QCD thermodynamics on the physical point with 2+1 flavor Möbius domain wall fermions

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

Acknowledgements

Codes used:

- Grid (HMC)
- BQCD (Measurements)
- Bridge++ (Measurements)
- Hadrons (Measurements)

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- KAKANHI – (FY2020-2024) - QCD phase diagram explored by chiral fermions – 20H01907
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- supercomputer **Fugaku** at R-CCS (hp210032,hp220108,hp220233; hp200130, hp230207)

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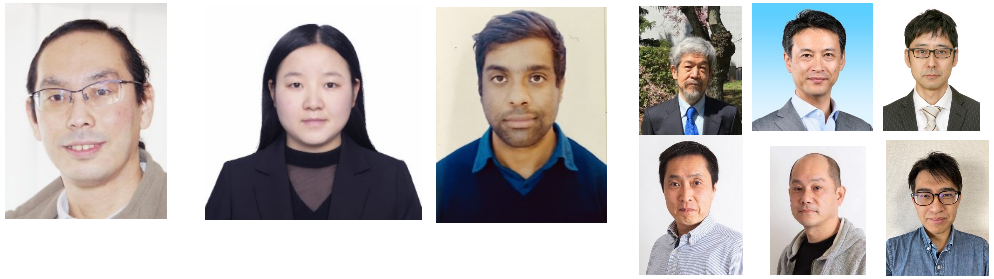
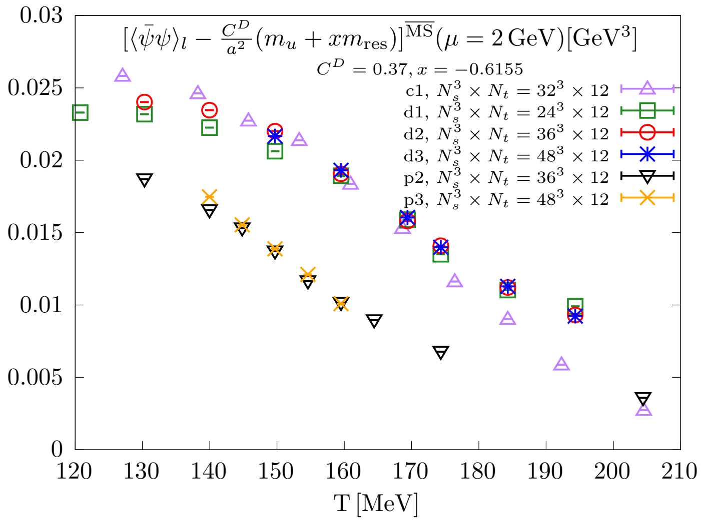
(3): KEK
(4): SOKENDAI
(5): Kobayashi-Maskawa Institute, Nagoya Univ.
(6): Bielefeld University

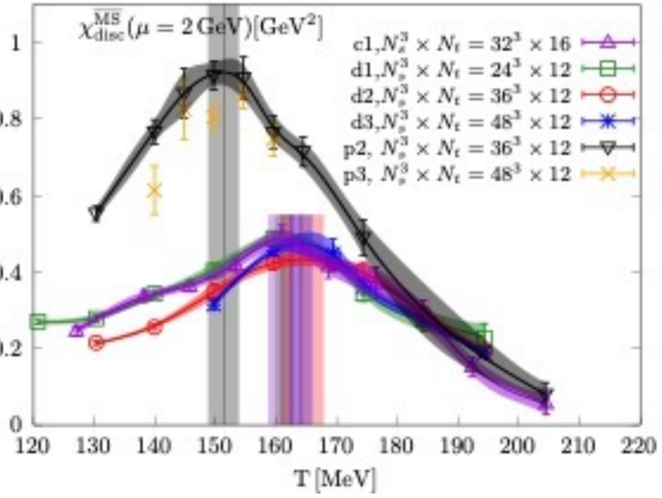
QCD phase transition near and on the physical point

- 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 →



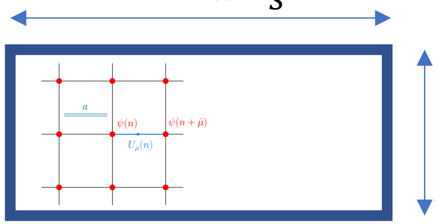


Modes of Simulations

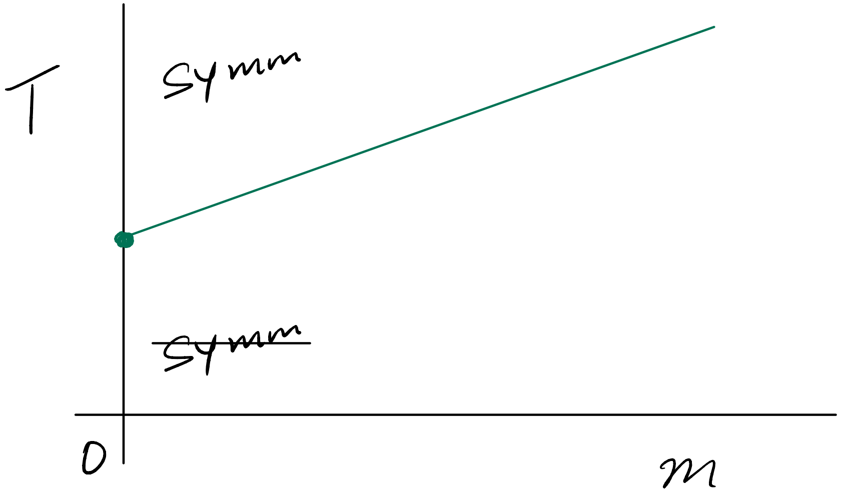
to locate phase transition

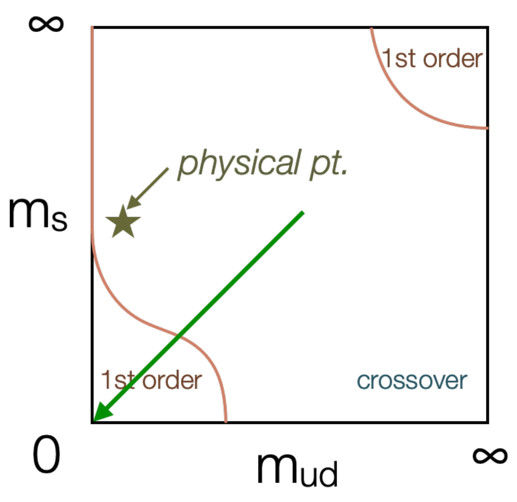
- tune parameters near transition
- ➢ T: fixed, change m
- ➢ m: fixed, change T

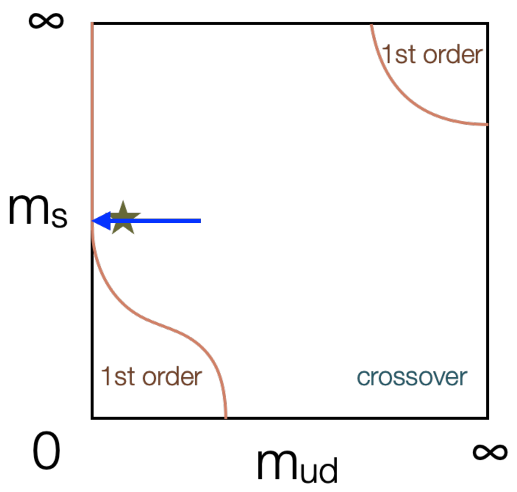
$L = aN_s$



$\frac{1}{T} = aN_t$







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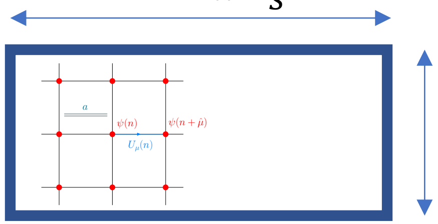

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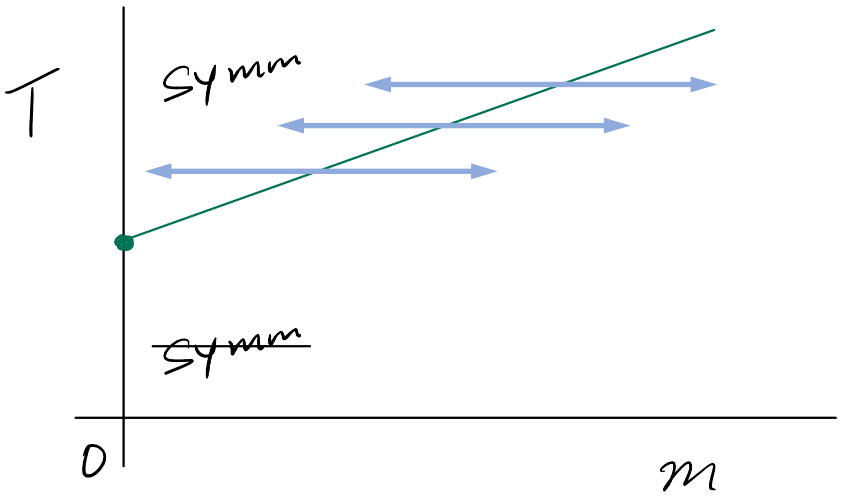
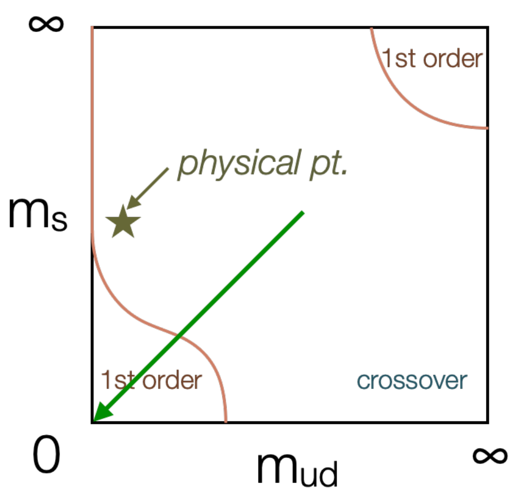
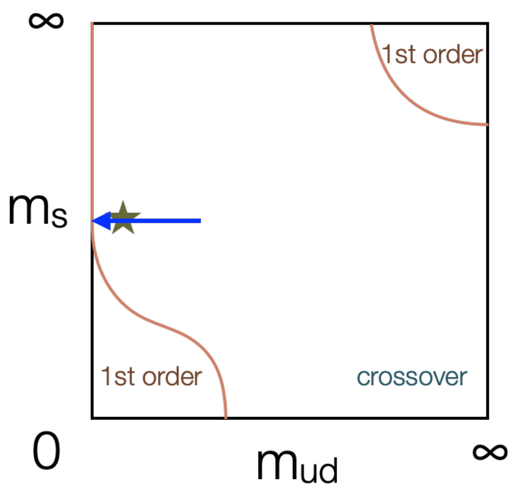






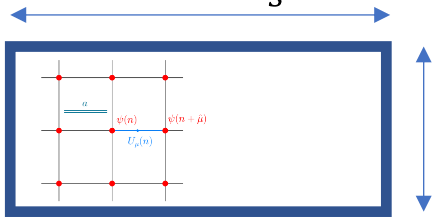
Modes of Simulations

Nf=2: Ward Thu. morning
Nf=3: Zhang Tue. morning

to locate phase transition

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

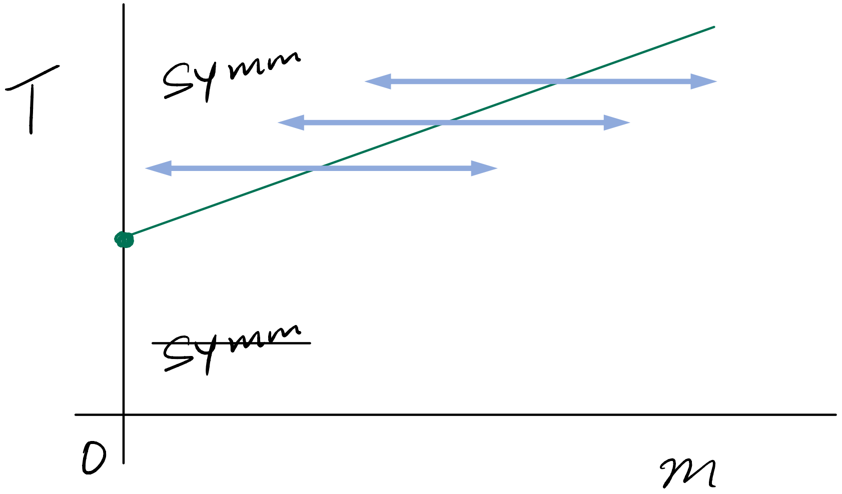
$L = aN_s$

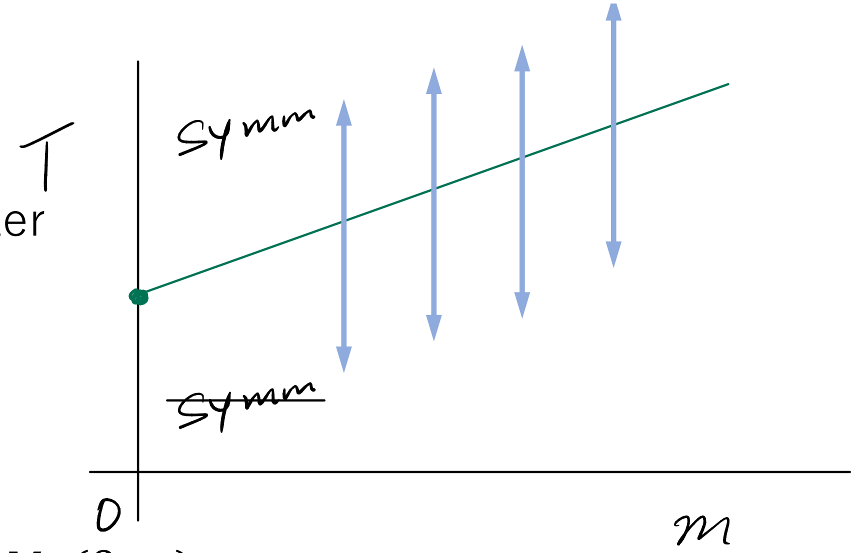


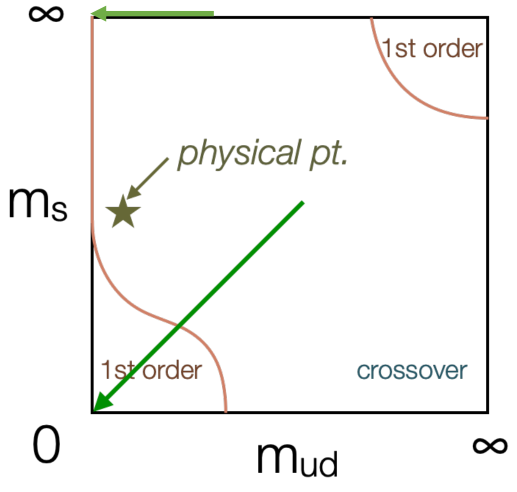
$$\frac{1}{T} = aN_t$$

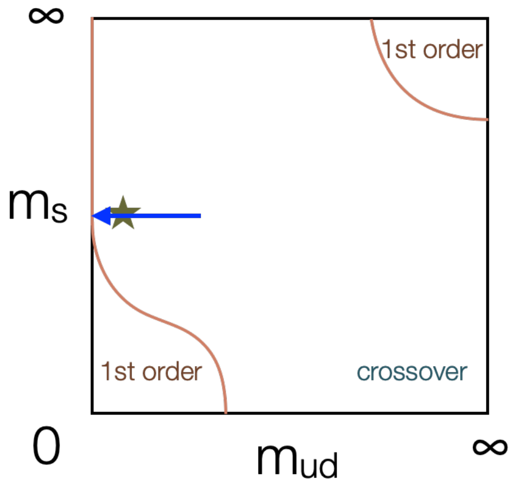
Fixing / changing the controlling parameter

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









N_f=2+1 Möbius DWF LCP for **FY2023-**

For the **L**ine of **C**onstant **P**hysics: $\boldsymbol{am_s(\beta)}$ with $\boldsymbol{a(\beta)}$

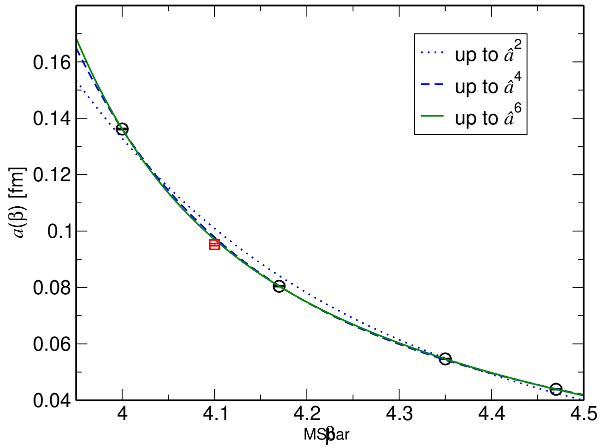
- Step 1: determine $\boldsymbol{a(\beta)}$ [fm] with t_0 (BMW) input
  - at $\beta = \mathbf{4.0}$, ~~4.1~~*, $4.17, 4.35, 4.47$

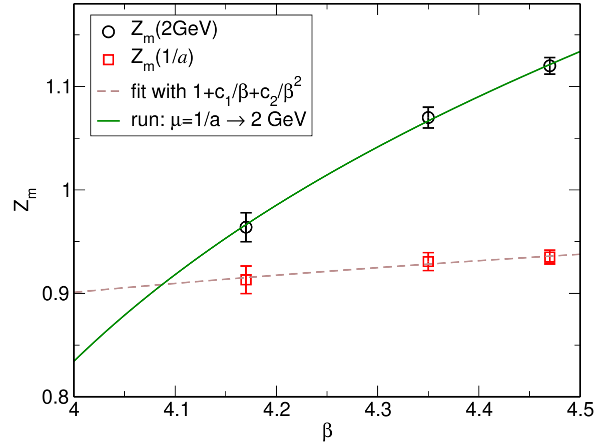
    * β=4.0 new data (previous step5), to add support at small β
- Step 2: determine $Z_m(\beta)$ using NPR results
  - at $\beta =$ $4.17, 4.35, 4.47$
  - And use $Z_m(\beta)$ so obtained for $\beta \geq 4.0$: $\beta < 4.17$ region is extrapolation
  - $1/Z_m(\beta)$ will be used to renormalize scalar operator, **chiral condensate**
- Step 3: solve $\boldsymbol{am_s(\beta)}$ with input (*quark mass input*):
  - $m_s^R = Z_m \cdot am_s^{latt} \cdot a^{-1} = 92$ 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.

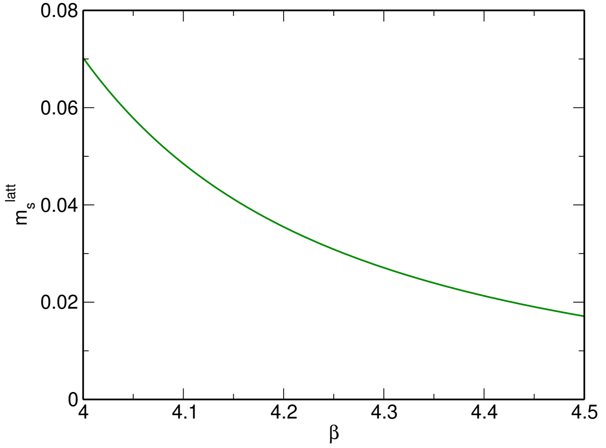
Do simulation

- Step 4: proper tuning of input mass: correct m_{res}

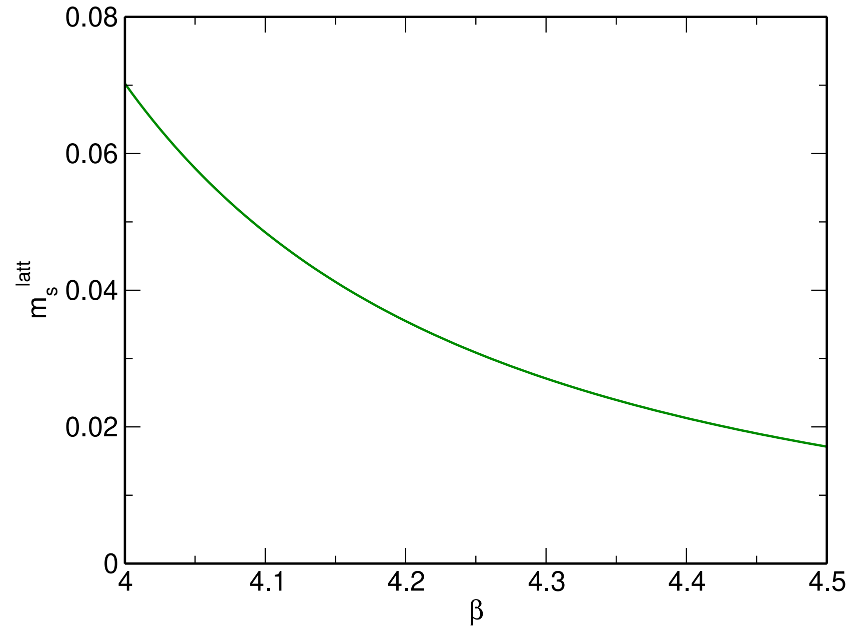
Do simulation 2nd round / correction with reweighting + valence meas.







LCP remarks for **FT2023-**

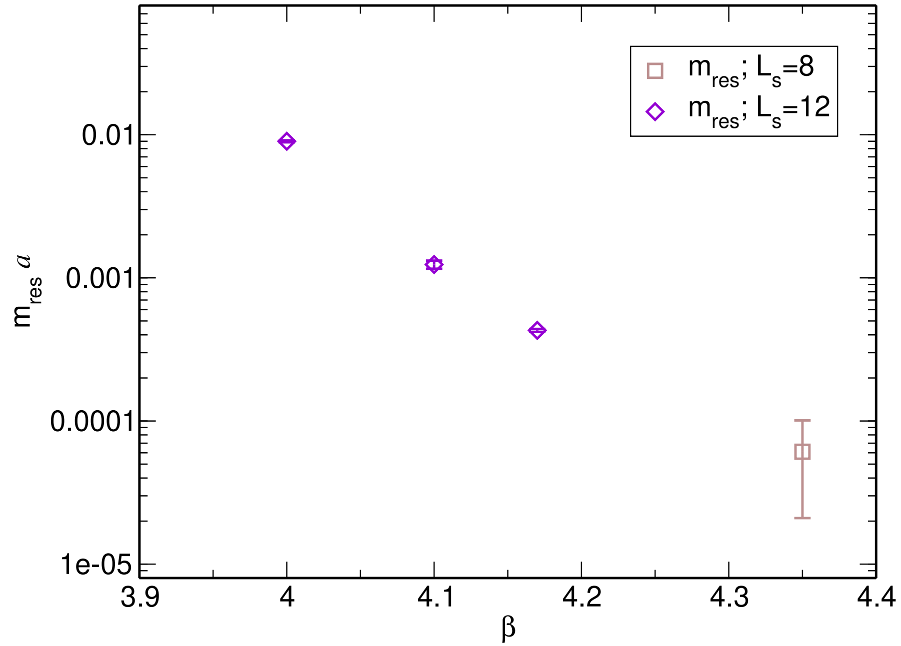


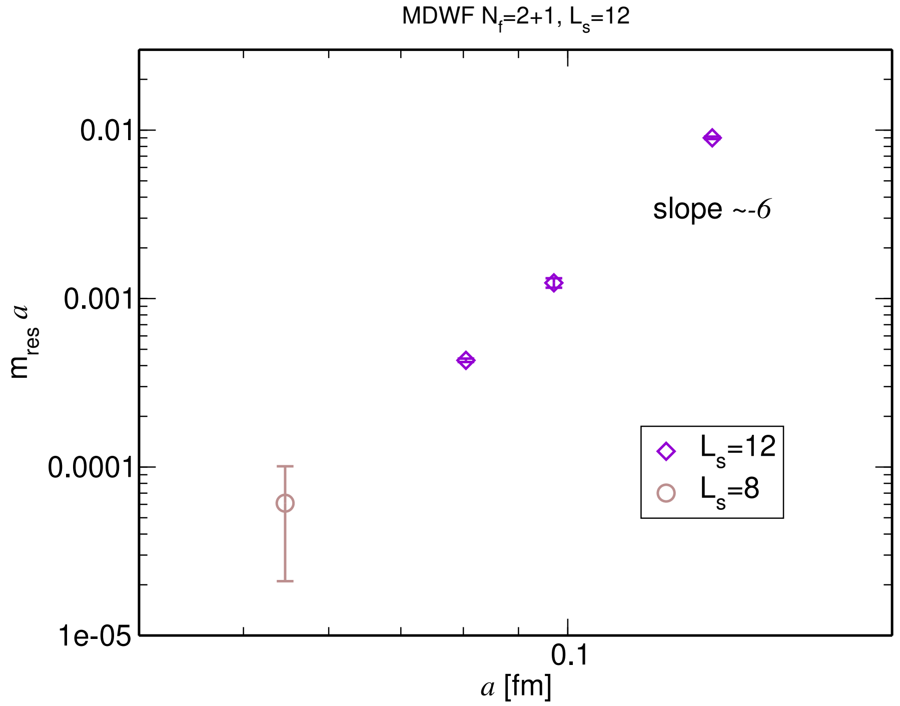
Features

- Fine lattice: use of existing results ($0.04 \le a \le 0.08$ 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} \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
  - Δm_K ~ ~~10 %~~ at $\beta = 4.0$ ($a \simeq 0.14$ fm) → Δm_K ~ a few %
  - Δm_K ~ 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 $a \to 0$
  - 1st (dumb) approximation: forget about m_{res}
  - Better : $m_f^{cont} \leftrightarrow (m_f + m_{res})$ but, this is not always enough

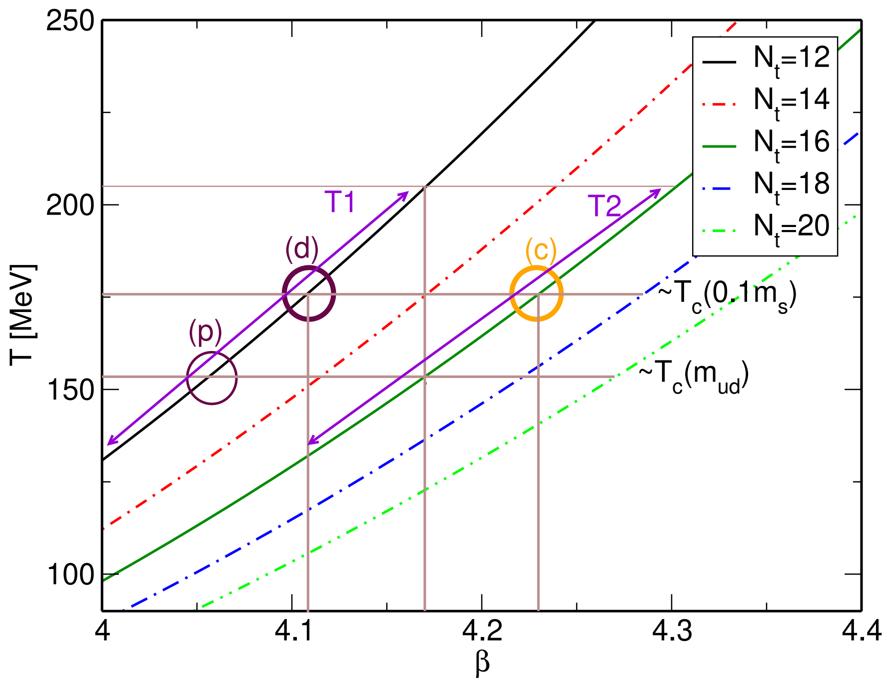


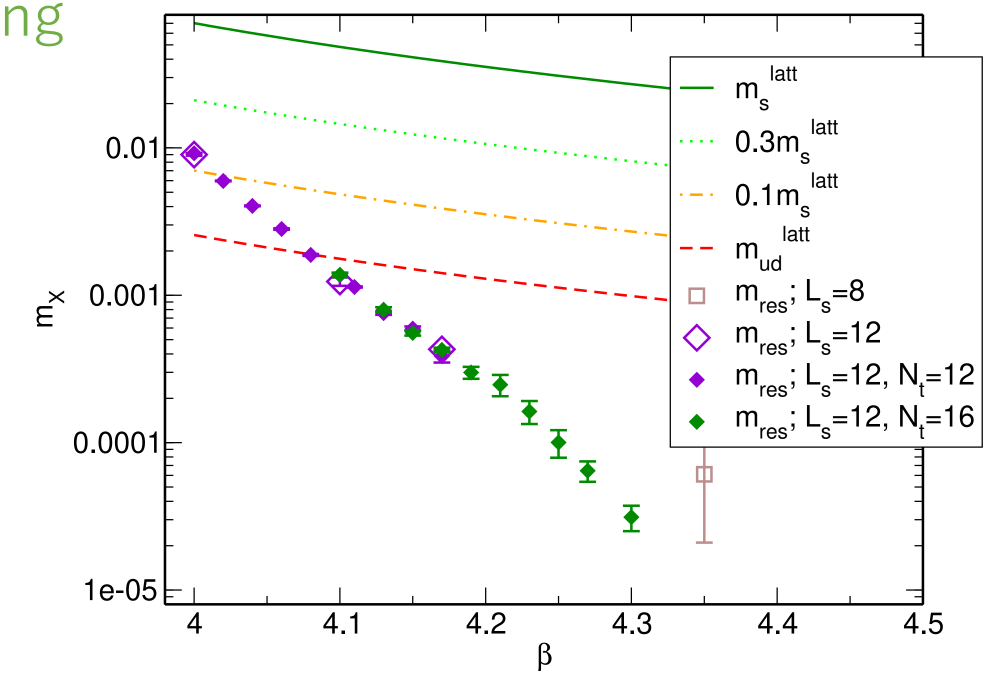


Simulation plan: 2^{nd} round w/ treatment of m_{res} effect

$L_s = 12$ fixed throughout this study

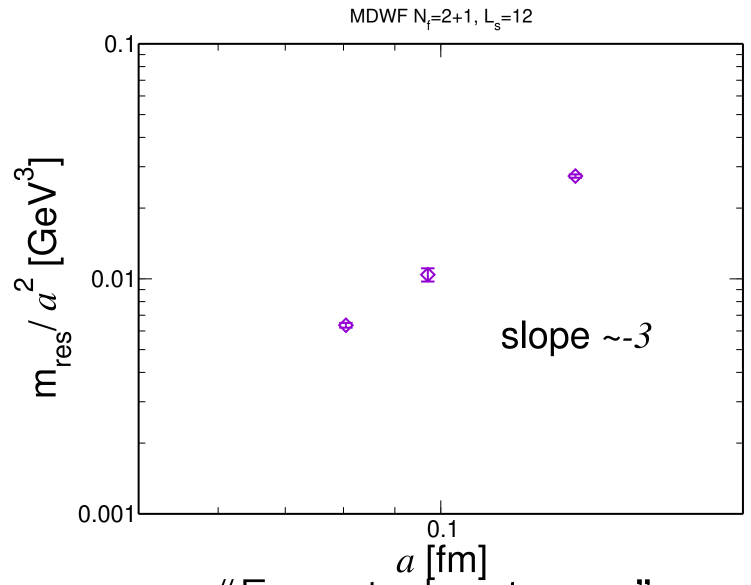
- T1-(d)
  - $N_t = 12$
  - $m_l = 0.1 m_s$
  - $m_q^{input} = m_q^{LCP} - m_{res}$
  - $V_s = 24^3, 36^3$
- T2-(c)
  - $N_t = 16$
  - $m_l = 0.1 m_s$
  - m_{res} shift by reweighting
  - $V_s = 32^3$
- T1-(p)
  - $N_t = 12$
  - $m_l = m_{ud}$
  - $m_q^{input} = m_q^{LCP} - m_{res}$
  - $V_s = 36^3,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





Light quark $\Sigma = -\langle\overline{\psi}\psi\rangle$: 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 very expensive proposition." – S. Sharpe.



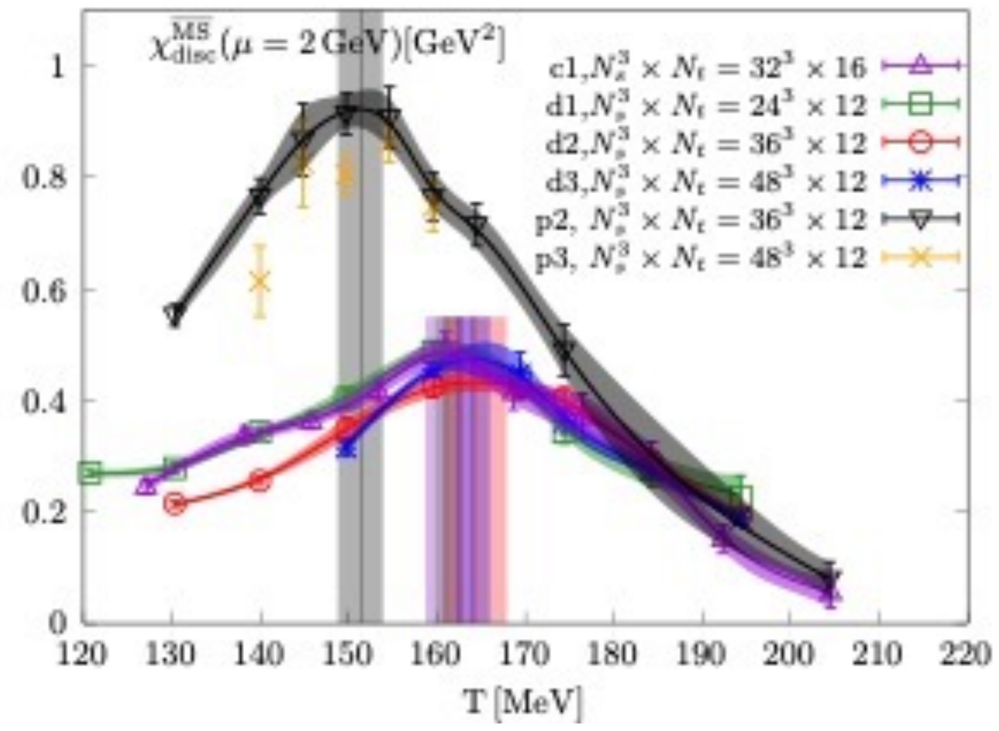
- $\Sigma|_{DWF} \to C_D \frac{x m_{res}}{a^2} + \Sigma|_{cont.} + \cdots$; $(m_f \to 0)$
- $\Sigma|_{DWF} \to C_D \frac{-(1-x) m_{res}}{a^2} + \Sigma|_{cont.} + \cdots$; $(m_f \to -m_{res})$

"Forget about m_{res}" is dumber for Σ, but⋯

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 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
- $\chi_{total} = \langle\overline{\psi}\psi \cdot \overline{\psi}\psi\rangle - \langle\overline{\psi}\psi\rangle\,\langle\overline{\psi}\psi\rangle$
  - has power divergence everywhere
  - needs to understand the power divergence of $\Sigma = -\langle\overline{\psi}\psi\rangle$ first

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.
- $\boldsymbol{T_{pc}} = \mathbf{151\ (3)}$ MeV (preliminary) on $\mathbf{36^3{\times}12}$, compared with
  - $\boldsymbol{T_{pc}} = \mathbf{155\ (1)(8)}$ w/ DWF ($\mathbf{N_t{=}8}$) by HotQCD (2014)
  - $\boldsymbol{T_{pc}} = \mathbf{156.5\ (1.5)}$ w/ HISQ by HotQCD (2019)
  - $\boldsymbol{T_{pc}} = \mathbf{158.0\ (0.6)}$ w/ stout staggered by Budapest-Wuppertal (2020)

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 very expensive proposition." – S. Sharpe.

- We propose another way to estimate $x m_{res}$ using m'_{res}

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

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

  $m'_{res} = \frac{\sum_x \langle J_{5q}(x) P(0)\rangle}{\sum_x \langle P(x)\, P(0)\rangle}$ ($\leftrightarrow$ $m_{res} = \frac{\sum_{\vec{x}} \langle J_{5q}(\vec{x},t) P(0)\rangle}{\sum_{\vec{x}} \langle P(\vec{x},t)\, P(0)\rangle} \rightarrow \frac{\langle 0|J_{5q}|\pi\rangle}{\langle 0|P|\pi\rangle}$ (large t))

  $m_f = -m_{res}'$ is a zero of $\Sigma|_{DWF}$ ($\leftrightarrow$ $m_f = -m_{res}$ is a zero of , m_π^2)

  Due to Axial WT identity: $(m_f + m'_{res}) \sum_x \langle P(x)\, P(0)\rangle = \Sigma$

  From: $\Delta_\mu \langle A_\mu(x)\, P(0)\rangle = 2 m_f \langle P(x)\, P(0)\rangle + 2 \langle J_{5q}(x)\, P(0)\rangle - 2\,\Sigma\,\delta_{x,0}$

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

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- Yet another way for the subtraction including $x m_{res}$ using $\boldsymbol{N_f = 3, T = 0}$ information

  →see the talk by Yu Zhang

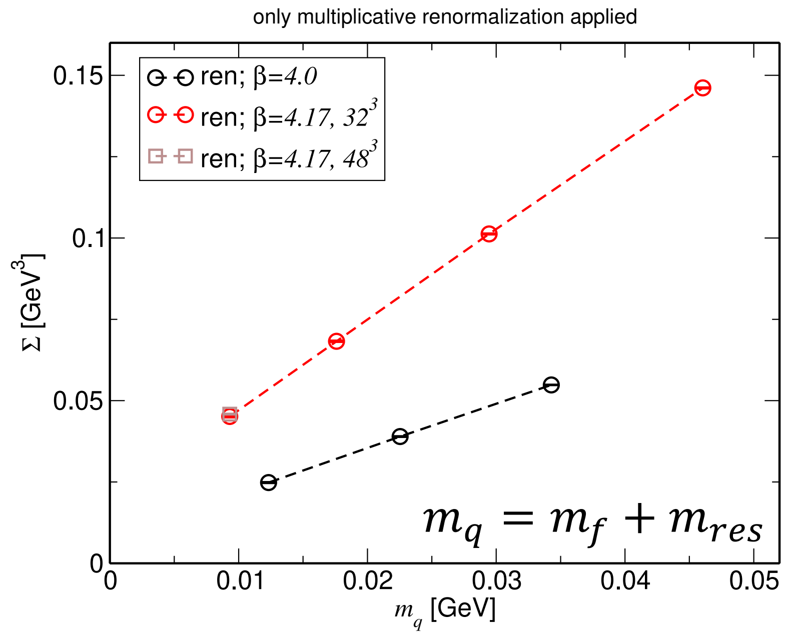
  1. Prepare several different lattice spacing
  2. Compute coefficient linear in m_f : $\Sigma|_{DWF} \sim const. + (\frac{C_D}{a^2} + C_R) m_f + \cdots$
  3. Separate divergent term : *linear fit in* a^2 *of*: $C_D + a^2 C_R \rightarrow \boldsymbol{C_D = 0.37(2)}$
  4. Estimate x through $\Sigma|_{DWF}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

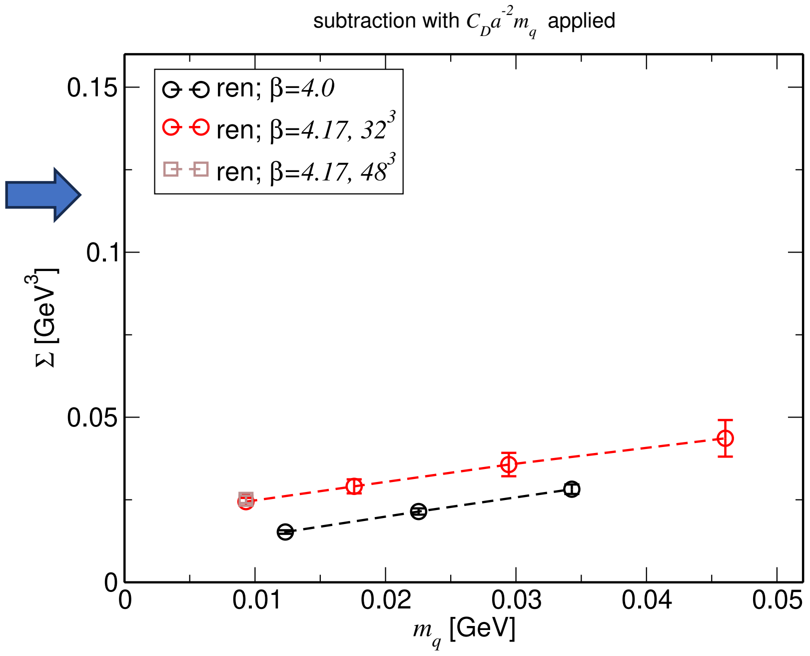
     this is meant to impose renorm. cond. $\Sigma|_{cont.} = 0$

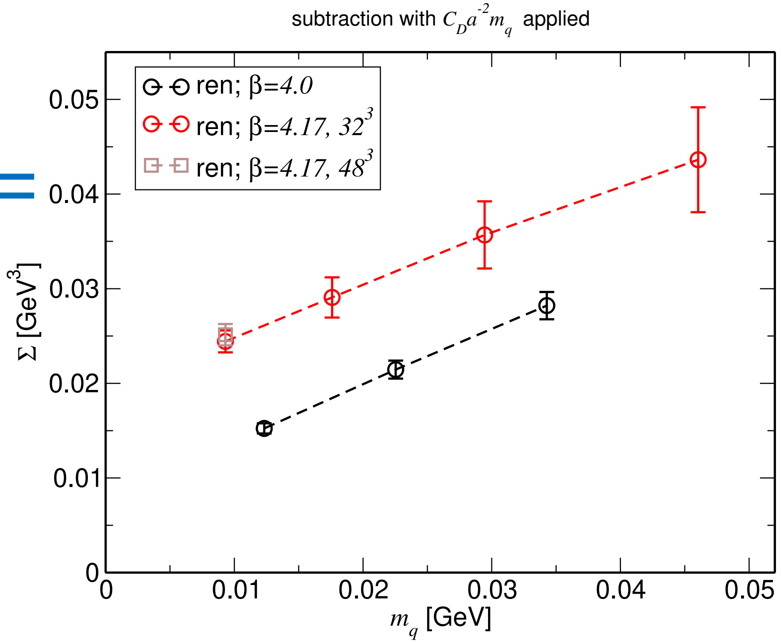
  → $\boldsymbol{N_f = 3}$; $\boldsymbol{\beta = 4.0}$ estimate: $\boldsymbol{x = -0.6(1)}$

  - In general, $\boldsymbol{x}$ may depend on $\boldsymbol{\beta}$, for now use this value as a reference for all $\boldsymbol{\beta}$
  - 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





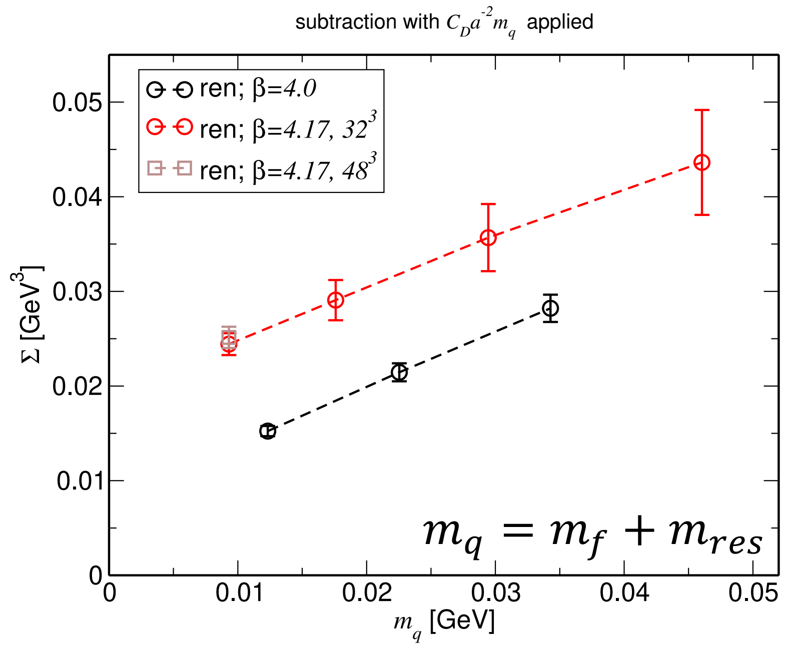


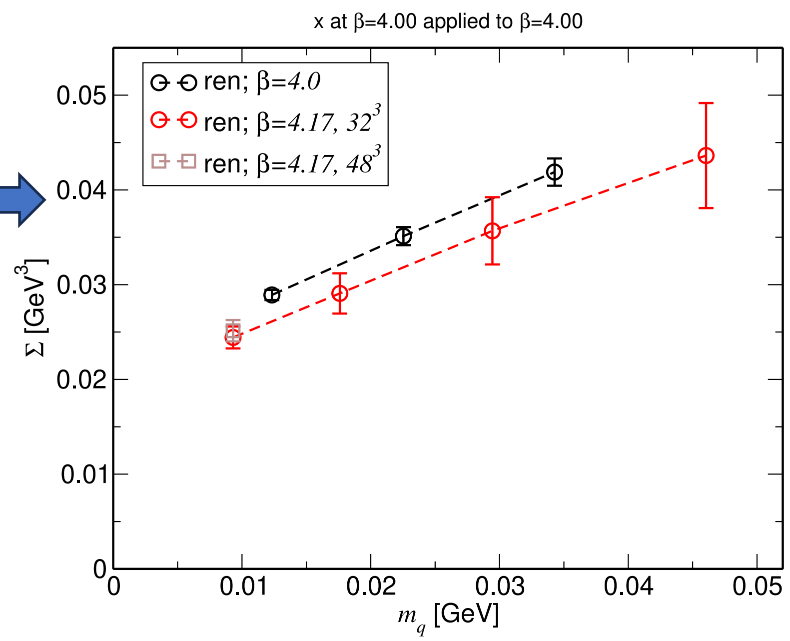
only multiplicative renormalizations applied

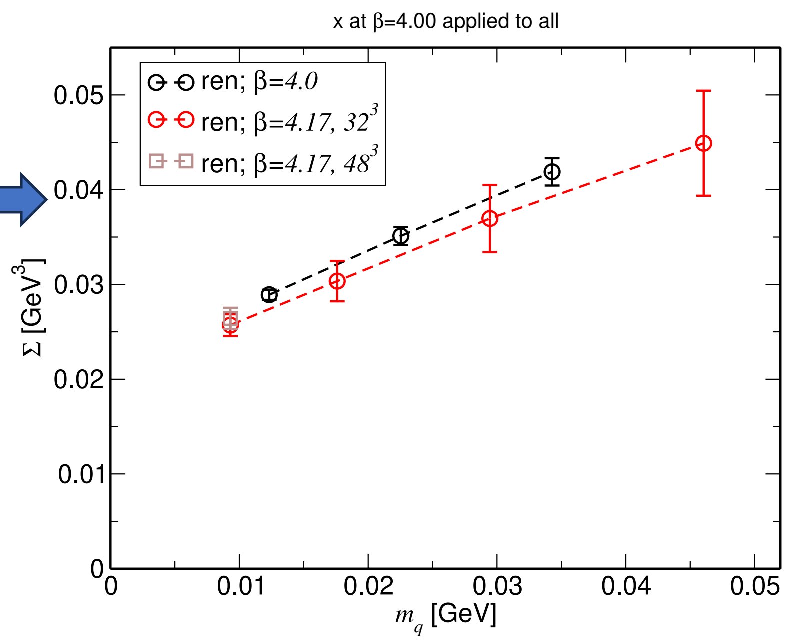
$C_D a^{-2} m_q$ subtraction applied

changing y-axis range

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







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

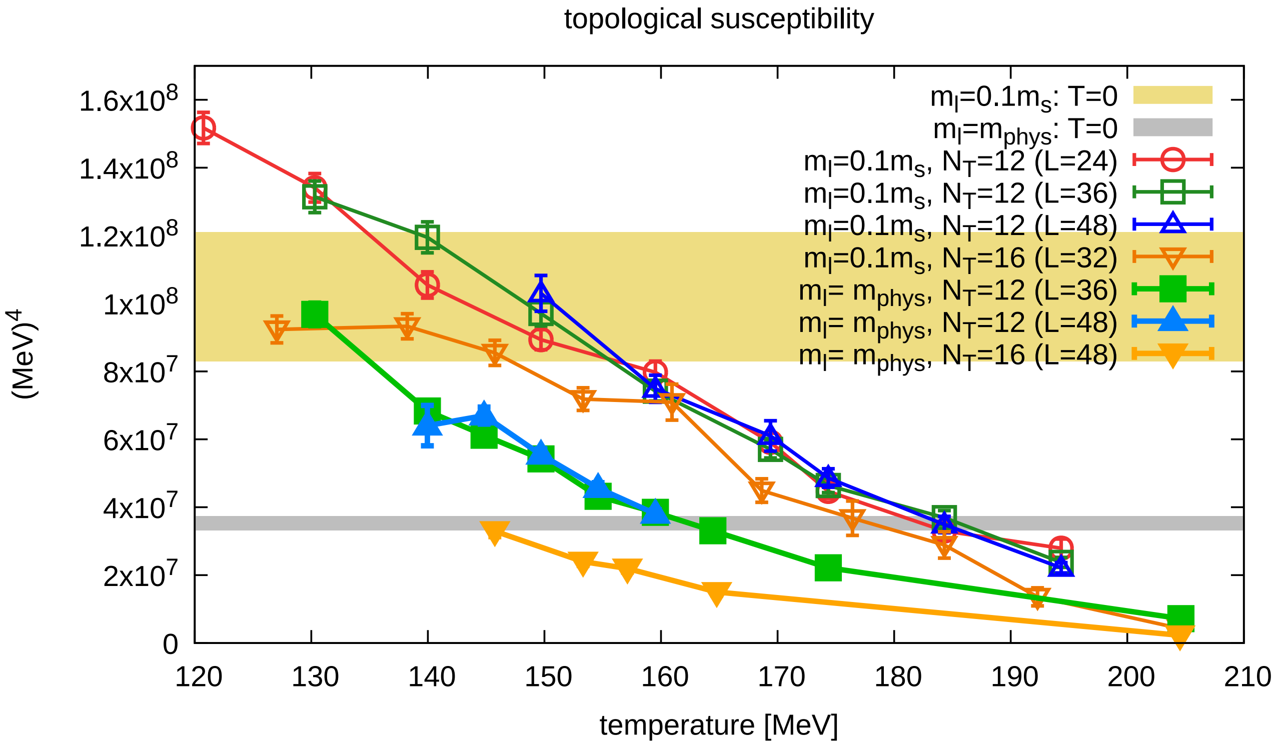
$C_D a^{-2}(1-x) m_{res}$ subtraction applied only to $\beta = 4.0$

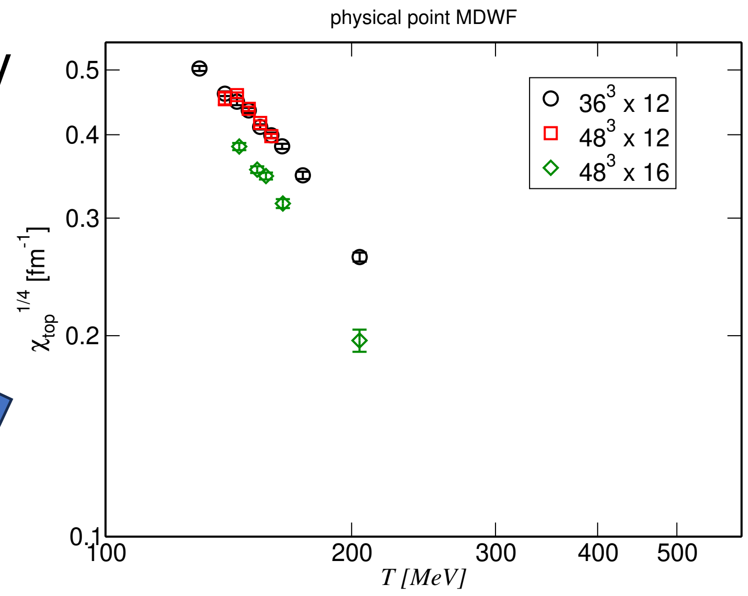
$C_D a^{-2}(1-x) m_{res}$ subtraction applied to all assuming x is universal

Seemingly, both conventional and residual divergence are controlled, but

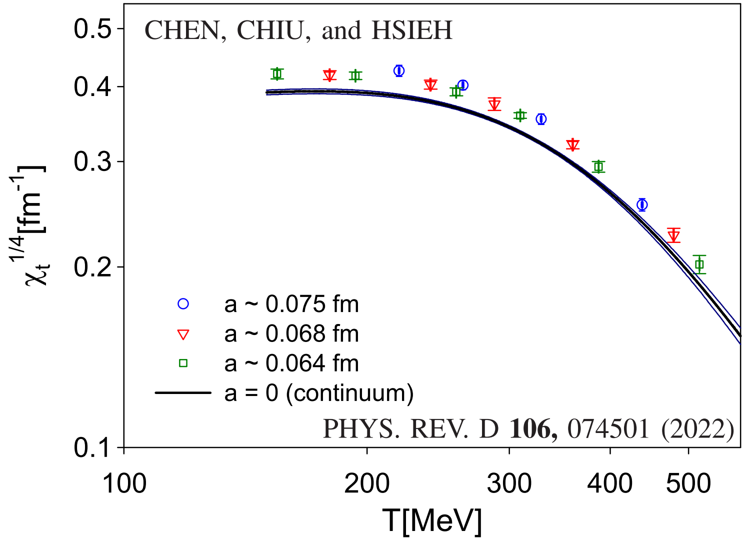
- need to check if x does not depend much on β
- refinement of precision and check applicability range of C_D necessary

topological susceptibility





MDWF
N_f=2+1



optimal DWF
N_f=2+1+1

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

Summary and Outlook

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

- use LCP, determined with T=0 JLQCD knowledge
- 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
- Topological susceptibility showing large lattice artifact for Nt=12. Nt=16 promising.

These are what's new's from Lattice 2022

Outlook

- refinement of power divergence subtraction using T=0 information of very fine MDWF
- 483 for Nt=12 and 16 are being run on Fugaku
- plan to be completed by the end of FY2025.
- use of these configuration underway
  - see talk by Goswami on Friday on charge fluctuation