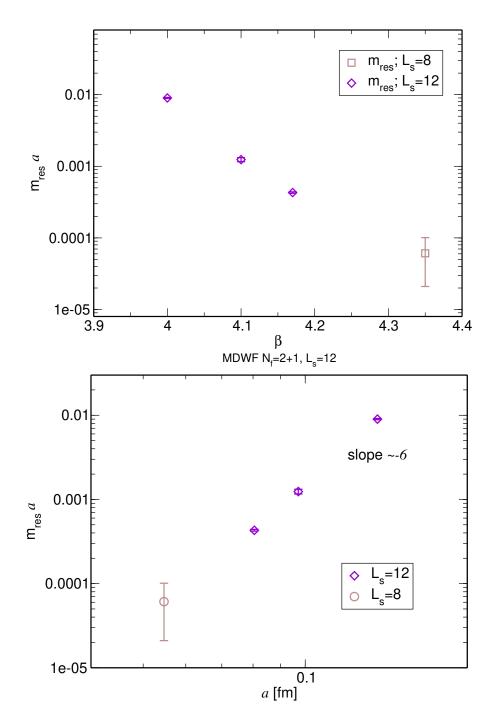
### Features

- Fine lattice: use of existing results  $(0.04 \le a \le 0.08 \text{ fm})$ 
  - Granted preciseness towards continuum limit
- Coarse lattice parametrization is an extrapolation
  - Preciseness might be deteriorated
  - Newly computing  $Z_m$  e.g. at  $\beta=4.0$  (lower edge) might improve, but not done so far
    - NPR of  $Z_m$  at  $a^{-1} \approx 1.4$  GeV may have sizable error (window problem) anyway
- Smooth connection from fine to coarse should not alter leading  $O(a^2)$ 
  - Difference should be higher order
- Error estimated from Kaon mass (at physical point)
  - $\Delta m_K \sim 10 \%$  at  $\beta = 4.0$   $(a \simeq 0.14 \text{ fm}) \rightarrow \Delta m_K \sim \text{a few } \%$
  - $\Delta m_K^2 \sim$  a few % at  $\beta = 4.17$  ( $a \simeq 0.08$  fm)



## Domain wall fermions

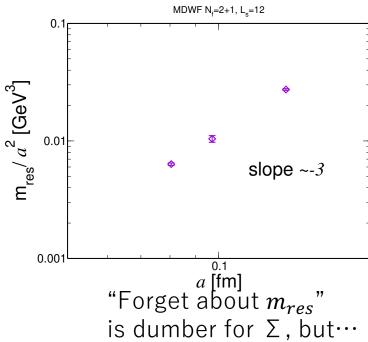
- Möbius DWF → OVF by reweighting
  - Successful (w/ error growth) at  $\beta = 4.17$  ( $a \simeq 0.08$  fm)
    - See Lattice 2021 JLQCD (presenter: K.Suzuki)
  - Questionable for
    - · Coarser lattice: rough gauge, DWF chiral symmetry breaking
    - Finer lattice: larger V (# sites)
- Chiral fermion with continuum limit
  - A practical choice is to stick on DWF
- Controlling chiral symmetry breaking with DWF
  - WTI residual mass  $m_{res}$ :  $m_{\pi}^2 \propto (m_f + m_{res})(1 + h.o.)$
  - Understanding  $m_{res}(\beta)$  with fixed  $L_s$  (5-th dim size)
- $m_{res}[MeV] \sim a^X$ , where  $X \sim 5$ 
  - Vanishes quickly as  $a \rightarrow 0$
  - 1st (dumb) approximation: forget about  $m_{res}$
  - Better:  $m_f^{cont} \leftrightarrow \left(m_f + m_{res}\right)$  but, this is not always enough



# Light quark $\Sigma = -\langle \overline{\psi} \psi \rangle$ : conventional and residual power divergence

• 
$$\Sigma|_{DWF} \sim C_D \frac{m_f + x m_{res}}{a^2} + \Sigma|_{cont.} + \cdots$$
 S. Sharpe (arXiv: 0706.0218)

- $m_{res} \neq x m_{res}$ ;  $x = O(1) \neq 1$ 
  - "Since x is not known, this term gives an uncontrolled error in the condensate. It can be studied and reduced only by increasing  $L_s$  a <u>very expensive proposition</u>." S. Sharpe.
- cf:  $m_{\pi}^2 \propto \left(m_f + m_{res}\right)$  [1+h.o.]
- $\Sigma|_{DWF} \rightarrow C_D \frac{xm_{res}}{a^2} + \Sigma|_{cont.} + \cdots; (m_f \rightarrow 0)$
- $\Sigma|_{DWF} \rightarrow C_D \frac{-(1-x)m_{res}}{a^2} + \Sigma|_{cont.}; \quad (m_f \rightarrow -m_{res})$

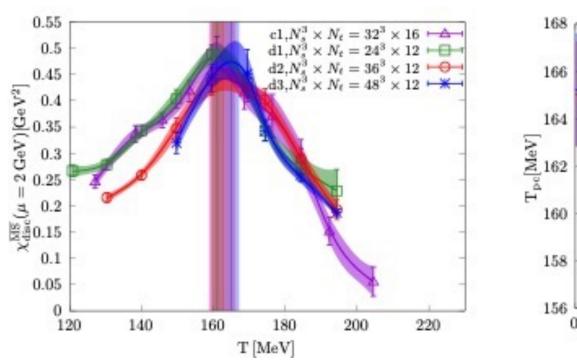


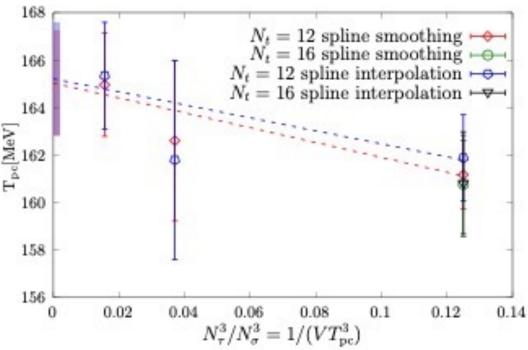
# Light quark $\Sigma = -\langle \overline{\psi} \psi \rangle$ : no power div. in disconnected susceptibility

- $\chi_{disc} = \langle \overline{u}u \cdot \overline{d}d \rangle \langle \overline{u}u \rangle \langle \overline{d}d \rangle$ 
  - power divergence in  $\langle \overline{\psi}\psi \rangle$  cancels out
  - no new divergence over  $\Sigma$  because no new contact terms
  - needs multiplicative renormalization for logarithmic divergence
  - $Z_S(\beta) = 1/Z_m(\beta)$
  - we stick for now on this quantity
- $\chi_{total} = \langle \overline{\psi}\psi \cdot \overline{\psi}\psi \rangle \langle \overline{\psi}\psi \rangle \langle \overline{\psi}\psi \rangle$ 
  - has power divergence everywhere
  - needs to understand the power divergence of  $\Sigma = -\langle \overline{\psi}\psi \rangle$  first

# Chiral susceptibility (disconnected)

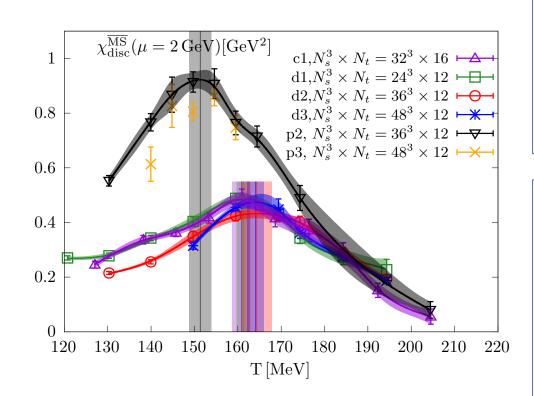
 $m_l = 0.1 m_{\scriptscriptstyle S}$  (about 3 time larger than physics u,d mass)





- no subtraction needed in addition to vacuum subtraction
- peak position: mild volume dependence → infinite volume limit
- observing no dependence for  $N_t=12$  and 16 (LT=2)
- $T_{pc} = 165$  (2) MeV from the disconnected chiral condensate

# Disconnected chiral susceptibility at average physical u and d quark mass



Likely NO phase transition at physical point with chiral fermions.

No surprise happened so far...

$$m_l = m_s / 10$$

•  $d1,d2,d3: N_t = 12, LT=2,3,4$ 

• c1 :  $N_t = 16$ , LT=2

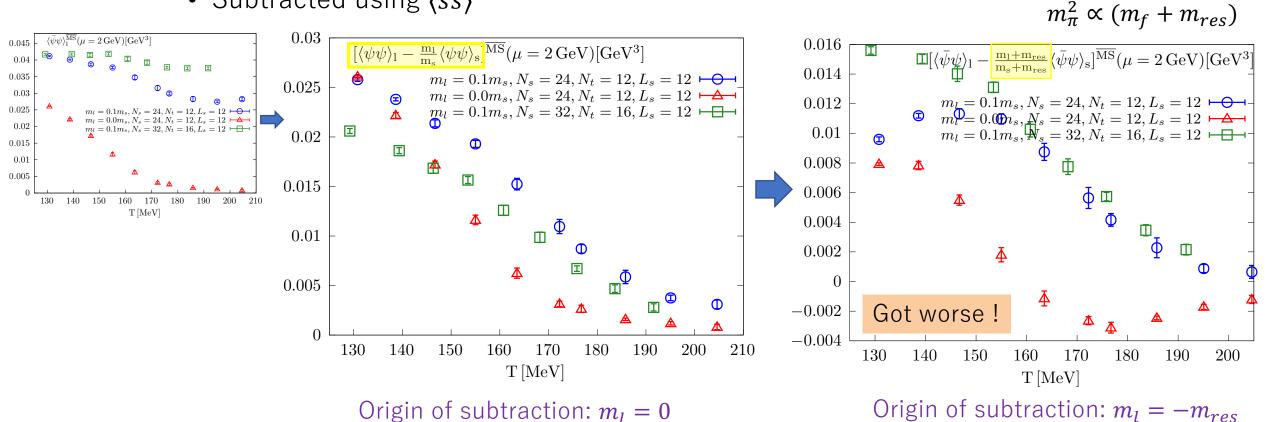
• good scaling  $N_t = 12$  -16 observed for LT=2

### $m_l = m_{ud}$

- p2,p3:  $N_t=12$ , aspect ratio LT = 3, 4
  - Statistics is ~20,000 MDTU for LT=3, sampled every 10 MDTU
  - LT=4 very preliminary, currently running to get to planned satat.
- $T_{pc} = 151$  (3) MeV (preliminary) on  $36^3 \times 12$ , compared with
  - $T_{pc} = 155 (1)(8)$  w/ DWF ( $N_t=8$ ) by HotQCD (2014)
  - $T_{pc} = 156.5 (1.5) \text{ w/ HISQ by HotQCD (2019) (} \simeq \text{disconnected)}$
  - $T_{pc} = 158.0 (0.6)$  w/ stout staggered by Budapest-Wuppertal (2020)

# Light quark $\Sigma = -\langle \overline{\psi}\psi \rangle$

- Two step UV renormalization necessary (naively)
  - Logarithmic divergence (multiplicative):  $Z_S(\overline{MS}, 2 \text{ GeV})$
  - Power divergence (additive):
    - Subtracted using  $\langle \overline{s}s \rangle$



 $\propto m_f a^{-2}$ 

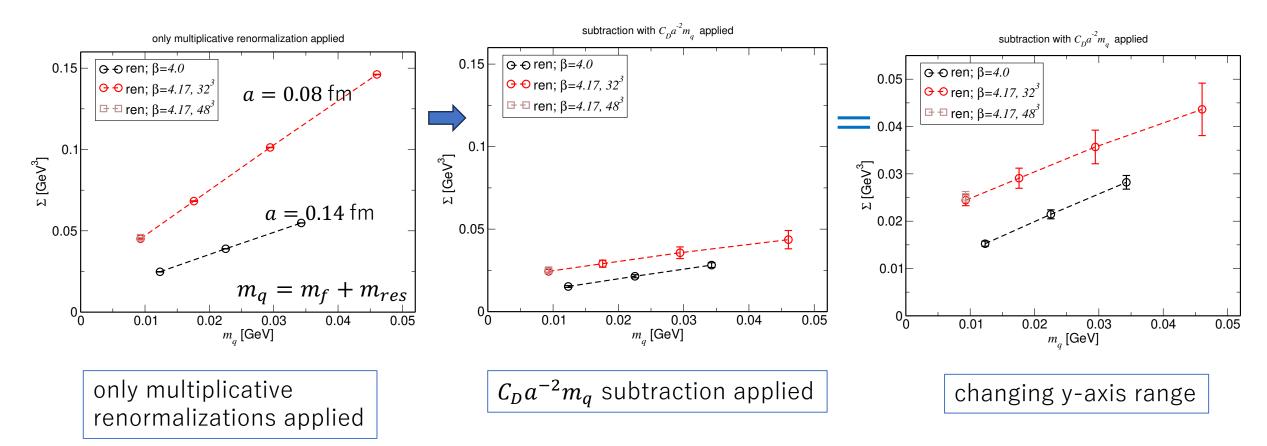
# Light quark $\Sigma = -\langle \overline{\psi}\psi \rangle$ : residual power divergence

• 
$$\Sigma|_{DWF} = C_D \frac{m_f + x m_{res}}{a^2} + \Sigma|_{cont.} + \cdots$$
 S. Sharpe (arXiv: 0706.0218)

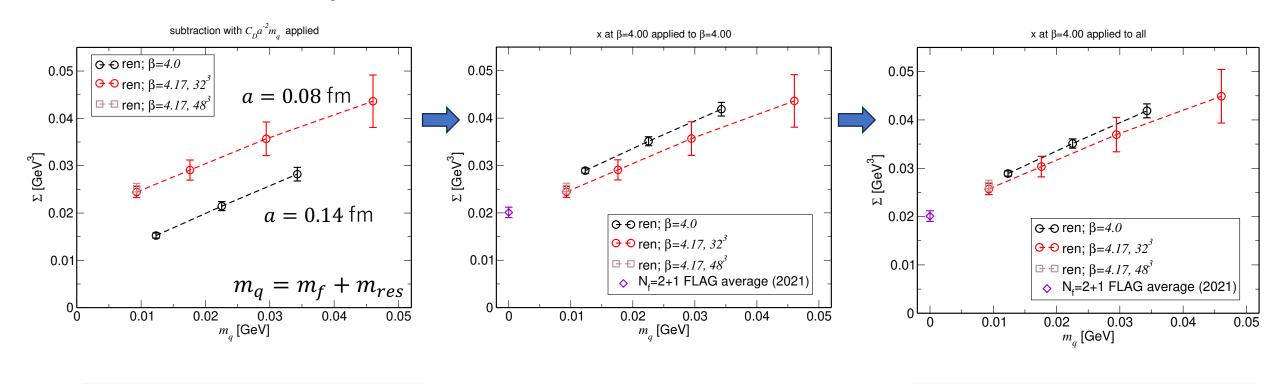
$$m_{res} \neq x m_{res}; \quad x = O(1) \neq 1$$

- "Since x is not known, this term gives an uncontrolled error in the condensate. It can be studied and reduced only by increasing  $L_s$  a <u>very expensive proposition</u>." S. Sharpe.
- (we proposed another way to utilize  $m'_{res}$ , which end up mixing T=0  $C_R$  into high T)
- Yet another way of subtraction including  $xm_{res}$  using  $N_f=3$ , T=0 &  $T>T_c$  information —see the talk by Yu Zhang
  - 1. Prepare several different lattice spacing for T = 0
  - 2. Compute coefficient linear in  $m_f$ :  $\Sigma|_{DWF} \sim const. + (\frac{C_D}{a^2} + C_R)m_f + \cdots$
  - 3. Separate divergent term : linear fit in  $a^2$  of.  $C_D + a^2 C_R \rightarrow C_D = 0.37(2)$
  - 4. Estimate x using  $T > T_c$  through  $\Sigma|_{DWF} \to \frac{-C_D(1-x)m_{res}}{a^2} = 0$   $(m_f \to -m_{res})$  [ren.cond.  $\Sigma|_{cont.} = 0$ ]
  - $\rightarrow$   $N_f = 3; \beta = 4.0 \text{ estimate: } x = -0.6(1)$ 
    - In general, x may depend on  $\beta$ , for now use this value as a reference for all  $\beta$
    - We also use  $C_D$  (single flavor normalization) of  $N_f=3$  for  $N_f=2+1$

# test on $N_f=2+1$ , T=0 measurements



# test on $N_f=2+1$ , T=0 measurements



Seemingly, both conventional and residual divergence are controlled, but

applied only to  $\beta = 4.0$ 

 $C_D a^{-2} (1-x) m_{res}$  subtraction

 $C_D a^{-2} (1-x) m_{res}$  subtraction

assuming x is universal

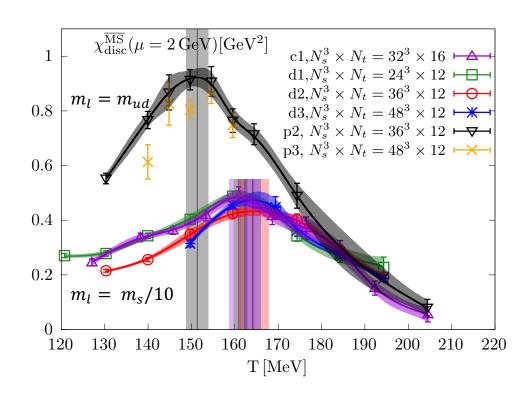
applied to all

• need to check if x does not depend much on  $\beta$ 

 $C_D a^{-2} m_a$  subtraction applied

• refinement of precision and check applicability range of  $C_D$  necessary

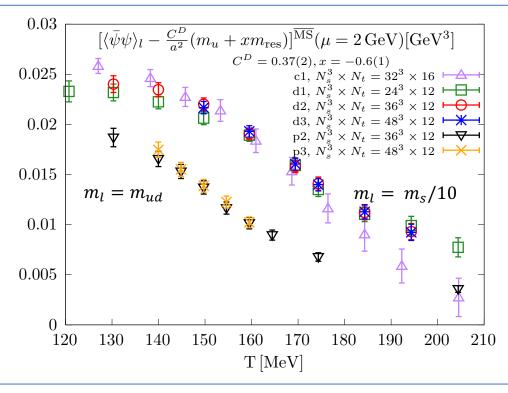
Disconnected chiral susceptibility and chiral condensate



Likely NO phase transition at physical point with chiral fermions.

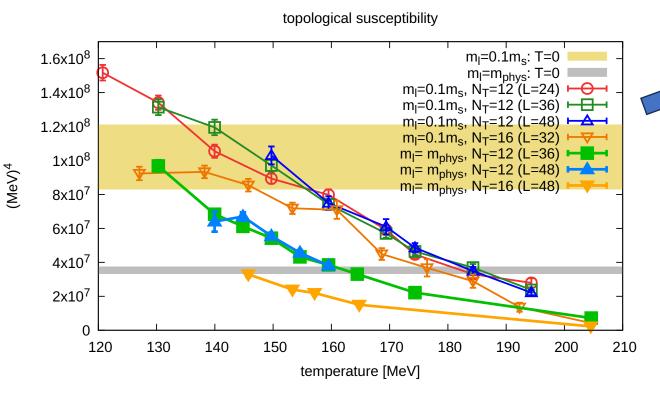
No surprise happened so far..

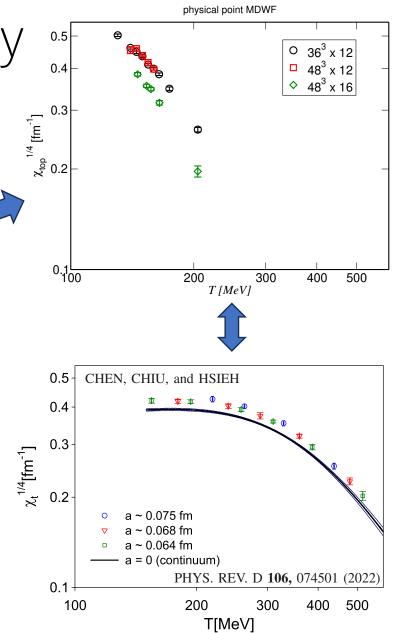
all divergences subtracted assuming x is universal



$$m_l = m_{ud}$$

- p2,p3:  $N_t=12$ , aspect ratio LT = 3, 4
  - Statistics is ~20,000 MDTU for LT=3, sampled every 10 MDTU
  - LT=4 very preliminary, currently running to get to planned satat.
- $T_{nc} = 151 (3) \text{ MeV (preliminary) on } 36^3 \times 12$



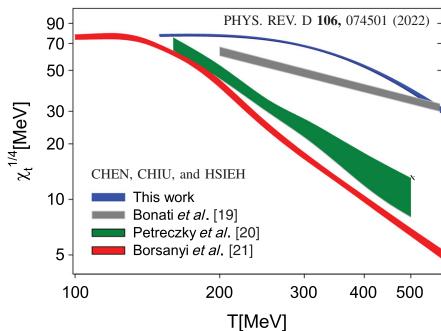


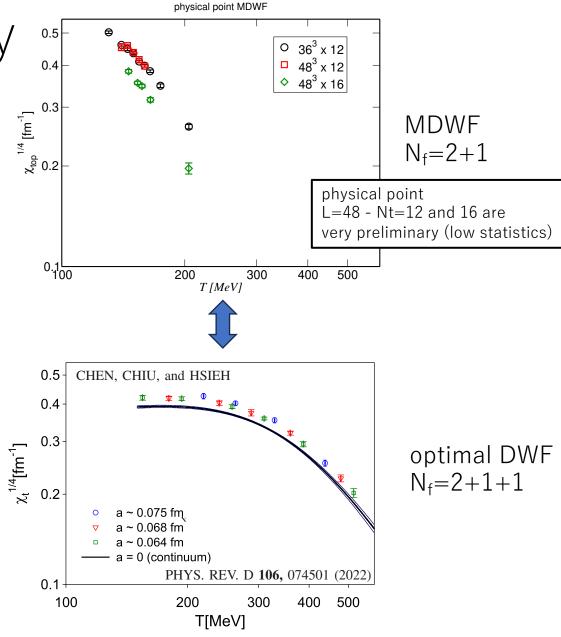
 $\begin{array}{c} MDWF \\ N_f = 2 + 1 \end{array}$ 

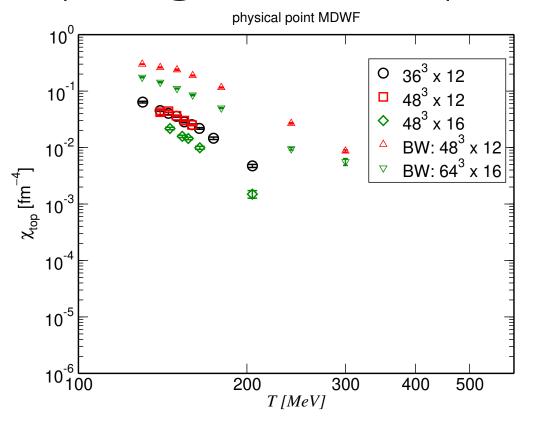
optimal DWF  $N_f=2+1+1$ 

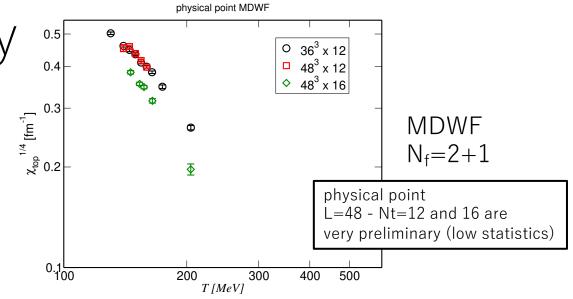
physical point L=48 - Nt=12 and 16 are very preliminary (low statistics)

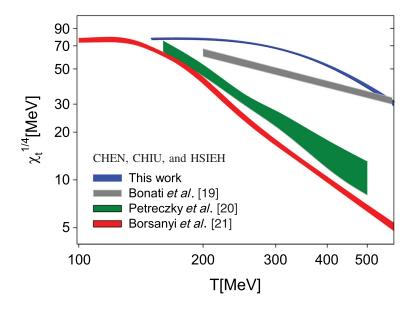
## Summary by Chen et al (TWQCD)

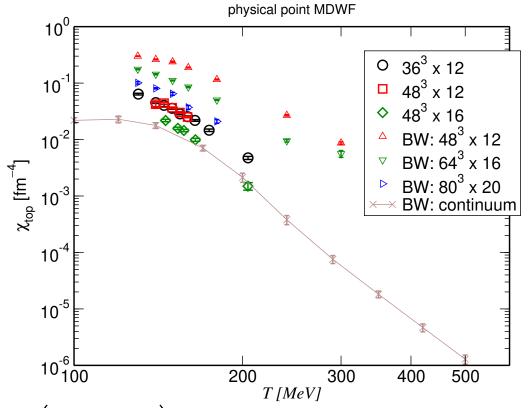


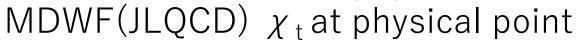




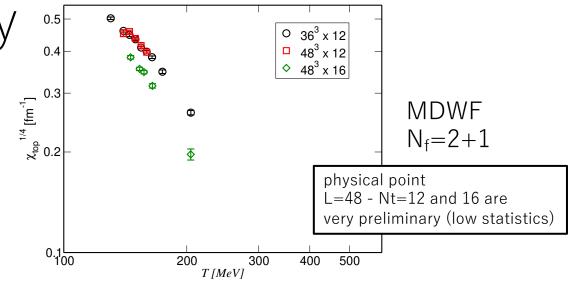




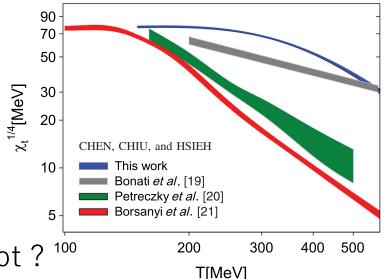




- inconsistent with Chen et al (optimal DWF)
- getting closer to BW[continuum] for  $a \rightarrow 0$
- $N_t$ =16 already ~continuum or even undershoot? 100
- more detailed study needed



physical point MDWF





### Summary and Outlook



### Nf=2+1 Physical point computation of QCD thermodynamics with Möbius DWF

- use LCP, determined with T=0 JLQCD knowledge
- no surprise on the existence/non-existence on the transition
- machinery to treat power divergence, residual chiral symmetry effect is being finalized
- seemingly the both types of "divergence" are under control using Nf=3 results
- further improvement underway
- Disconnected chiral susceptibility show no hint of phase transition for Nt=12
  - $T_{pc} \simeq T_{pc}$  (staggered)
  - no surprise so far with chiral fermions
- Topological susceptibility showing large lattice artifact for Nt=12. Nt=16 promising.

### **Outlook**

- refinement of power divergence subtraction using T=0 information of very fine MDWF
- 48<sup>3</sup> for Nt=12 and 16 are being run on Fugaku
- plan to be completed by the end of FY2025 with a few additional points on  $64^3 \times 16$ .
- use of these configuration underway
  - > see eg. talk by Goswami on charge fluctuation

thank you for your attention

# Light quark $\Sigma = -\langle \overline{\psi}\psi \rangle$ : residual power divergence

•  $\Sigma|_{DWF} \sim \frac{m_f + x m_{res}}{a^2} + \Sigma|_{cont.} + \cdots$  S. Sharpe (arXiv: 0706.0218)

$$m_{res} \neq x m_{res}$$
;  $x = O(1) \neq 1$ 

- "Since x is not known, this term gives an uncontrolled error in the condensate. It can be studied and reduced only by increasing  $L_s$  a <u>very expensive proposition</u>." S. Sharpe.
- We propose another way to estimate  $xm_{res}$  using  $m'_{res}$  If chiral symmetry is restored  $\rightarrow \Sigma|_{cont.} = 0$   $\rightarrow m_f = -xm_{res} \text{ is a zero of } \Sigma|_{DWE} \text{ which is related with}$

$$m_{res} = \frac{\sum_{\vec{x}} \langle J_{5q}(\vec{x},t)P(0)\rangle}{\sum_{\vec{x}} \langle P(\vec{x})P(0)\rangle} \qquad (\Leftrightarrow m_{res} = \frac{\sum_{\vec{x}} \langle J_{5q}(\vec{x},t)P(0)\rangle}{\sum_{\vec{x}} \langle P(\vec{x},t)P(0)\rangle} \rightarrow \frac{\langle 0|J_{5q}|\pi\rangle}{\langle 0|P|\pi\rangle}$$

$$m_f = -m_{res}'$$
 is a zero of  $\Sigma|_{DWF}$   $(\Leftrightarrow m_f = -m_{res})$  is a zero of  $m_\pi^2$  Due to Axial WT identity:  $(m_f + m_{res}') \sum_x \langle P(x) P(0) \rangle = \Sigma$   
From:  $\Delta_\mu \langle A_\mu(x) P(0) \rangle = 2m_f \langle P(x) P(0) \rangle + 2 \langle J_{5g}(x) P(0) \rangle - 2 \sum_x \delta_{x,0}$ 

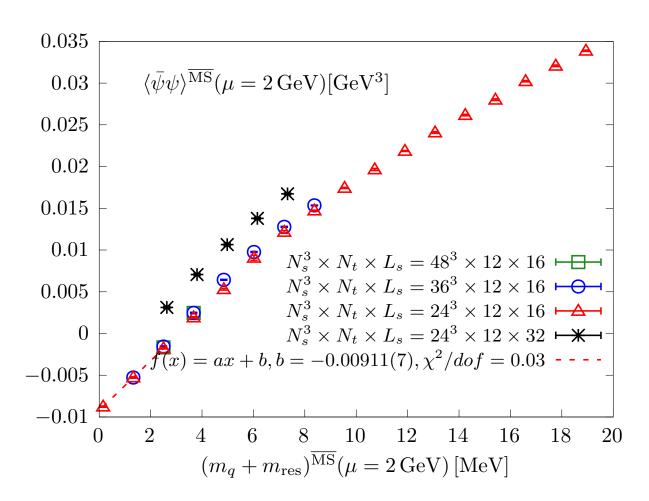
Light quark 
$$\Sigma = -\langle \overline{\psi}\psi \rangle$$
: residual power divergence

• 
$$\Sigma|_{DWF} = C_D \frac{m_f + x m_{res}}{a^2} + \Sigma|_{cont.} + \cdots$$
 S. Sharpe (arXiv: 0706.0218)

$$m_{res} \neq x m_{res}; \quad x = O(1) \neq 1$$

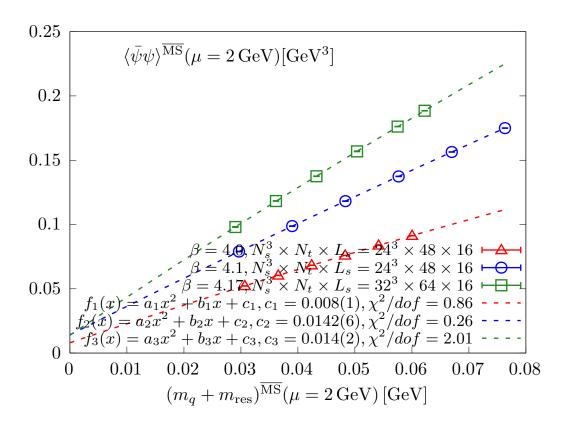
- "Since x is not known, this term gives an uncontrolled error in the condensate. It can be studied and reduced only by increasing  $L_s$  a <u>very expensive proposition</u>." S. Sharpe.
- $N_f = 3$  case
  - T>0 problem @  $\beta = 4.0$
  - T=0 exercise @  $\beta$  =4.0, 4.1, 4.17
  - T>0 div free  $\Sigma$

# $N_f=3$ , $N_t=12$ chiral condensate



- only multiplicative renormalization applied
- quark mass: m<sub>res</sub> shift applied
- @T=0:  $m_{\pi} \rightarrow 0$  ,  $(m_q + m_{res}) \rightarrow 0$
- $L_s = 16$ 
  - three volumes: 24<sup>3</sup>, 36<sup>3</sup>, 48<sup>3</sup>
- $L_s = 32$ 
  - smaller  $m_{res}$ ,  $24^3$
- Intercept =  $C_D \frac{-(1-x)m_{res}}{a^2} < 0$ 
  - need to be subtracted

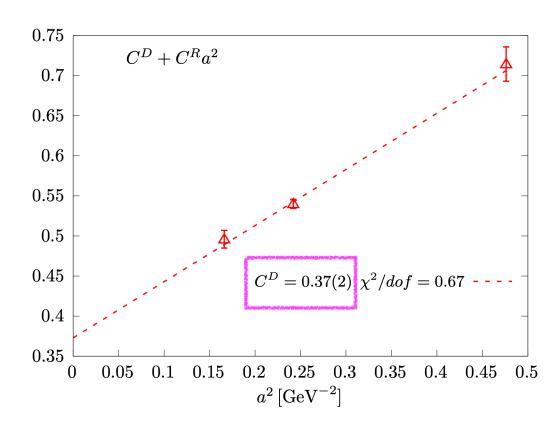
## Nf=3, T=0 chiral condensate



• 
$$\Sigma(m) = C_0 + C_1 m + C_2 m^2$$
 fit

• 
$$C_1 = \frac{C_D}{a^2} + C_R$$

•  $C_D/a^2$ : divergent,  $C_R$ : regular

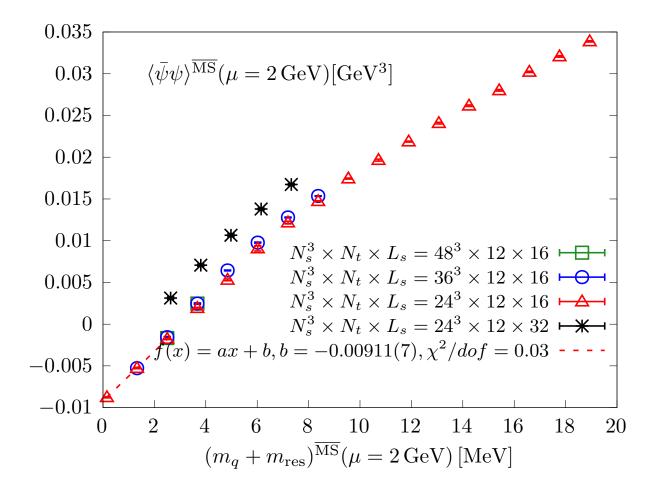


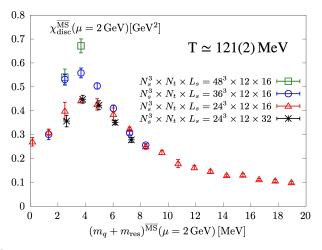
• 
$$\Sigma|_{DWF} = C_D \frac{m_f + x m_{res}}{a^2} + \Sigma|_{cont.} + \cdots$$

• 
$$C_D + C_R a^2$$

•  $C_D = 0.37(2)$  from linear fit

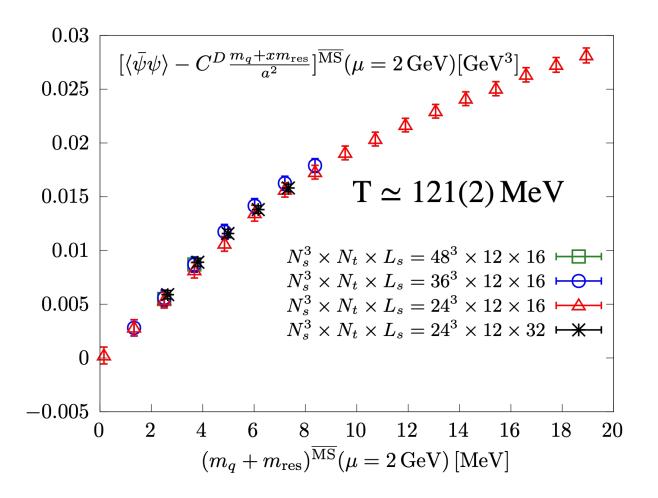
# $N_f=3$ , $N_t=12$ chiral condensate

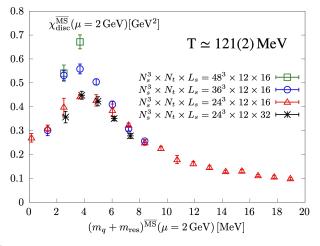




- $m_{pc} \simeq 4 \text{ MeV}$
- $m < m_{pc}$ : high T "phase"
- $\Sigma|_{DWF} \rightarrow C_D \frac{-(1-x)m_{res}}{a^2} + \Sigma|_{cont.};$  $(m_f \rightarrow -m_{res})$
- $\Sigma|_{cont.}=0$ : renormalization cond.
  - applied to determine x
  - x=-0.6(1) from  $24^3 \times 12 \times 16$

# $N_f=3$ , $N_t=12$ chiral condensate

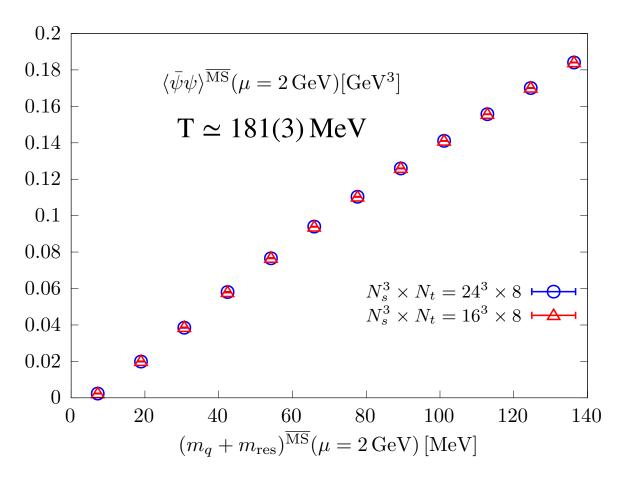




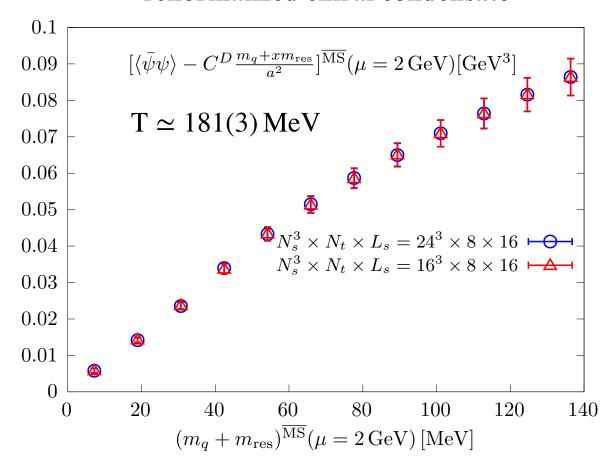
- $m_{pc} \simeq 4 \text{ MeV}$
- $m < m_{pc}$ : high T "phase"
- $\Sigma|_{DWF} \rightarrow C_D \frac{-(1-x)m_{res}}{a^2} + \Sigma|_{cont.};$  $(m_f \rightarrow -m_{res})$
- $\Sigma|_{cont.}=0$ : renormalization cond.
  - applied to determine x
  - x=-0.6(1) from  $24^3x12x16$
- subtraction using these to all sets
  - note: consistency  $L_s=16 <-> 32$

## Renormalized chiral condensate

### Multiplicatively renormalized chiral condensate



## Additive and multiplicatively renormalized chiral condensate



Subtracted chiral condensate vanishes in the chiral limit as expected since T> T<sub>c</sub>