

Finite temperature QCD explored with chiral fermions

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<https://www.r-ccs.riken.jp/labs/ftrt/>



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)

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 Lattice 2024 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



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Y. Nakamura⁽¹⁾, Y. Zhang⁽⁶⁾,,,,

(1): RIKEN Center for Computational Science

(2): Osaka University

(3): KEK

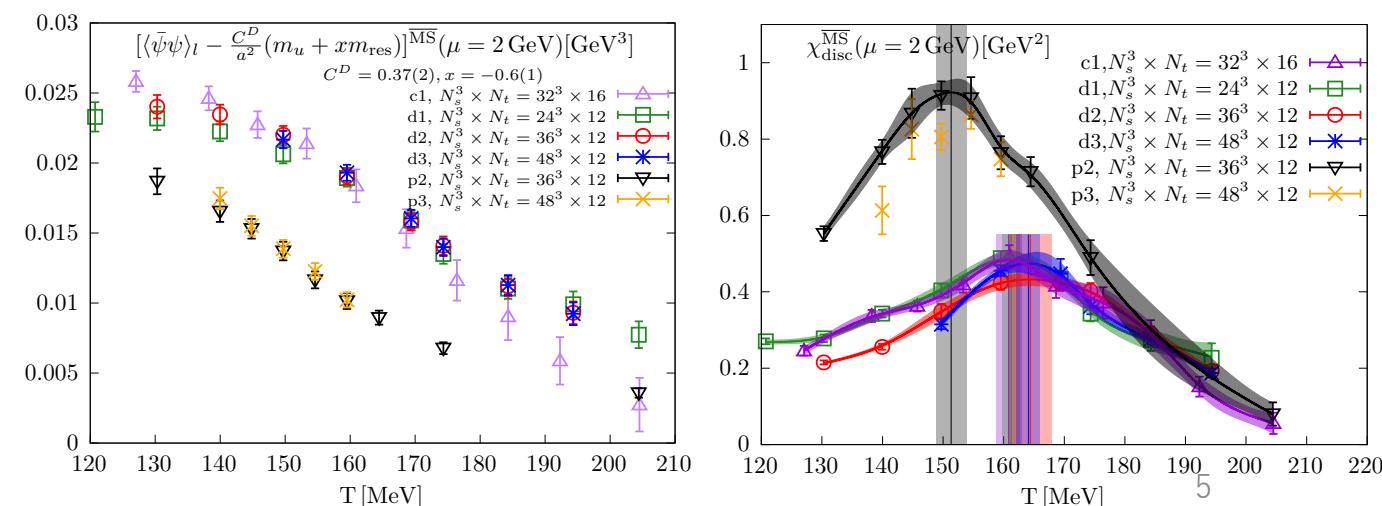
(4): SOKENDAI

(5): Kobayashi-Maskawa Institute, Nagoya Univ.

(6): Bielefeld University

QCD phase transition near and on the physical point

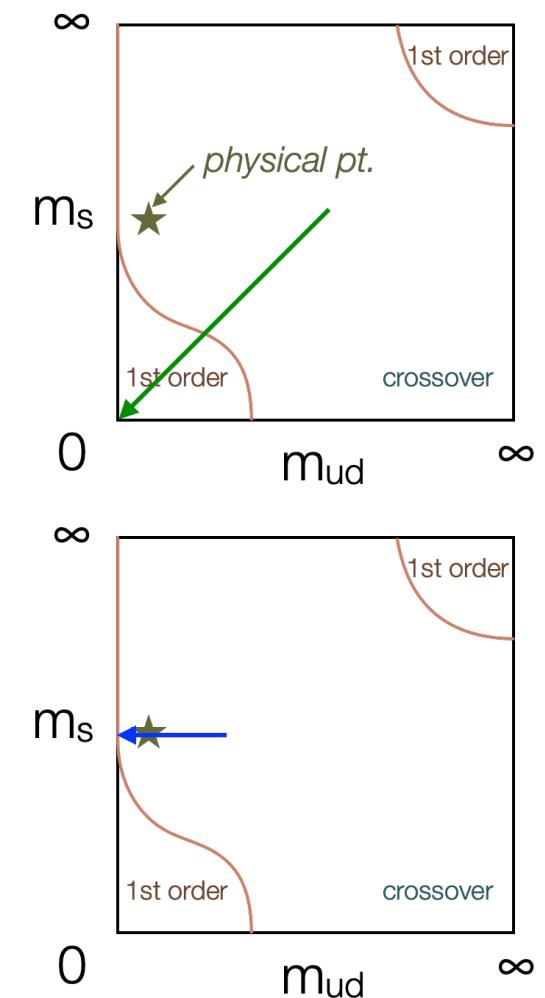
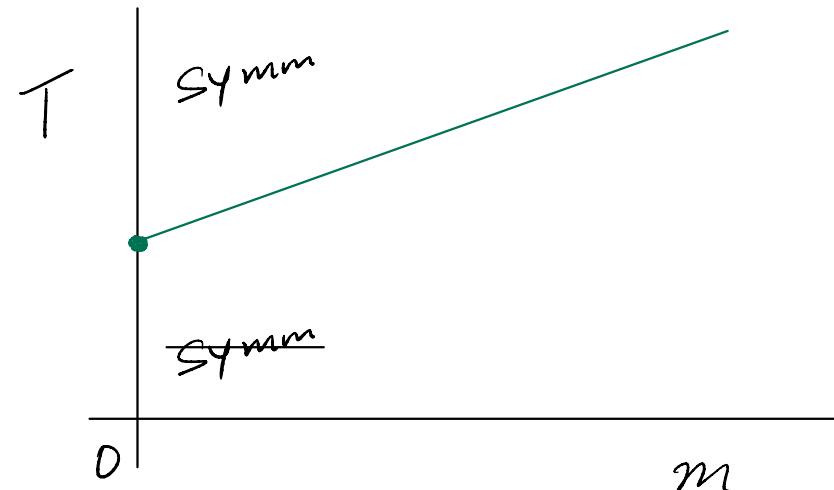
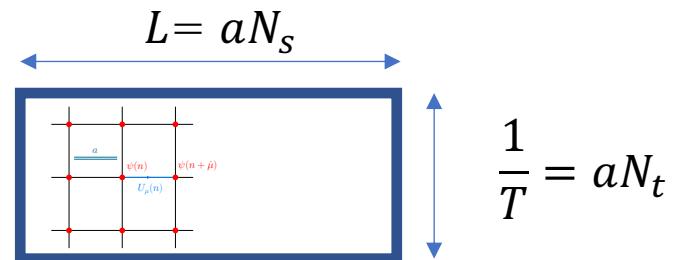
- $N_f=2+1$, 2 fine lattice DWF simulation and reweighting to overlap [PRD(2021), PTEP(2022)]
 - Profound relation among: chiral symmetry, axial anomaly and topological susceptibility
- R & D for the $N_f=2+1$ thermodynamics with Line of Constant Physics (LCP)
 - Codes: Grid, Hadrons, Bridge++
 - LCP / Reweighting
 - Chiral order parameter and renormalization
 - Quark number susceptibility
- $N_f=2+1$ - thermodynamics with LCP (mass = $m_s/10$ = 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

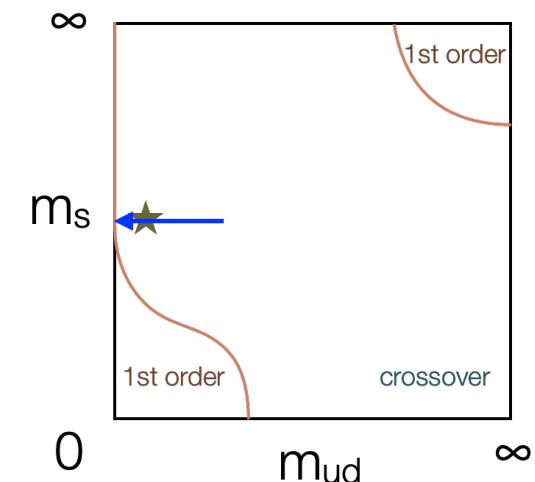
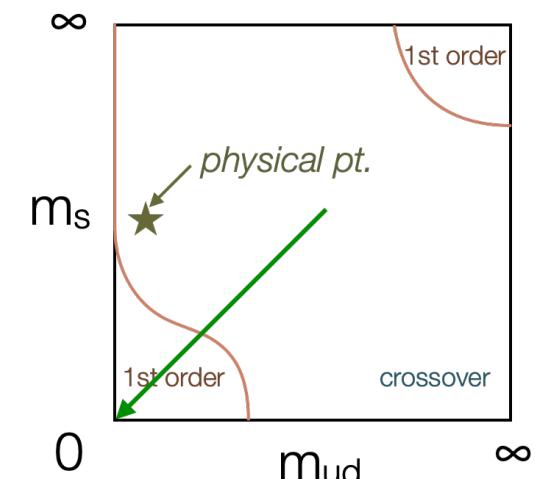
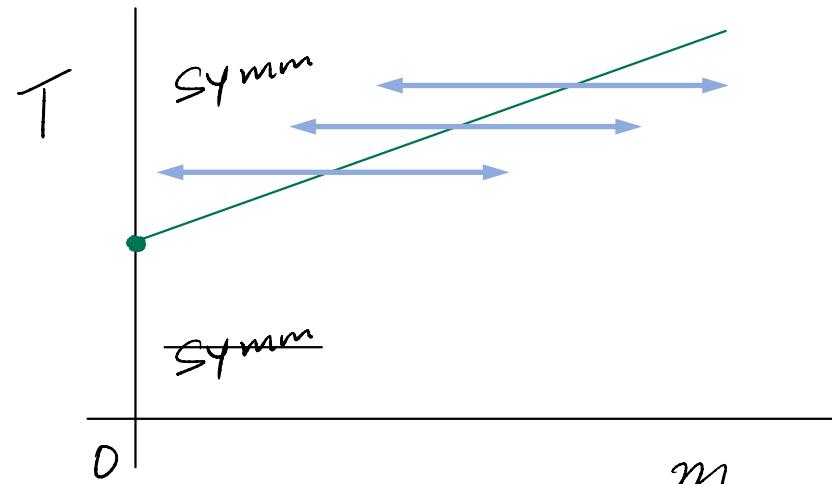
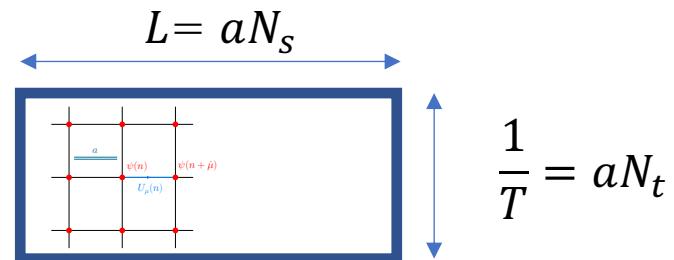
- tune parameters near transition
- T: fixed, change m
- m: fixed, change T



Modes of Simulations

to locate phase transition

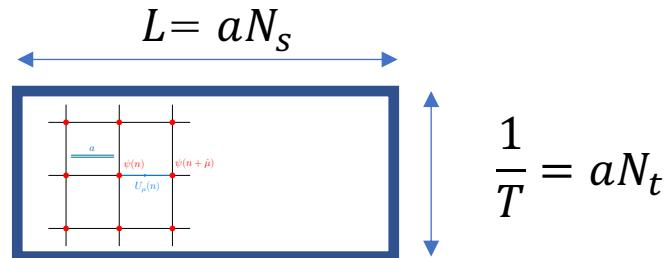
- tune parameters near transition
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Modes of Simulations

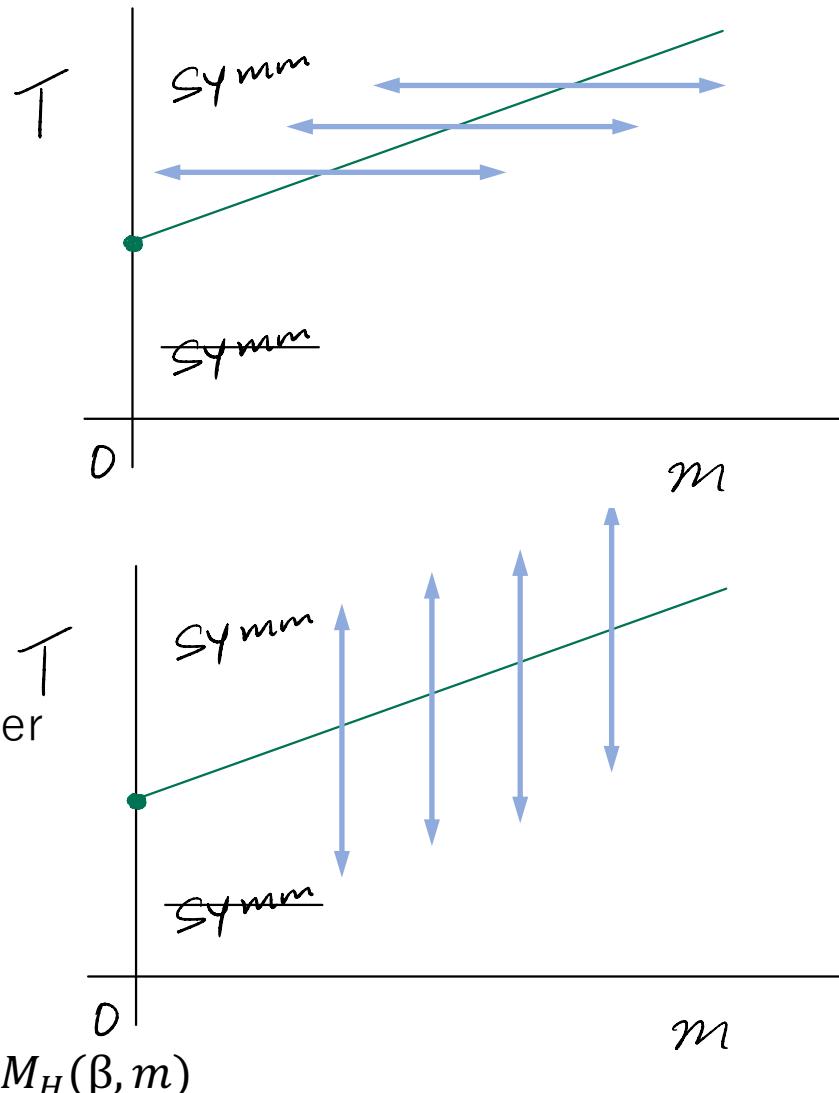
to locate phase transition

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

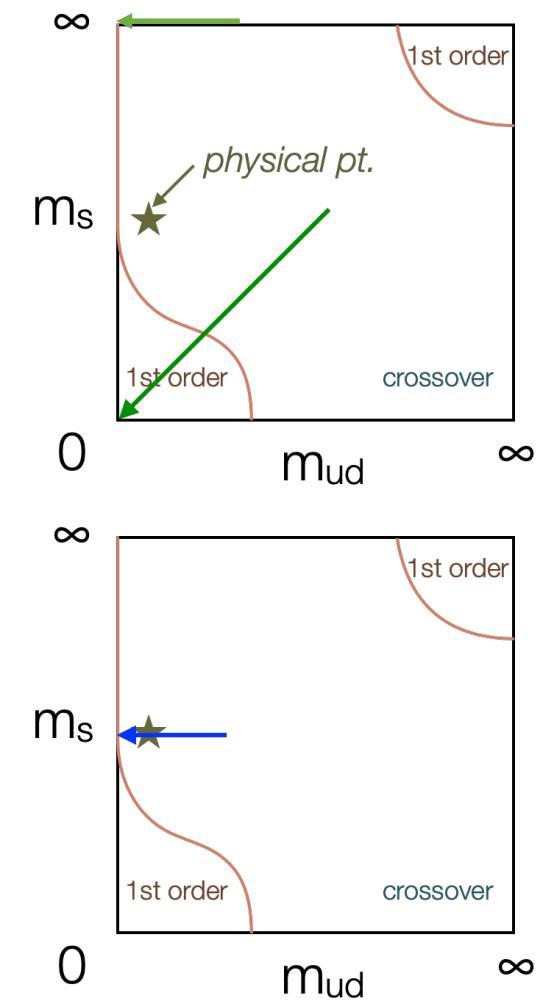


Fixing / changing the controlling parameter

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



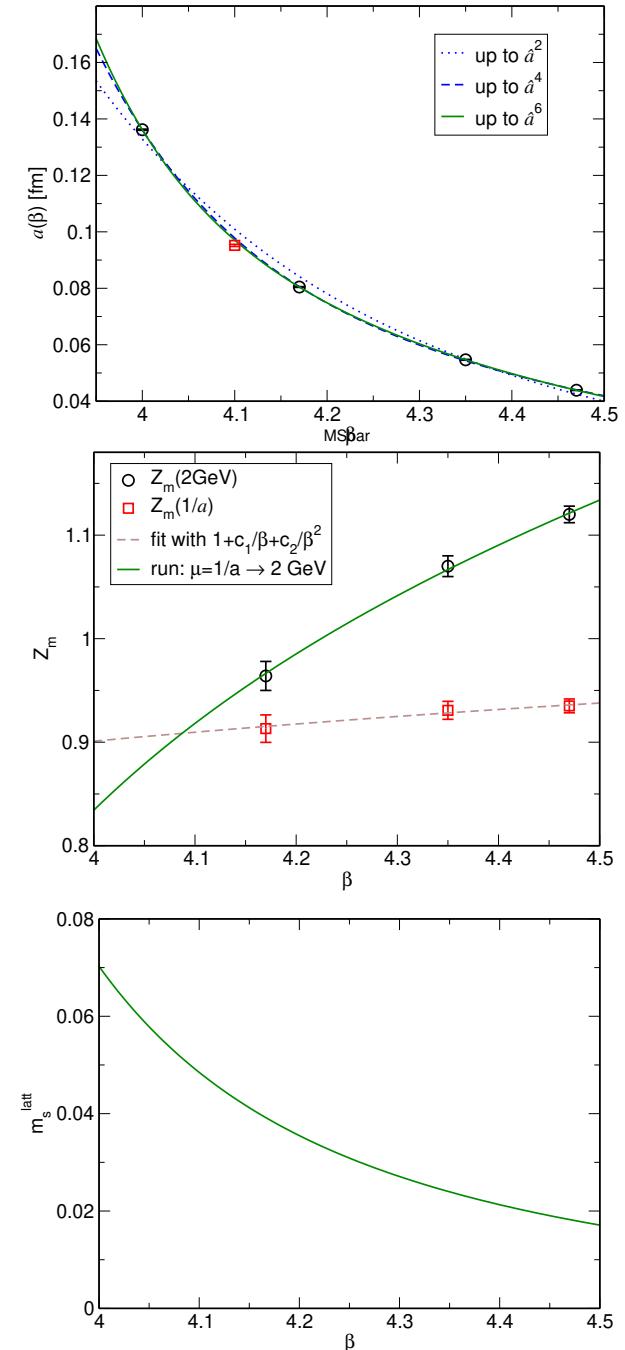
Nf=2: Ward (Lattice 2024)
Nf=3: Zhang



$N_f=2+1$ Möbius DWF LCP for 2023-

For the Line of Constant Physics: $\mathbf{am}_s(\beta)$ with $\mathbf{a}(\beta)$

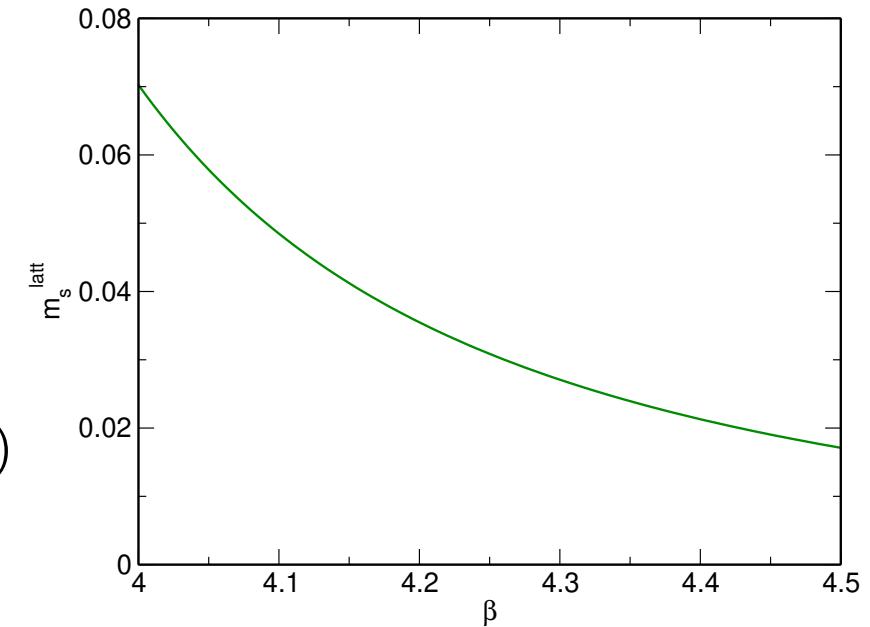
- Step 1: determine $\mathbf{a}(\beta)$ [fm] with t_0 (BMW) input
 - at $\beta = 4.0, 4.1^*, 4.17, 4.35, 4.47$
 - * $\beta=4.0$ new data, to add support at small β
 - * $\beta=4.1$ old pilot study data, removed - small volume and statistics
 - Step 2: determine $Z_m(\beta)$ using Non-Perturbative Renormalization results
 - at $\beta = 4.17, 4.35, 4.47$; Z_m with \overline{MS} 2 GeV are available
 - NNNLO running: $\mu = 2 \text{ GeV} \rightarrow 1/a$ & β polynomial fit & running back
 - use $Z_m(\beta)$ so obtained for $\beta \geq 4.0$: $\beta < 4.17$ region is extrapolation
 - $1/Z_m(\beta)$ will be used to renormalize scalar operator, **chiral condensate**
 - Step 3: solve $\mathbf{am}_s(\beta)$ with input (*quark mass input*):
 - $m_s^R = Z_m \cdot am_s^{latt} \cdot a^{-1} = 92 \text{ MeV}$
 - $\frac{m_s}{m_{ud}} = 27.4$ (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_{res}
- Do simulation 2nd round / correction with reweighting + valence meas.



LCP remarks for FT2023-

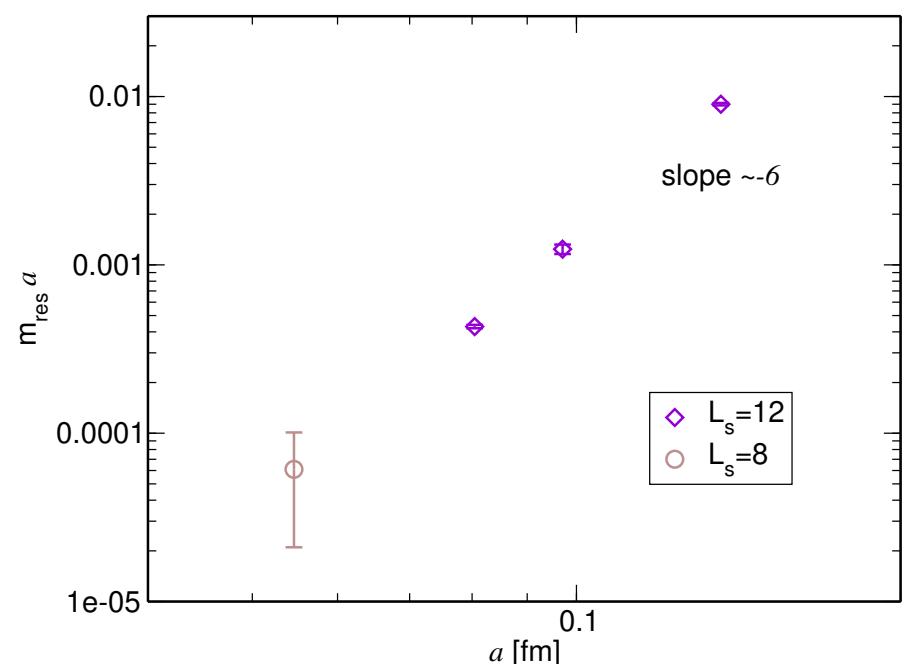
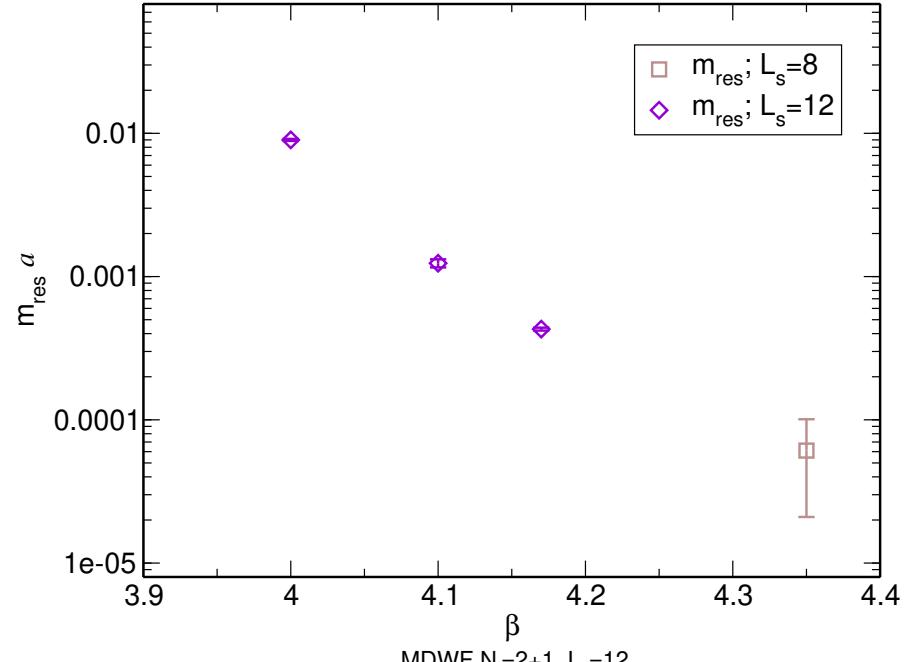
Features

- Fine lattice: use of existing results ($0.04 \leq a \leq 0.08$ fm)
 - Granted precision towards continuum limit
- Coarse lattice parametrization is an extrapolation
 - Precision 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 $a^{-1} \simeq 1.4$ 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
 - $\Delta m_K \sim 10\%$ at $\beta = 4.0$ ($a \simeq 0.14$ fm) $\rightarrow \Delta m_K \sim$ a few %
 - $\Delta m_K \sim$ a few % at $\beta = 4.17$ ($a \simeq 0.08$ fm)



Domain wall fermions

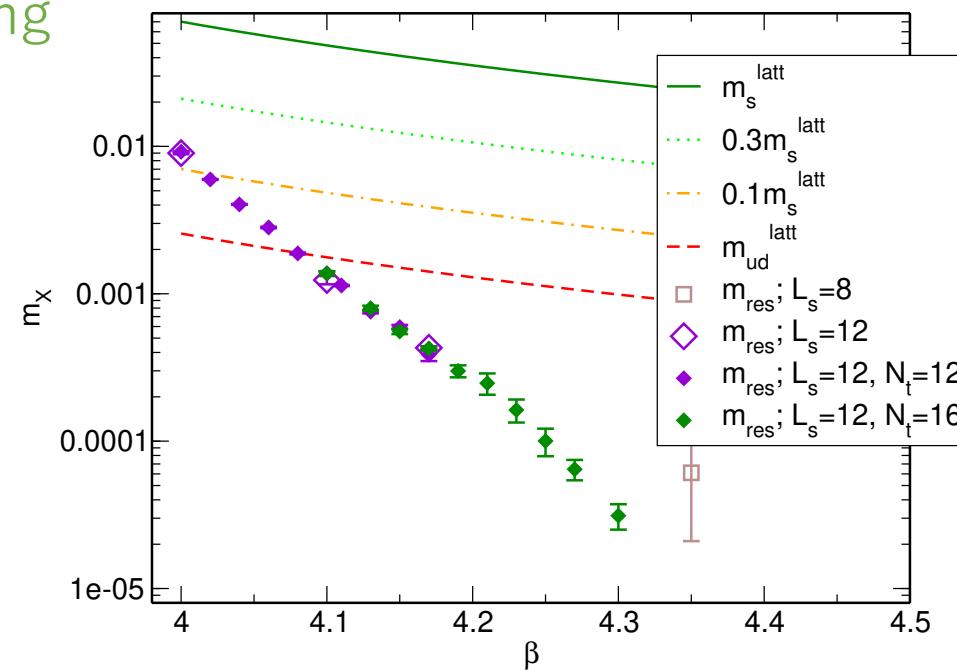
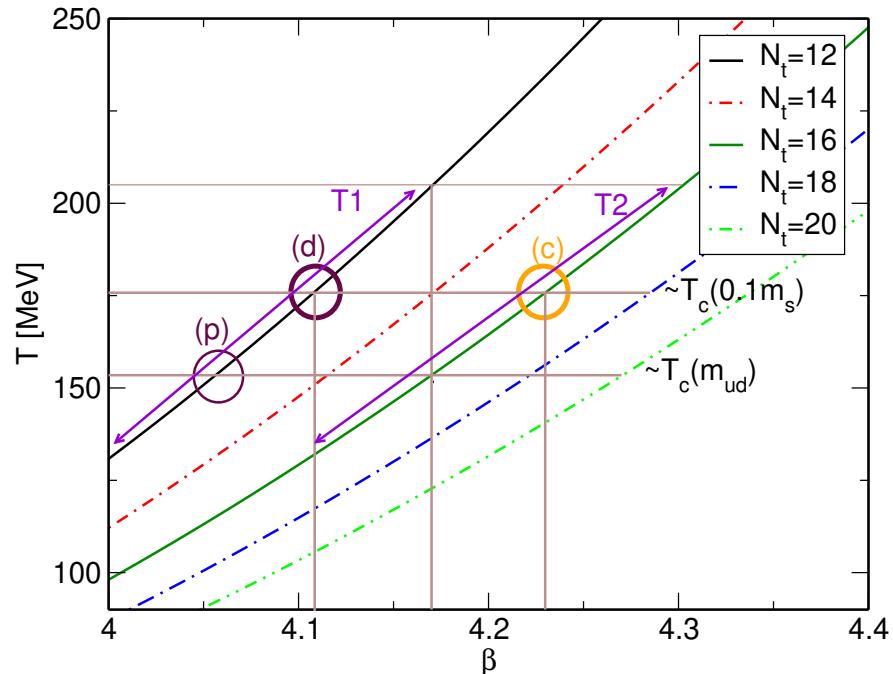
- Möbius DWF \rightarrow OVF by reweighting
 - Successful (w/ error growth) at $\beta = 4.17$ ($a \simeq 0.08$ fm)
 - See Lattice 2021 JLQCD (presenter: K.Suzuki)
 - Questionable for
 - Coarser lattice: rough gauge, DWF chiral symmetry breaking
 - Finer lattice: larger V (# sites)
- Chiral fermion with 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)
- $m_{res}[\text{MeV}] \sim a^X$, where $X \sim 5$
 - Vanishes quickly as $a \rightarrow 0$
 - 1st (dumb) approximation: forget about m_{res}
 - Better : $m_f^{cont} \leftrightarrow (m_f + m_{res})$ but, this is not always enough



Simulation plan: 2nd round w/ treatment of m_{res} effect

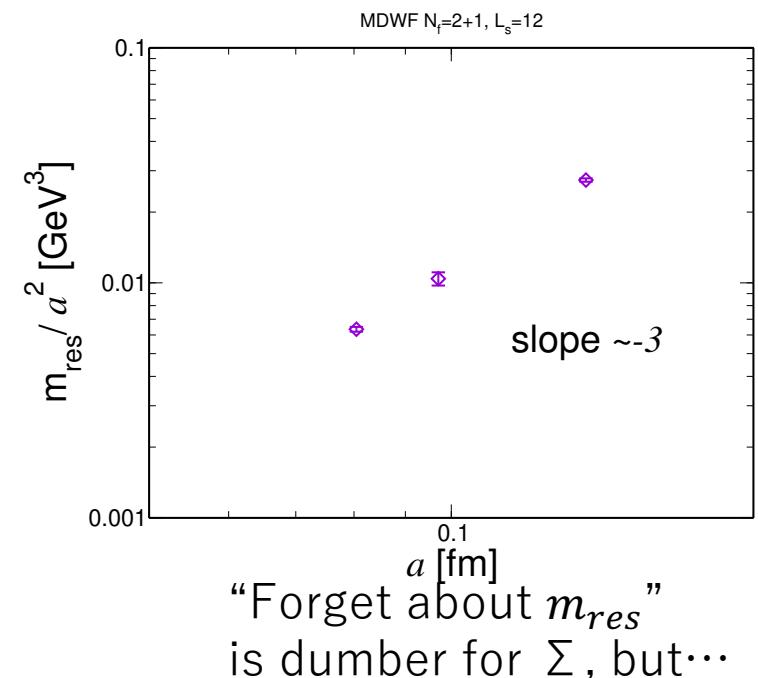
$L_s = 12$ fixed throughout this study

- T1-(d)
 - $N_t = 12$
 - $m_l = 0.1m_s$
 - $m_q^{input} = m_q^{LCP} - m_{res}$
 - $V_s = 24^3, 36^3$
- T2-(c)
 - $N_t = 16$
 - $m_l = 0.1m_s$
 - m_{res} shift by reweighting
 - $V_s = 32^3$
- T1-(p)
 - $N_t = 12$
 - $m_l = m_{ud}$
 - $m_q^{input} = m_q^{LCP} - m_{res}$
 - $V_s = 36^3, 48^3$
- T1-(q)
 - $N_t = 16$
 - $m_l = m_{ud}$
 - $m_q^{input} = m_q^{LCP} - m_{res}$
 - $V_s = 48^3$



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

- $\Sigma|_{DWF} \sim C_D \frac{m_f + xm_{res}}{a^2} + \Sigma|_{cont.} + \dots$ S. Sharpe (arXiv: 0706.0218)
- $m_{res} \neq xm_{res}$; $x = O(1) \neq 1$
 - “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 very expensive proposition.”
– S. Sharpe.
- $\Sigma|_{DWF} \rightarrow C_D \frac{xm_{res}}{a^2} + \Sigma|_{cont.} + \dots ; (m_f \rightarrow 0)$
- $\Sigma|_{DWF} \rightarrow C_D \frac{-(1-x)m_{res}}{a^2} + \Sigma|_{cont.} + \dots ; (m_f \rightarrow -m_{res})$



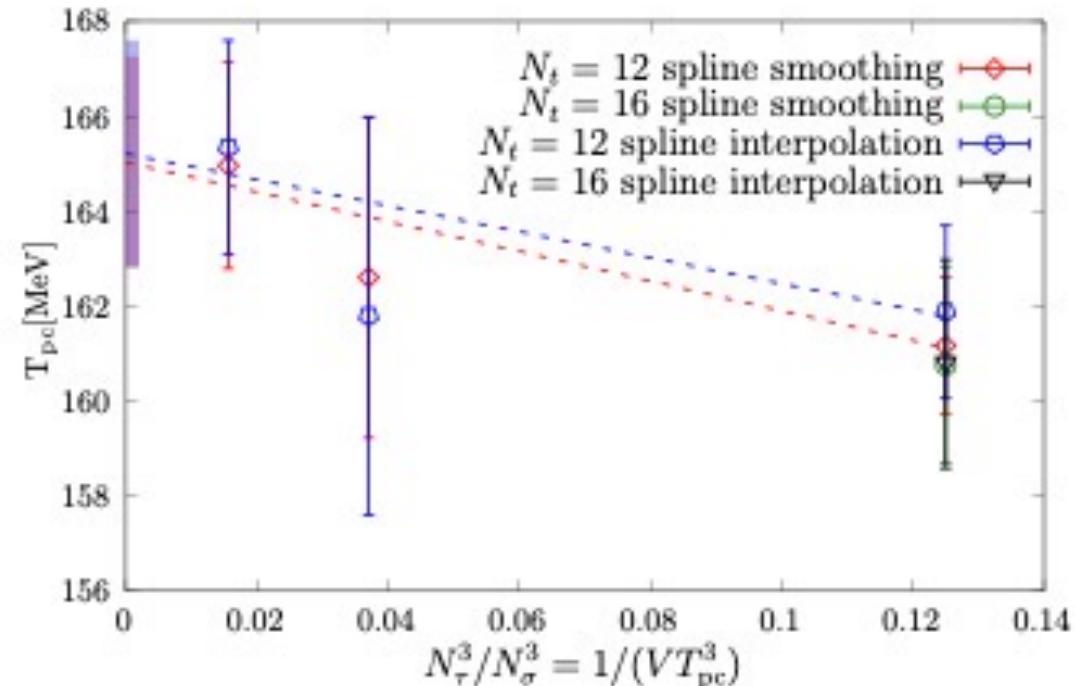
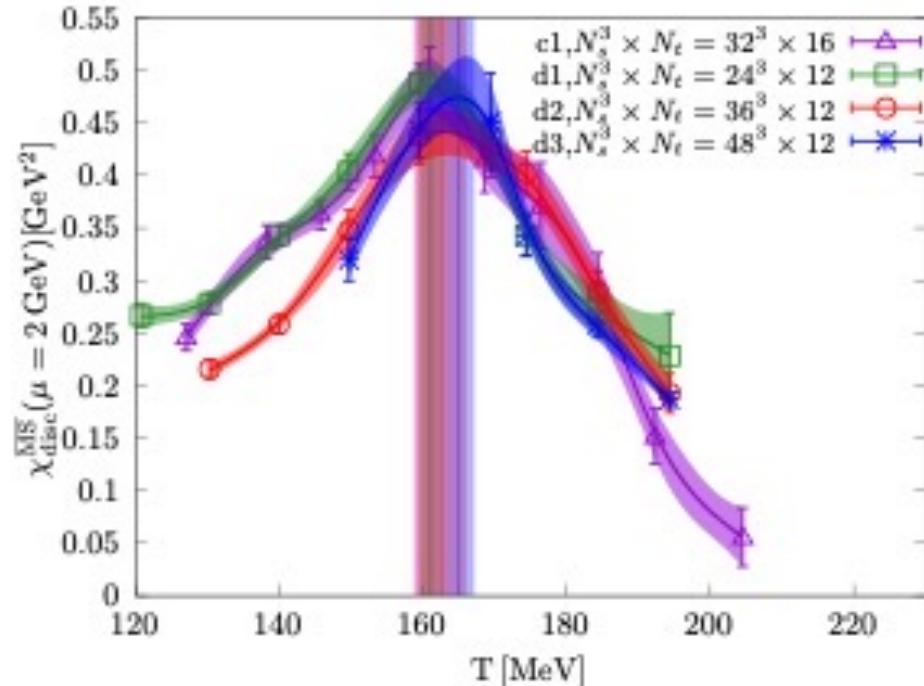
Light quark $\Sigma = -\langle \bar{\psi}\psi \rangle$:

no power div. in disconnected susceptibility

- $\chi_{disc} = \langle \bar{u}u \cdot \bar{d}d \rangle - \langle \bar{u}u \rangle \langle \bar{d}d \rangle$
 - power divergence in $\langle \bar{\psi}\psi \rangle$ cancels out
 - no new divergence over Σ 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
- $\chi_{total} = \langle \bar{\psi}\psi \cdot \bar{\psi}\psi \rangle - \langle \bar{\psi}\psi \rangle \langle \bar{\psi}\psi \rangle$
 - has power divergence everywhere
 - needs to understand the power divergence of $\Sigma = -\langle \bar{\psi}\psi \rangle$ first

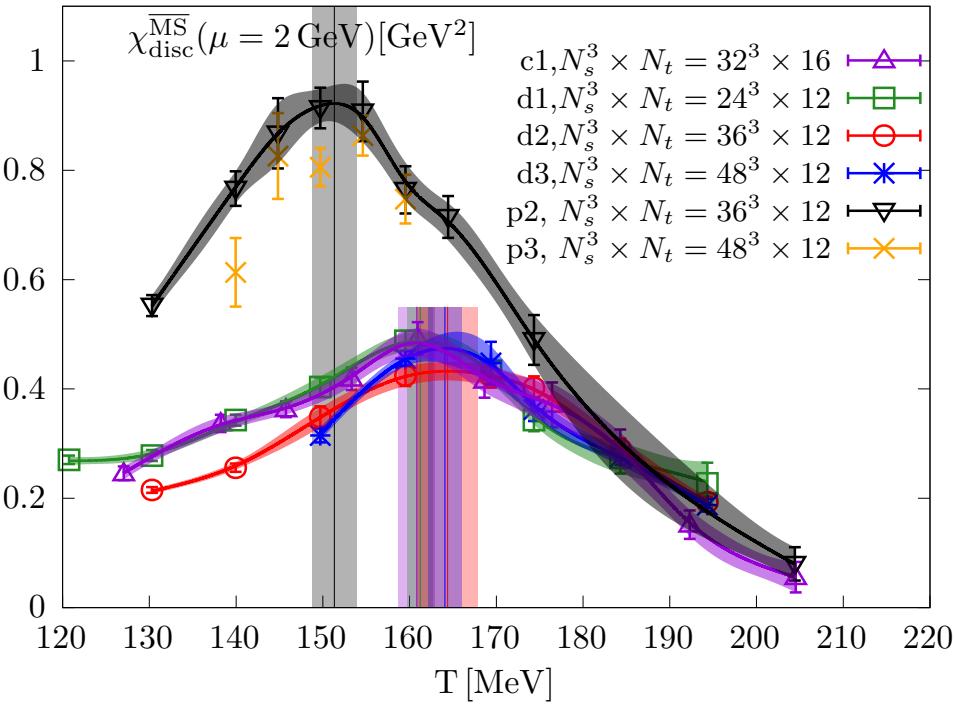
Chiral susceptibility (disconnected)

$m_l = 0.1m_s$ (about 3 time larger than physics u,d mass)



- no subtraction needed in addition to vacuum subtraction
- peak position : mild volume dependence \rightarrow 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..

$$m_l = m_s/10$$

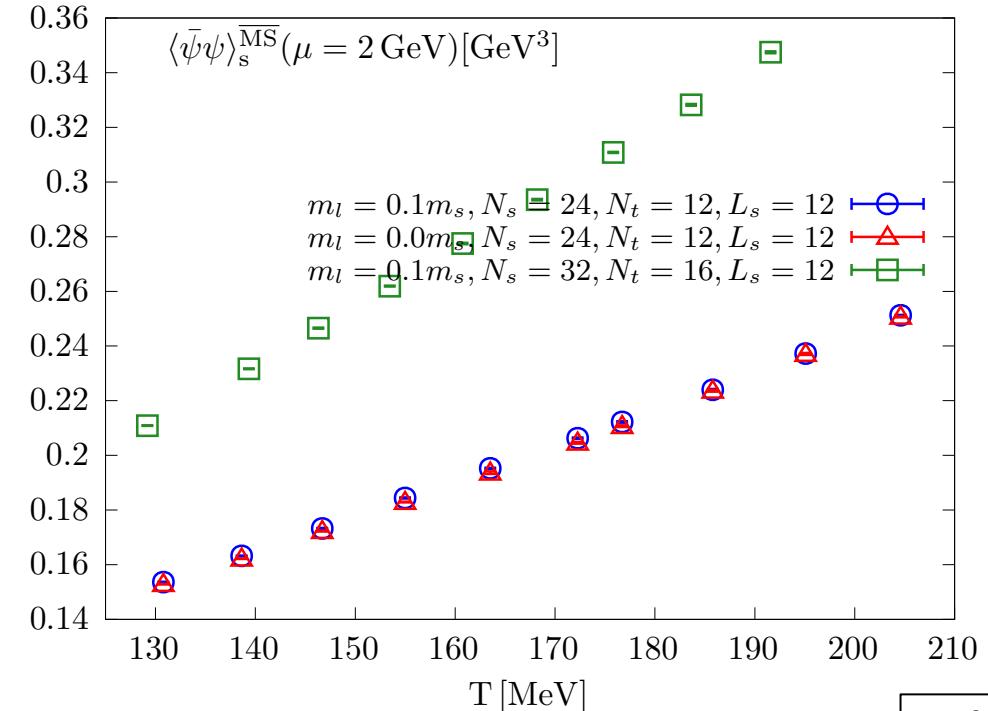
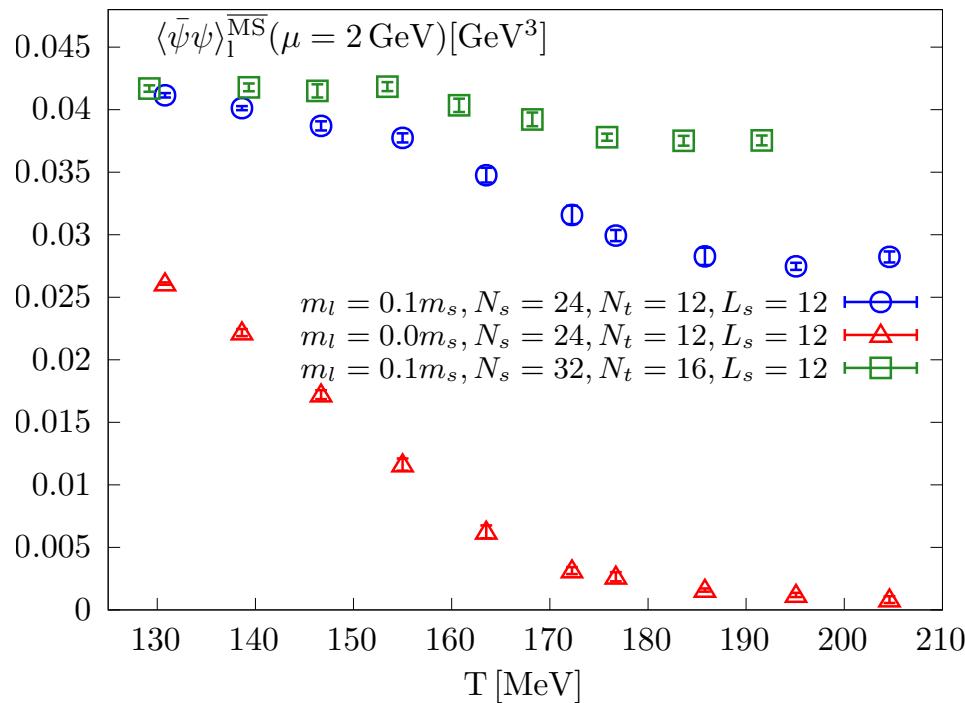
- d1,d2,d3 : $N_t = 12$, LT=2,3,4
- c1 : $N_t = 16$, LT=2
- good scaling $N_t = 12 - 16$ observed for LT=2

$$m_l = m_{ud}$$

- p2,p3: $N_t=12$, aspect ratio LT = 3, 4
 - Statistics is $\sim 20,000$ 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)
 - $T_{pc} = 156.5 (1.5)$ w/ HISQ by HotQCD (2019)
 - $T_{pc} = 158.0 (0.6)$ w/ stout staggered by Budapest-Wuppertal (2020)

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

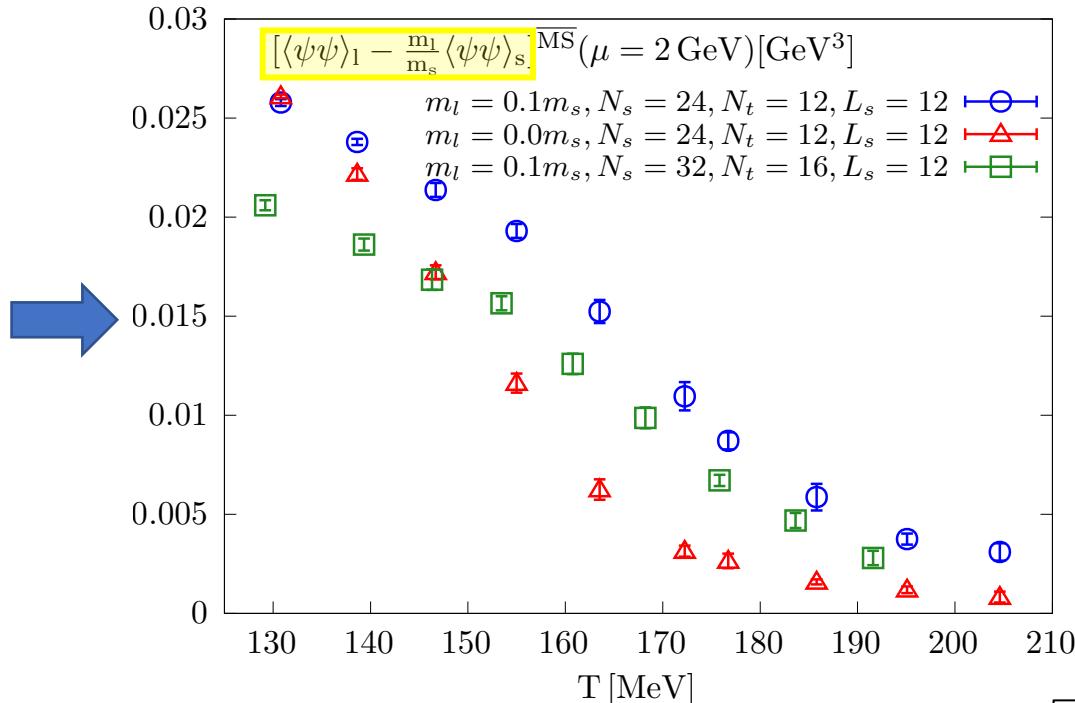
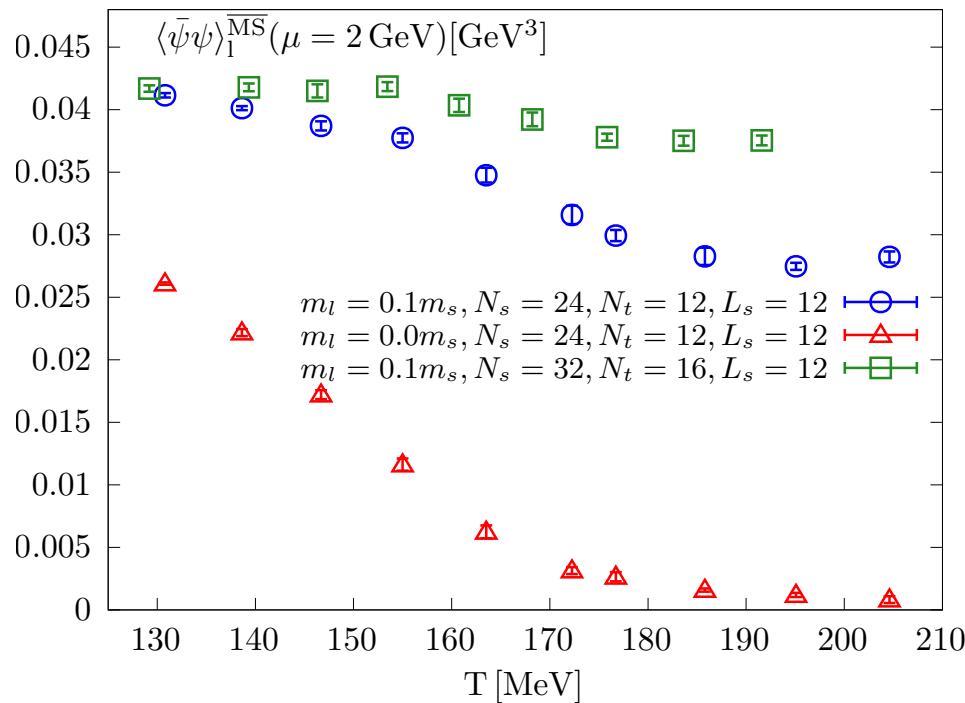
- Two step UV renormalization necessary (naively)
 - Logarithmic divergence (multiplicative): $Z_S(\overline{MS}, 2 \text{ GeV})$
 - Power divergence (additive): $\propto m_f a^{-2}$
 - Subtracted using $\langle \bar{s}s \rangle$



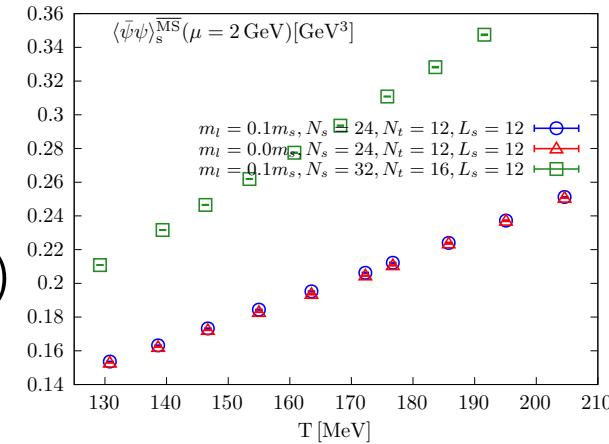
Before “step 4”

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

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



Before “step 4”

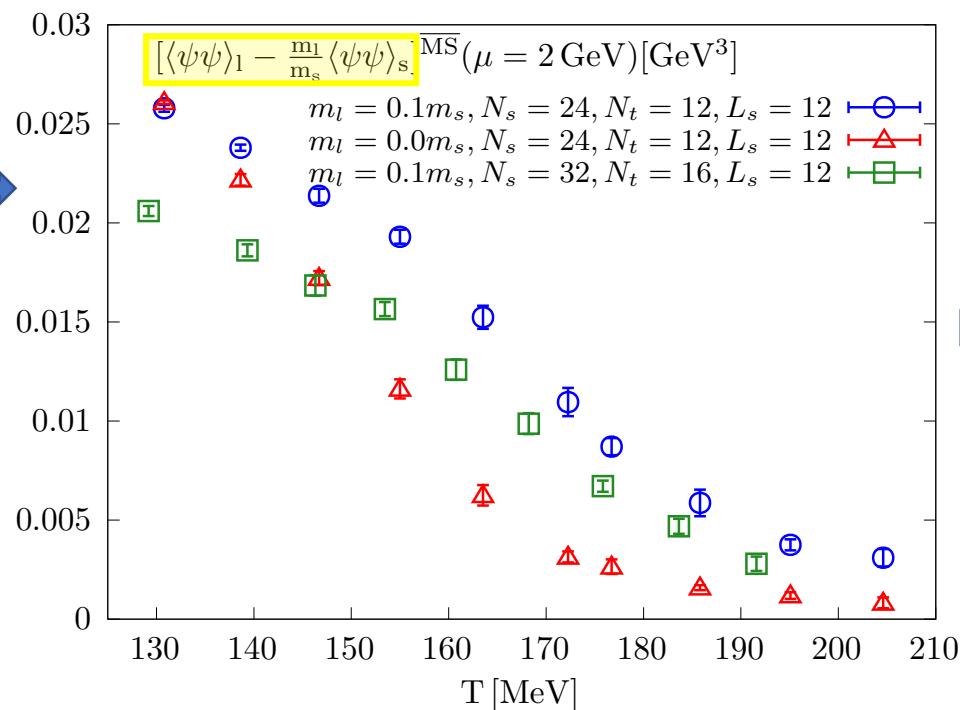
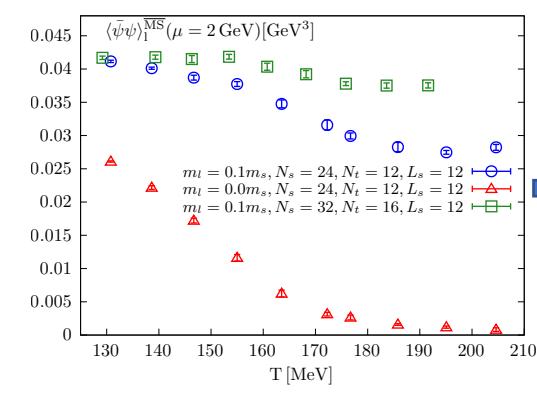


Light quark $\Sigma = -\langle \bar{\psi}\psi \rangle$

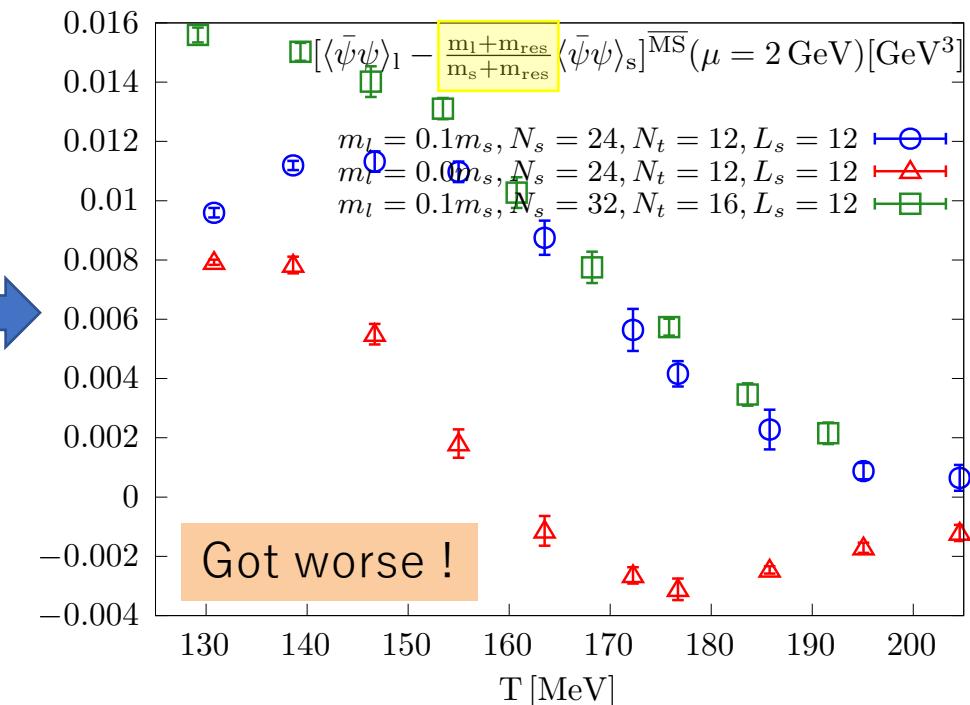
- Two step UV renormalization necessary (naively)
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 - Subtracted using $\langle \bar{s}s \rangle$

$$m_{res} = \frac{\langle 0 | J_{5q} | \pi \rangle}{\langle 0 | P | \pi \rangle}$$

$$m_\pi^2 \propto (m_f + m_{res})$$



Origin of subtraction: $m_l = 0$



Origin of subtraction: $m_l = -m_{res}$

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

- $\Sigma|_{DWF} \sim \frac{m_f + xm_{res}}{a^2} + \Sigma|_{cont.} + \dots$ S. Sharpe (arXiv: 0706.0218)

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

- “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 very expensive proposition.” – S. Sharpe.

- We propose another way to estimate xm_{res} using m'_{res}

If chiral symmetry is restored $\rightarrow \Sigma|_{cont.} = 0$

$\rightarrow m_f = -xm_{res}$ is a **zero** of $\Sigma|_{DWF}$ which is **related** with

$$(large \ t) \quad m'_{res} = \frac{\sum_x \langle J_{5q}(x) P(0) \rangle}{\sum_x \langle P(x) P(0) \rangle}$$

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

$m_f = -m'_{res}$ 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: $\Delta_\mu \langle A_\mu(x) P(0) \rangle = 2m_f \langle P(x) P(0) \rangle + 2 \langle J_{5q}(x) P(0) \rangle - 2 \sum \delta_{x,0}$

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

- $\Sigma|_{DWF} = C_D \frac{m_f + xm_{res}}{a^2} + \Sigma|_{cont.} + \dots$ S. Sharpe (arXiv: 0706.0218)

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

- “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 very expensive proposition.“ – S. Sharpe.

- Yet another way for the subtraction including xm_{res} using $N_f = 3, T = 0$ information
→ see the talk by Yu Zhang

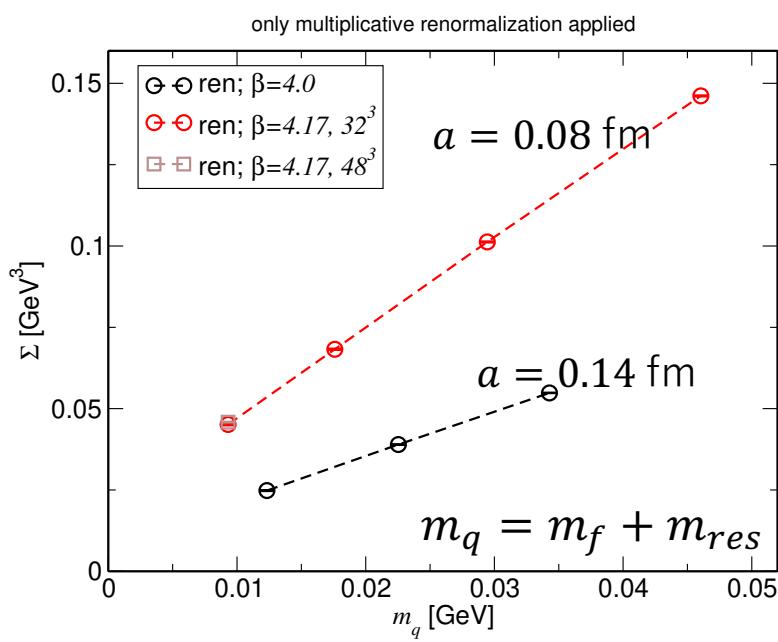
1. Prepare several different lattice spacing
2. Compute coefficient linear in m_f : $\Sigma|_{DWF} \sim const. + (\frac{C_D}{a^2} + C_R)m_f + \dots$
3. Separate divergent term : $linear fit in a^2 of. C_D + a^2 C_R \rightarrow C_D = 0.37(2)$
4. Estimate x through $\Sigma|_{DWF} \rightarrow \frac{-C_D(1-x)m_{res}}{a^2}$ for $m_f \rightarrow -m_{res}$ at $T > T_c$

this is meant to impose renorm. cond. $\Sigma|_{cont.} = 0$

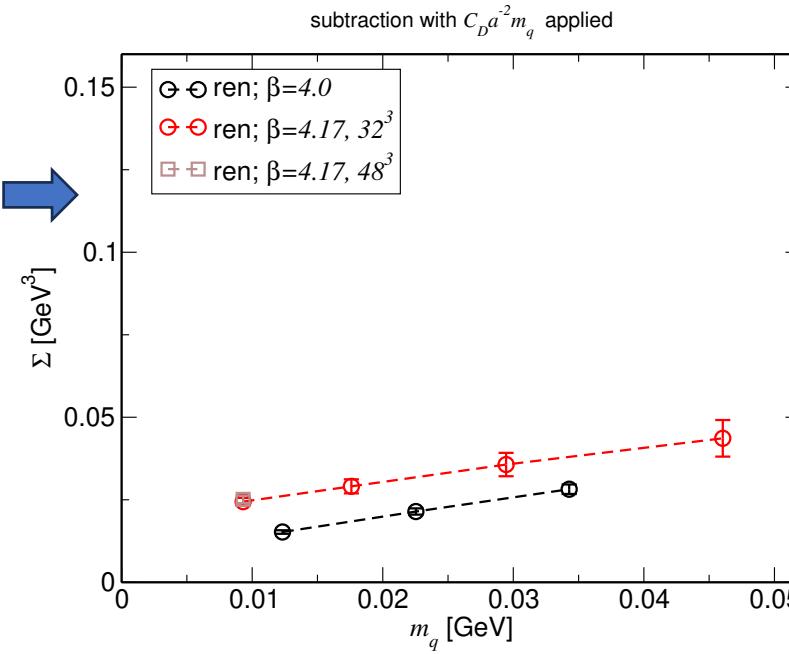
→ $N_f = 3; \beta = 4.0$ estimate: $x = -0.6(1)$

- In general, x may depend on β , for now use this value as a reference for all β
- We also use C_D (single flavor normalization) of $N_f = 3$ for $N_f = 2 + 1$

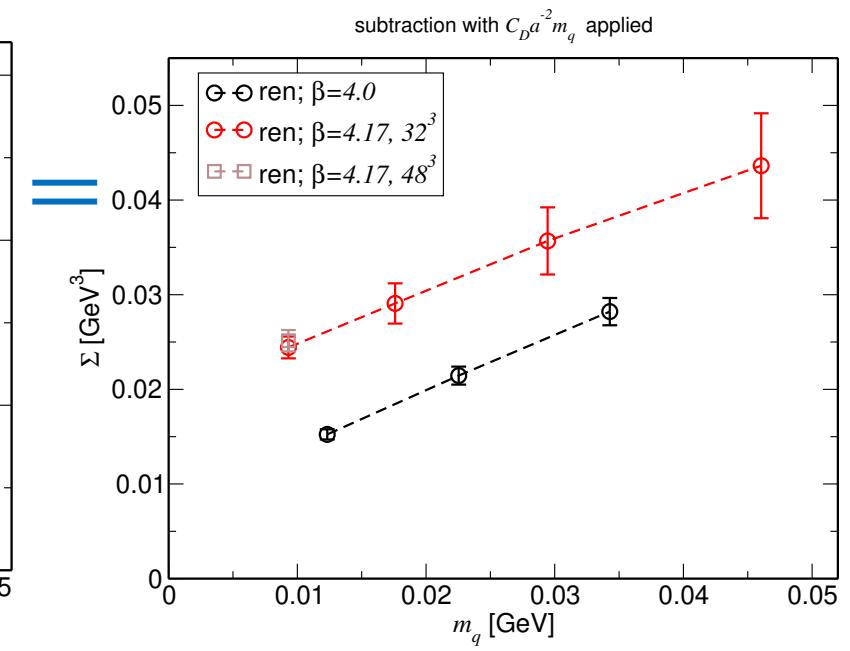
test on $N_f = 2 + 1, T = 0$ measurements



only multiplicative
renormalizations applied

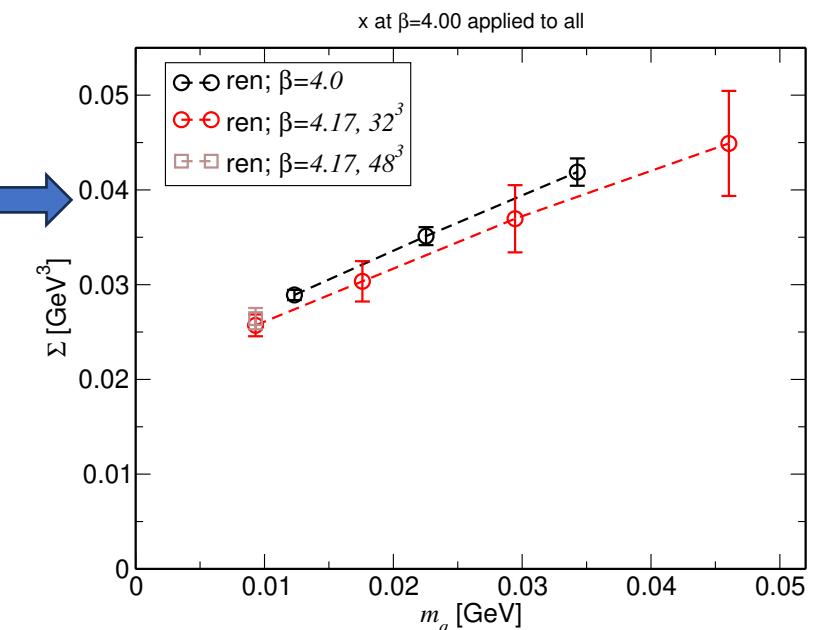
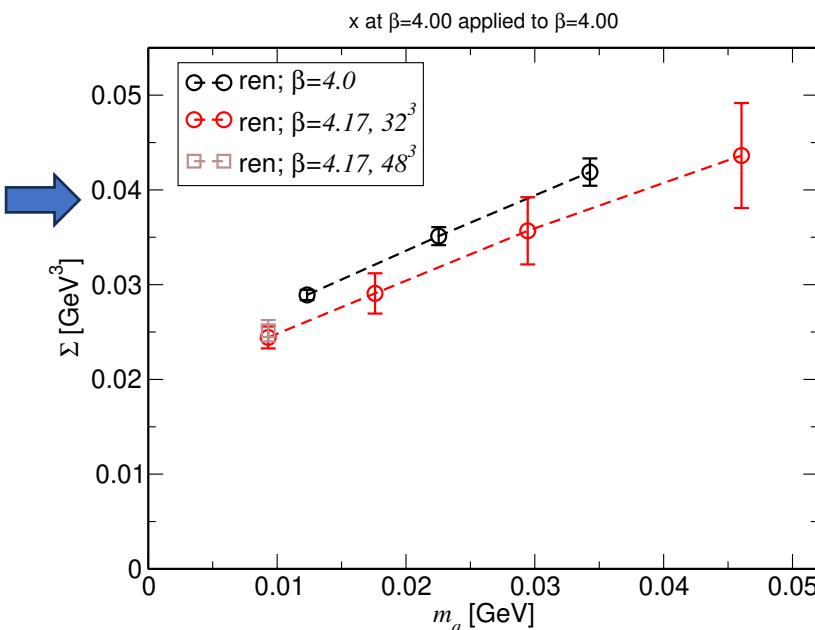
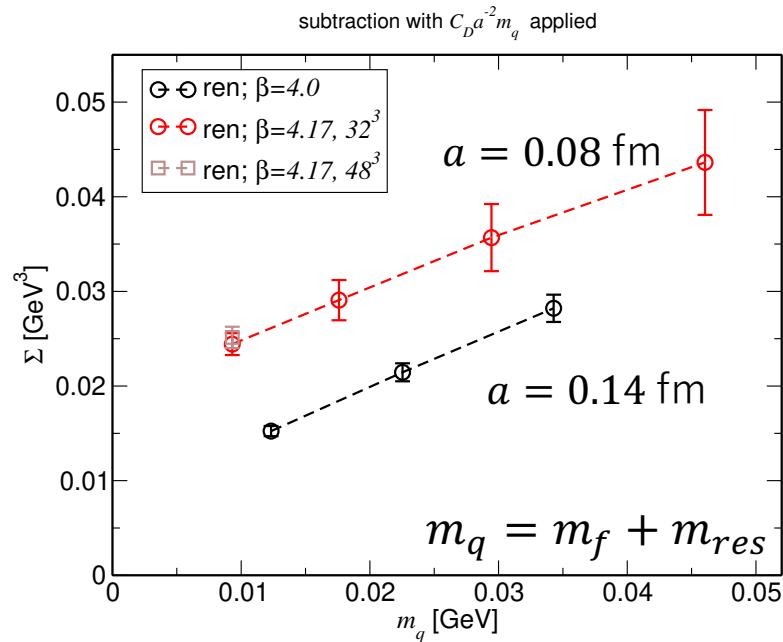


$C_D a^{-2} m_q$ subtraction applied



changing y-axis range

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



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

$C_D a^{-2}(1 - x)m_{res}$ subtraction applied only to $\beta = 4.0$

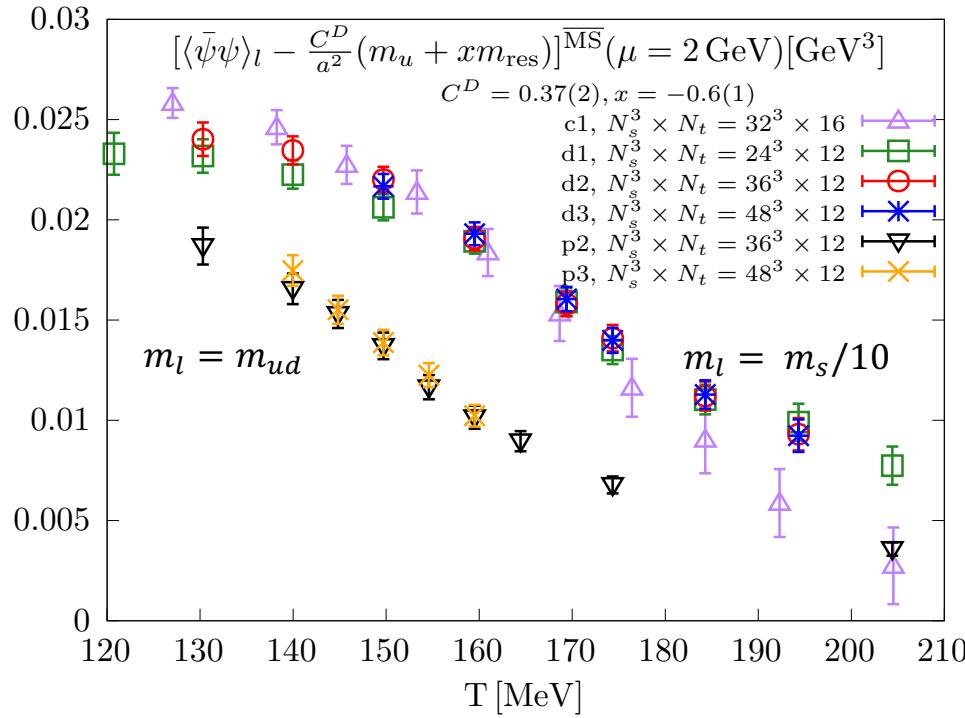
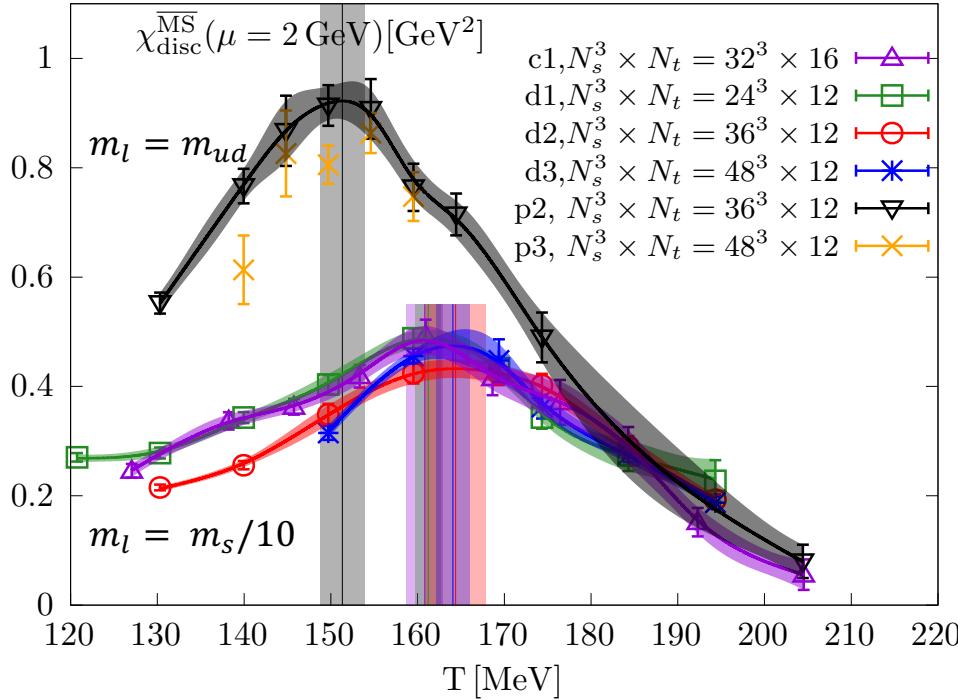
$C_D a^{-2}(1 - x)m_{res}$ subtraction applied to all assuming x is universal

Seemingly, both conventional and residual divergence are controlled, but

- need to check if x does not depend much on β
- refinement of precision and check applicability range of C_D necessary

Disconnected chiral susceptibility and chiral condensate

all divergences subtracted assuming x is universal

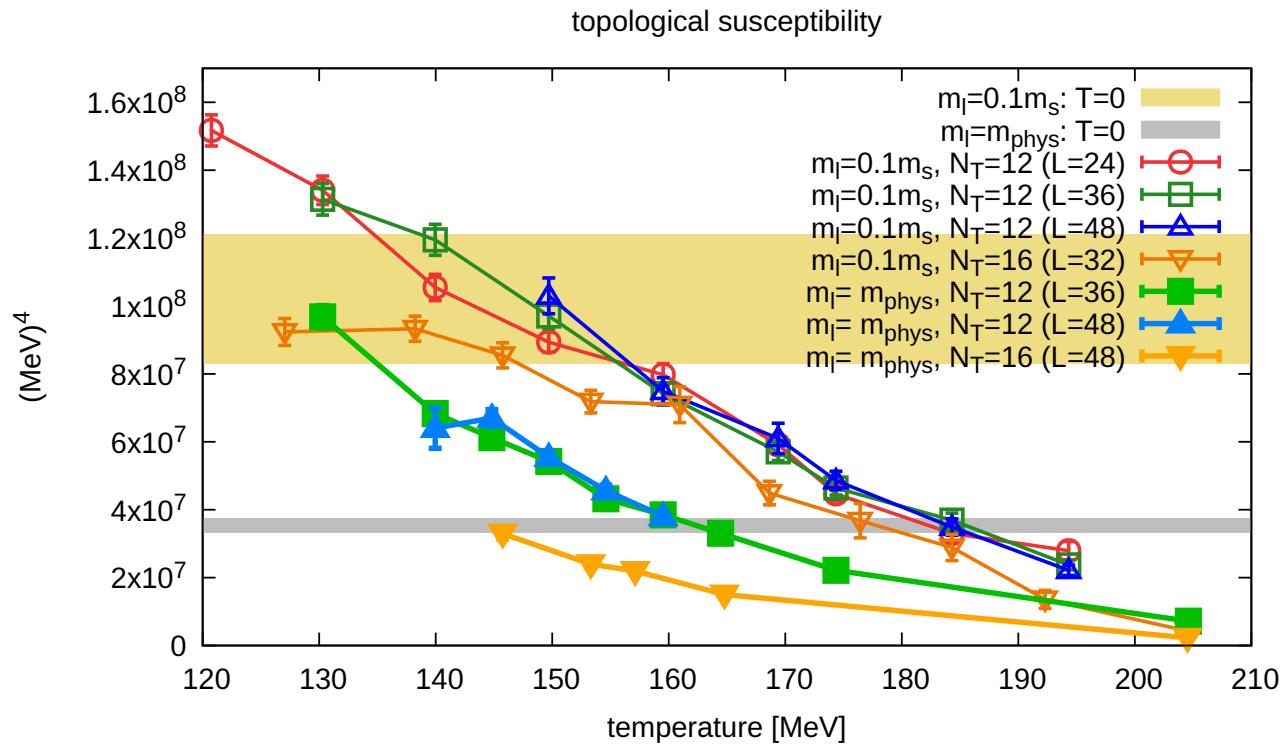


Likely NO phase transition at physical point with chiral fermions.
No surprise happened so far..

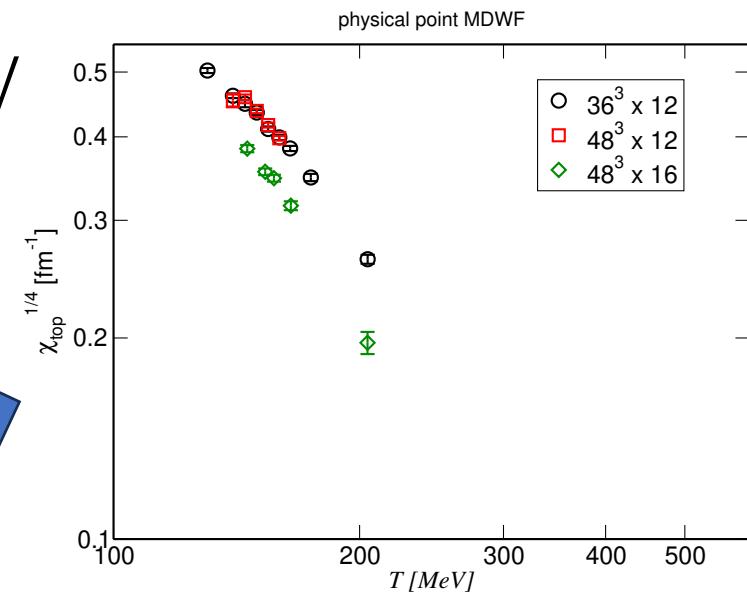
$m_l = m_{ud}$

- p2,p3: $N_t=12$, aspect ratio $LT = 3, 4$
 - Statistics is $\sim 20,000$ 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

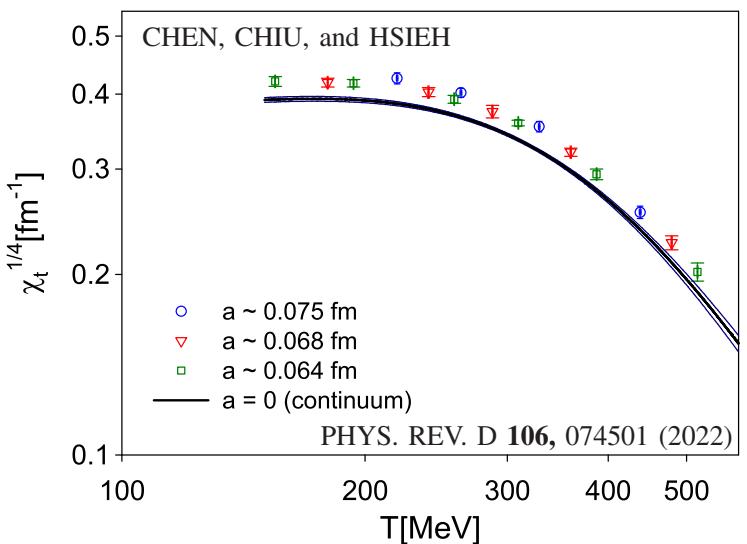
topological susceptibility



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

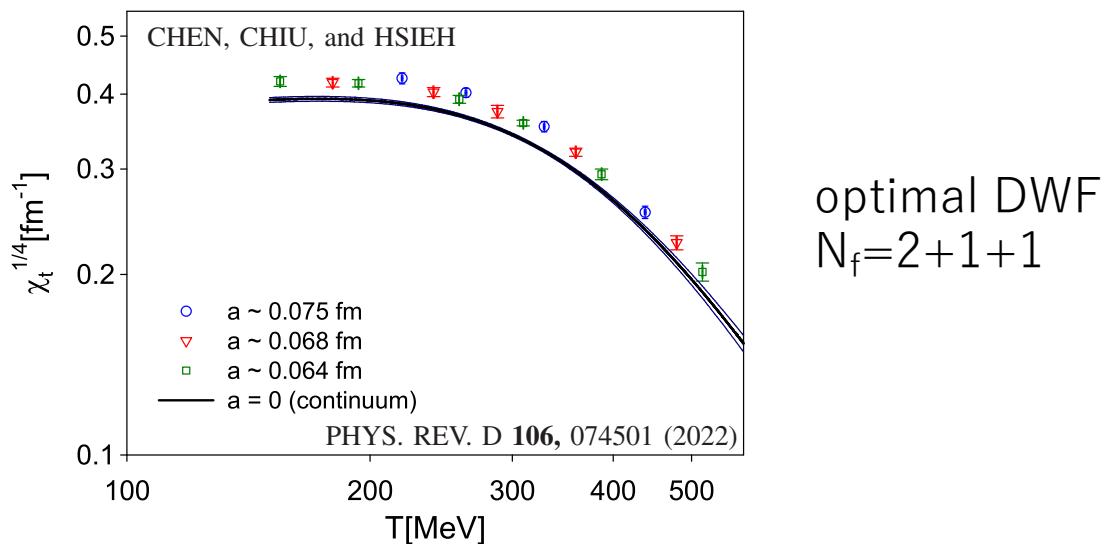
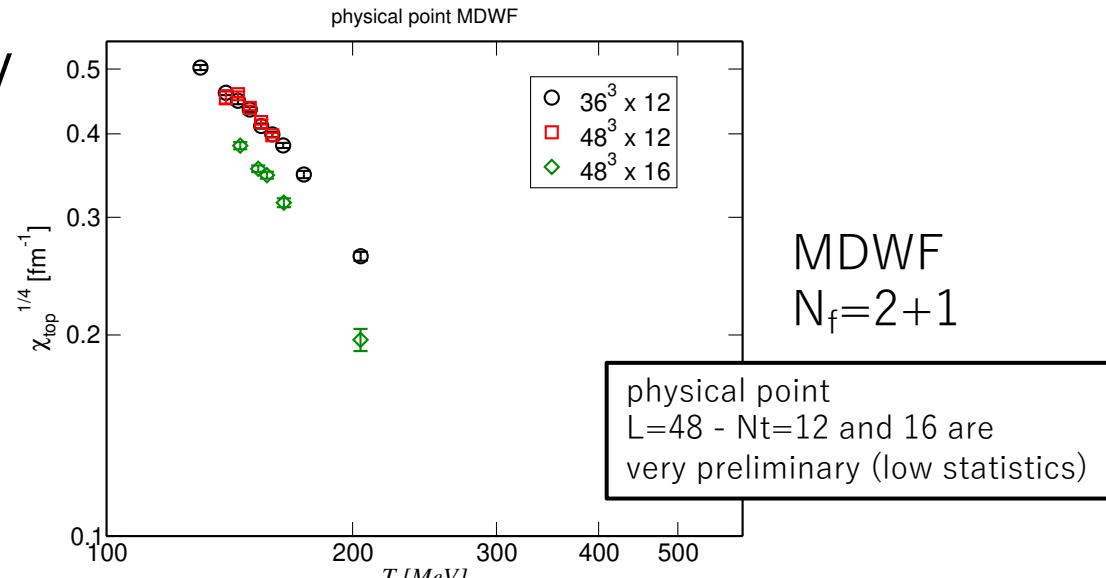
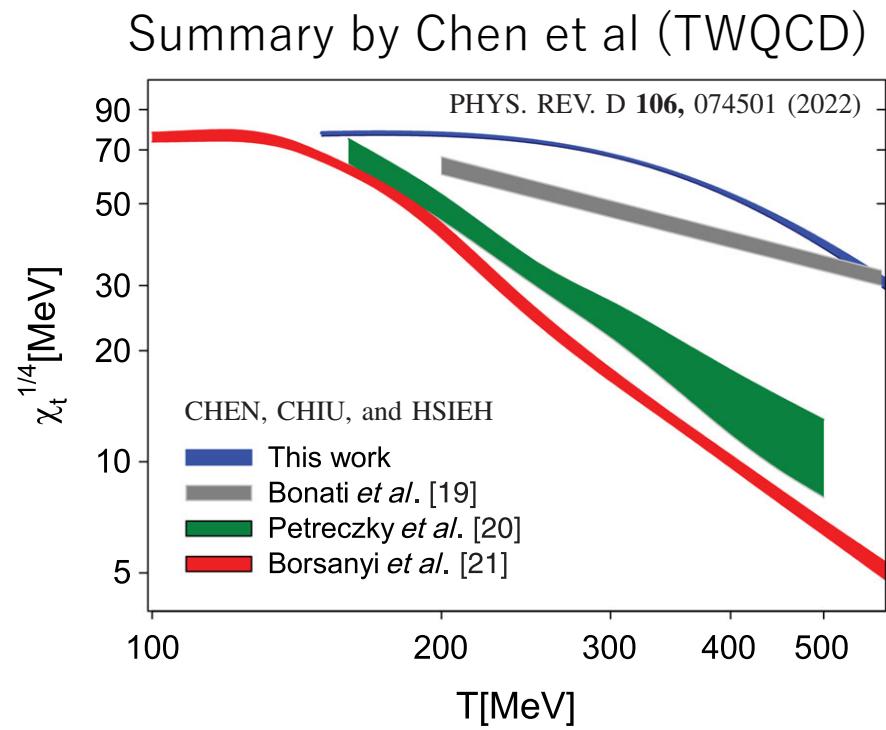


MDWF
 $N_f = 2+1$

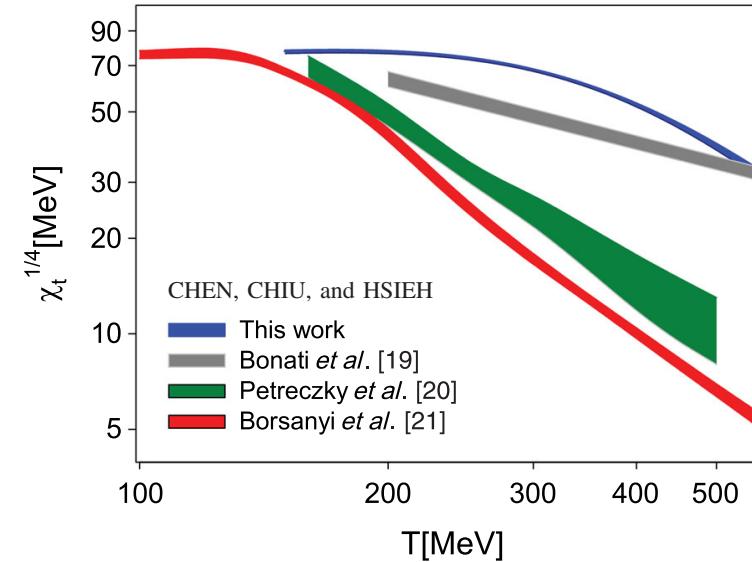
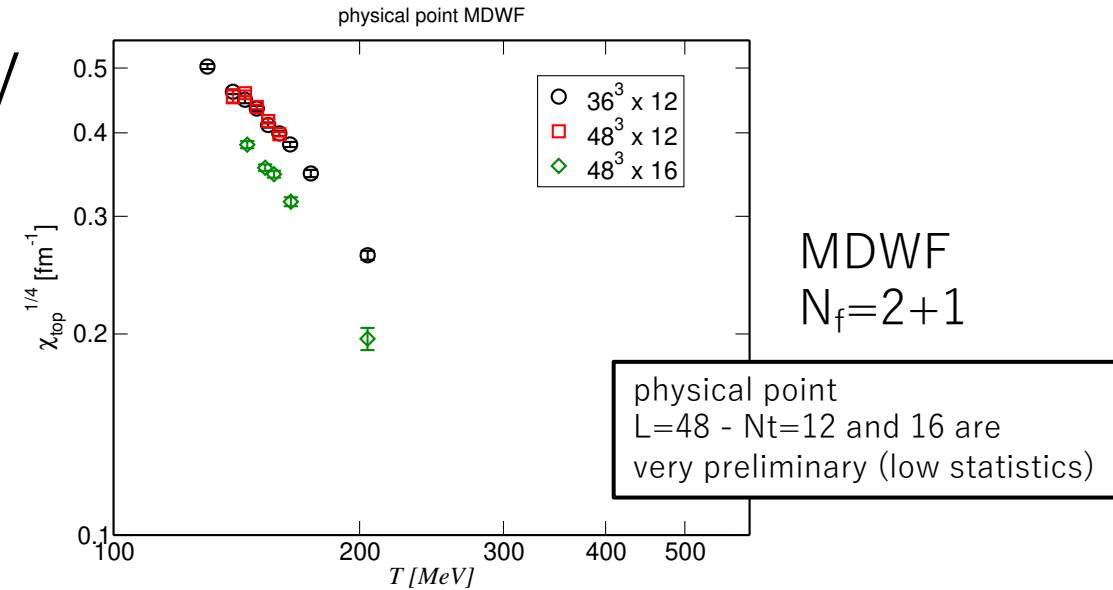
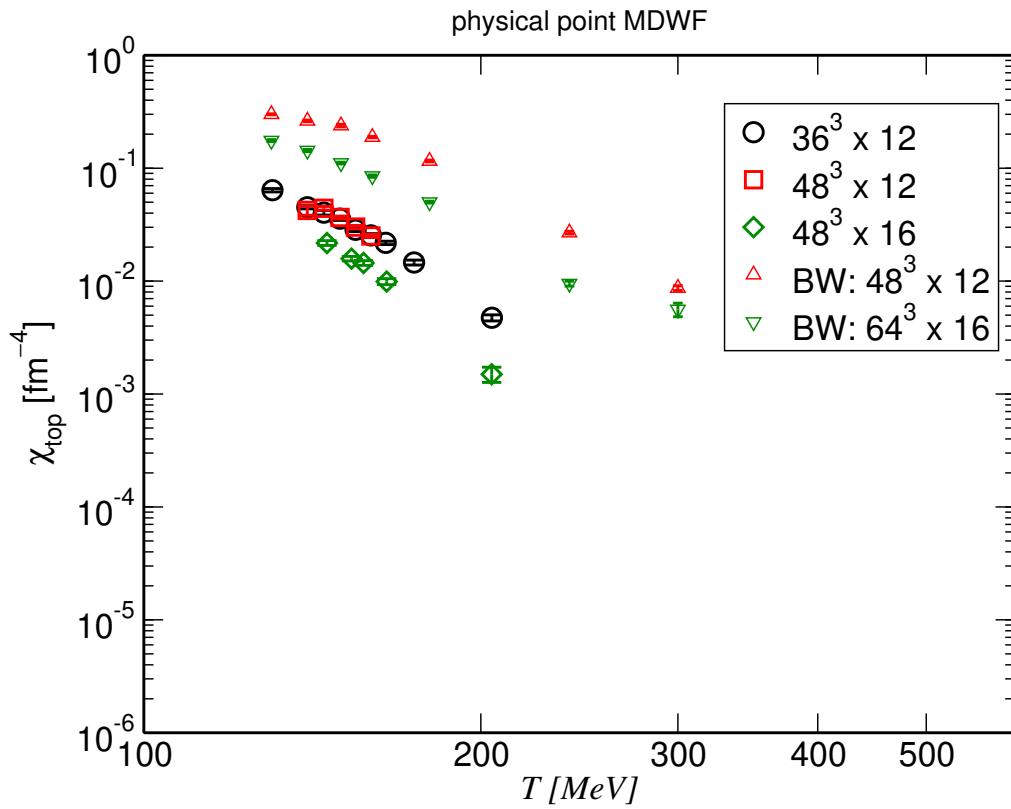


optimal DWF
 $N_f = 2+1+1$

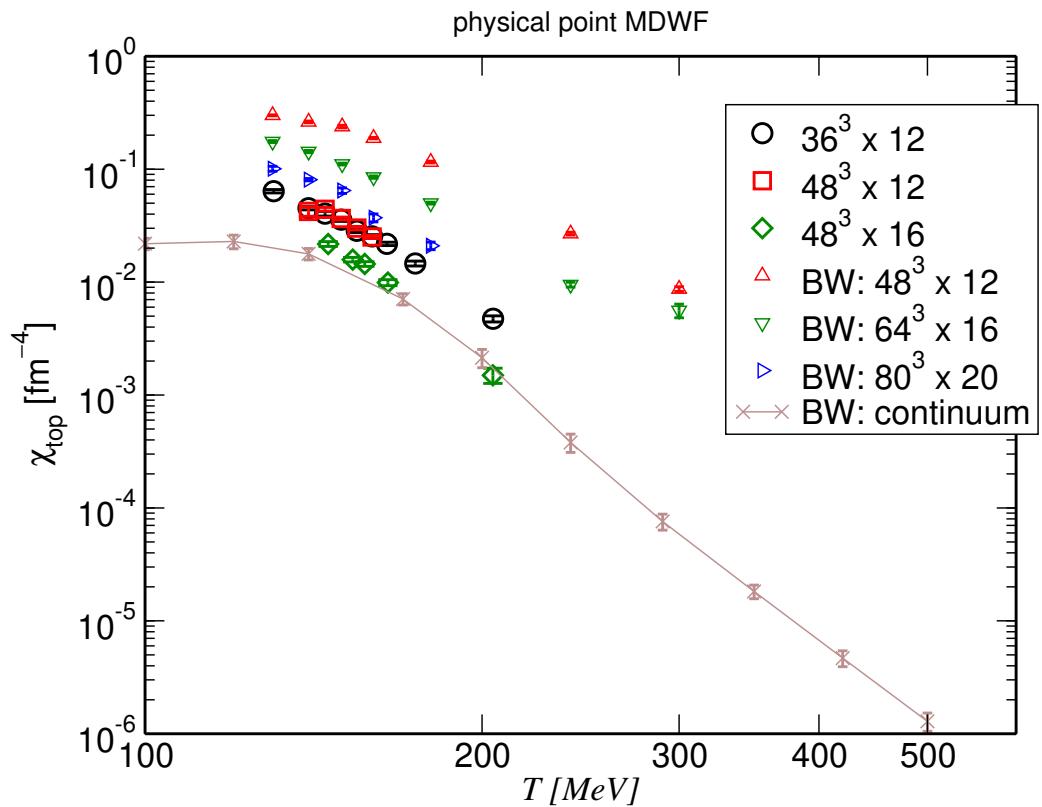
topological susceptibility



topological susceptibility

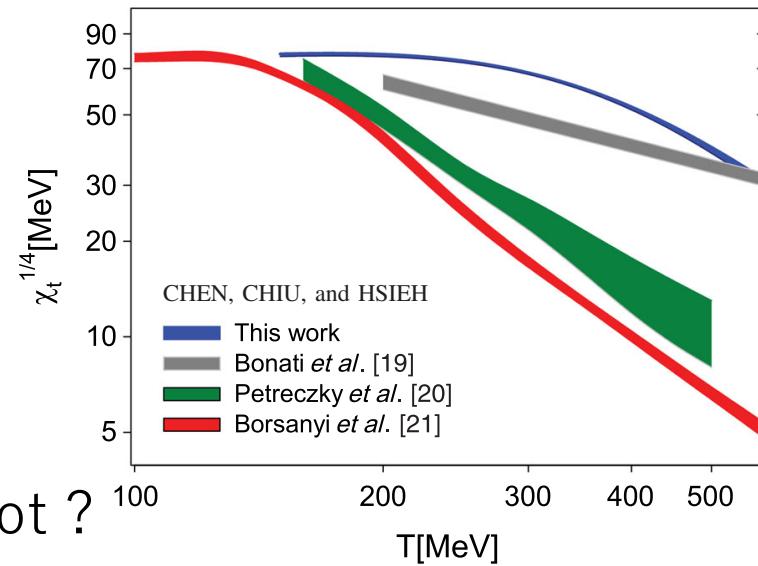
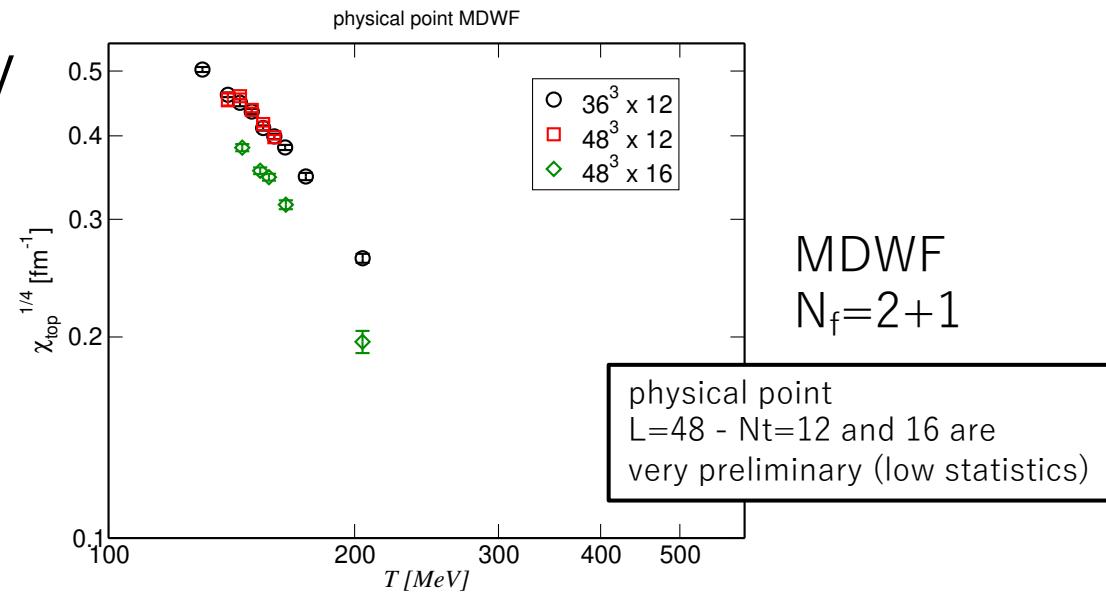


topological susceptibility



MDWF(JLQCD) χ_t at physical point

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



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, $T_{pc} \approx T_{pc}$ (staggered)
- machinery to treat power divergence, residual chiral symmetry effect is being finalized
- seemingly the both type of divergence are under control using Nf=3 results
- further improvement underway
- Disconnected chiral susceptibility show no hint of phase transition for Nt=12
 - $T_{pc} \approx T_{pc}$ (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
- 48^3 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. Lattice 2024 talk by Goswami on charge fluctuation