Finite temperature QCD phase transition with (2+1)- and 3-flavor Möbius domain wall fermions

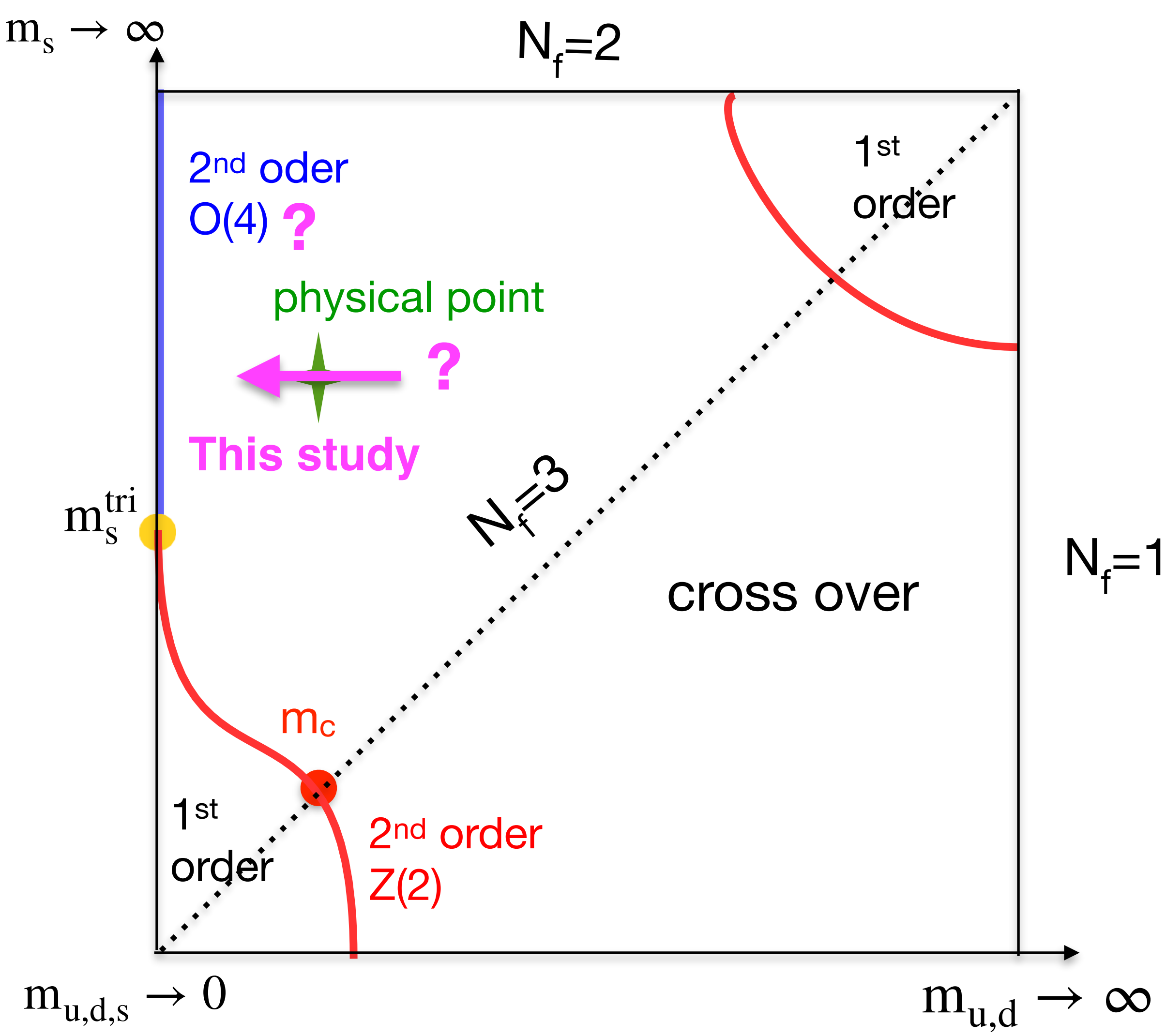
Yu Zhang
(RIKEN R-CCS)

Based on work with JLQCD collaboration:
S.Aoki, Y.Aoki, H.Fukaya, J.Goswami, S.Hashimoto, I.Kanamori, T.Kaneko, Y.Nakamura

Challenges and opportunities in Lattice QCD simulations and related fields
Feb.16, 2023, RIKEN R-CCS

The nature of QCD phase transition at $\mu_B = 0$

Columbia plot



The nature of chiral phase transition depends on whether the $U(1)_A$ symmetry is effectively restored or not at T_c

- $m_q = 0$:
- $U(1)_A$ symmetry broken at T_c → 2nd order O(4)
- $U(1)_A$ symmetry effectively restored at T_c
  → not O(4), $SU(2)_L \times SU(2)_R / U(2)_V$?
  → a possible 1st order [Pisarski, Wilczek PRD 84]

Recent study with non-chiral fermion (staggered fermions) gives evidence of O(4) scaling in the chiral limit of Nf=2+1 QCD [H.-T.Ding et al., PRL 21]

$T_c \sim 132$ MeV [HotQCD, PRL 19]

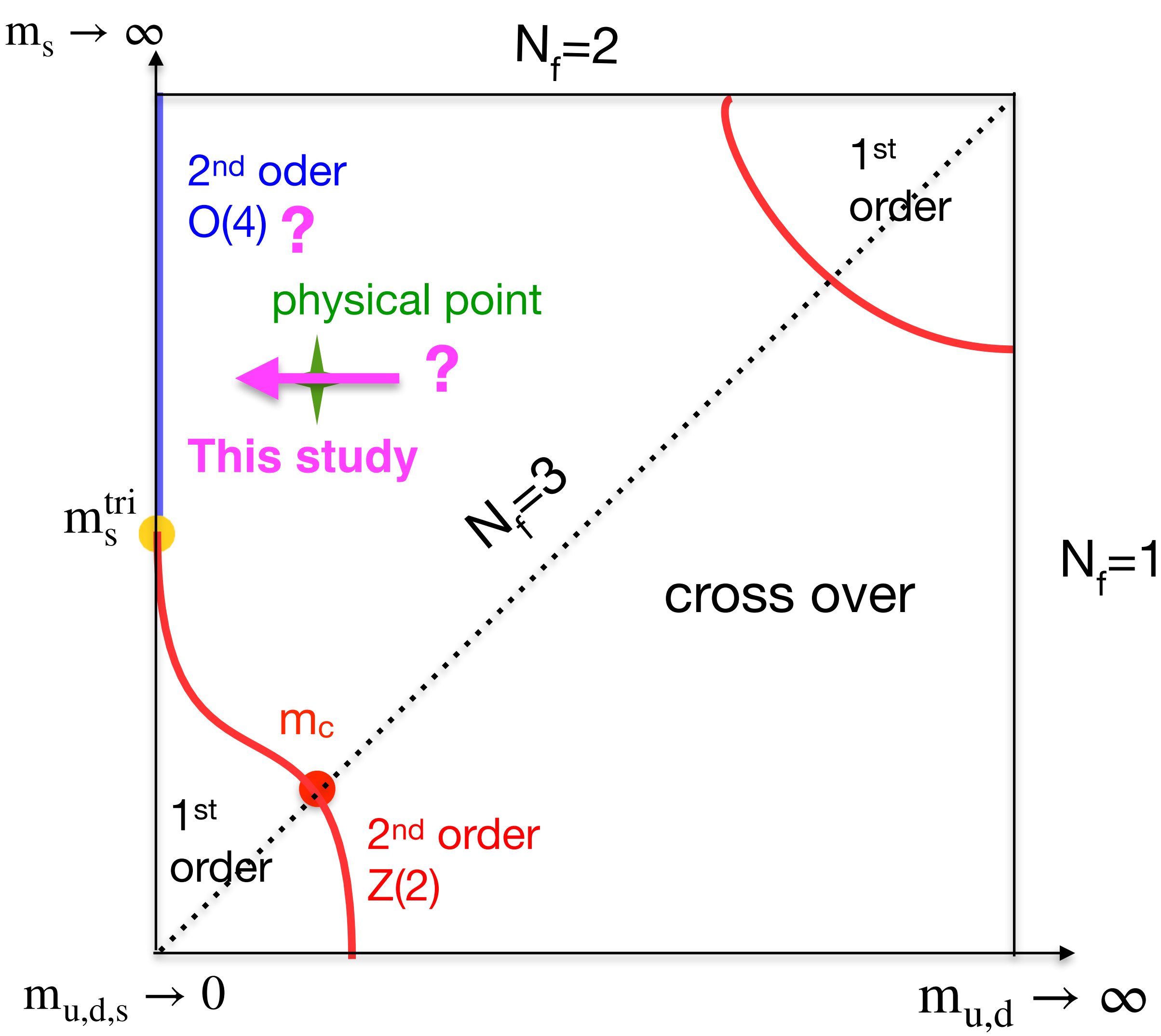
- m_q physical: crossover [Y.Aoki et al., Nature 06]

$T_{pc} \sim 156$ MeV [HotQCD, PLB 19]

- $N_f = 2 + 1$ & very light m_l: nature of transition?

The nature of QCD phase transition at $\mu_B = 0$

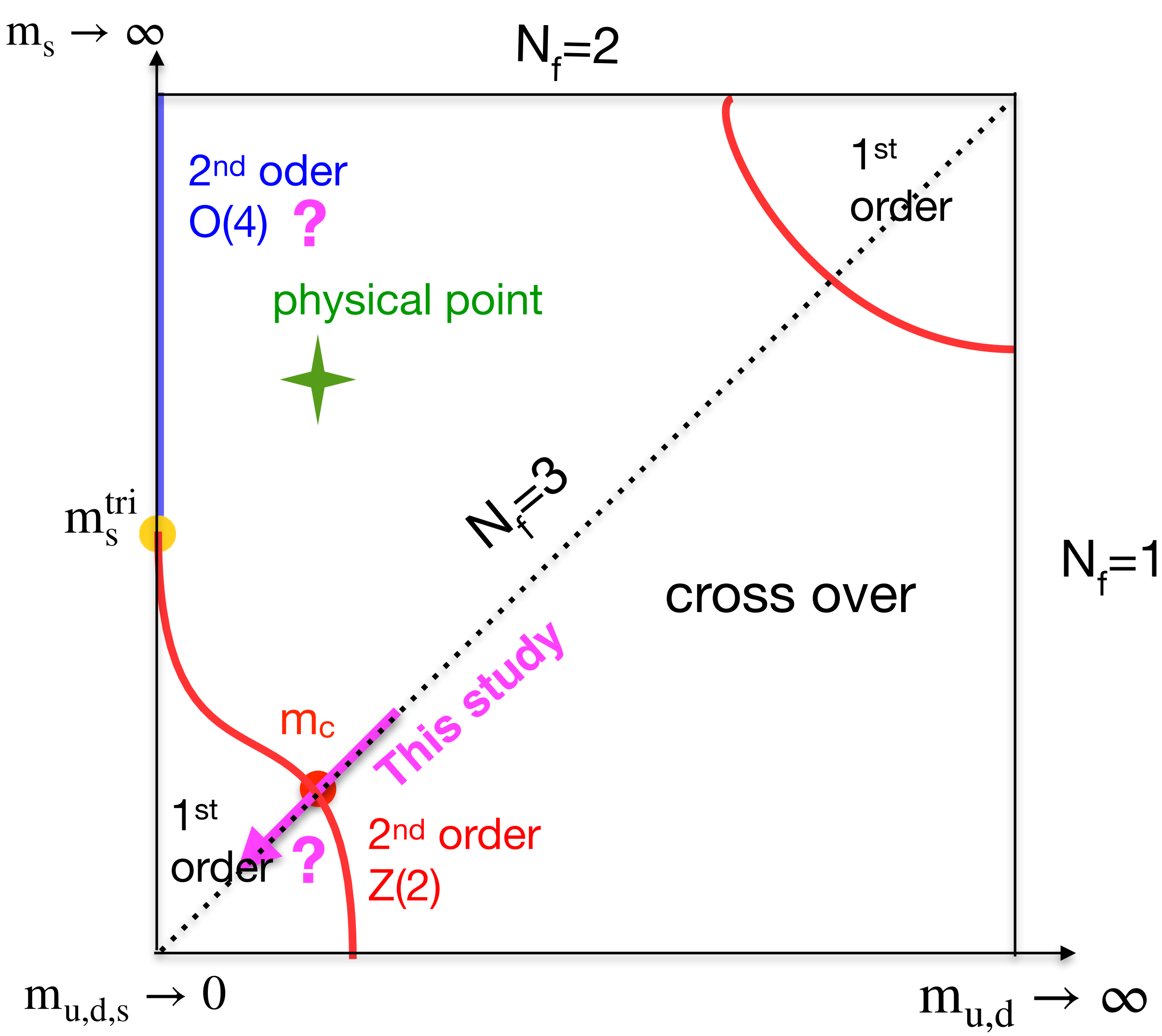
Columbia plot



- This work:
  - Order of phase transition near physical point using $N_f = 2 + 1$ Mobius domain wall fermion
  - The transition temperature
- Why DWF
  - Preserve chiral symmetry and $U(1)_A$ symmetry at finite a when $L_s \to \infty$
  - Reduced χ_{SB} parameterized by residual mass when L_s is finite

The nature of QCD phase transition at $\mu_B = 0$

Columbia plot



Order of phase transition depends on m_l, m_s & N_f

- ϵ expansion: 1st order phase transition in the chiral limit for $N_f = 3$
  [Pisarski, Wilczek PRD 84]

- RG flows of all couplings up to ϕ^6 in 3d Ginzburg-Landau potential for $N_f = 3$ in the chiral limit: a possible 2nd order phase transition
  [G. Fejos, PRD 22]

This work:

➡ Explore $N_f = 3$ chiral region using first-principle lattice QCD

Previous Nf=3 lattice QCD studies

Action	N_t	$m_\pi^{Z_2}$ [MeV]	Ref.
Wilson	4	$\lesssim 670$	Iwasaki et al. (1996)
Staggered	4	290	Karsch et al. (2001)
Staggered	6	150	de Forcrand et al. (2007)
HISQ	6	$\lesssim 50$	Bazavov et al. (2017)
Wilson-Clover	6-10	$\lesssim 170$	Jin et al. (2017)
Wilson-Clover	6-12	$\lesssim 110$	Kuramashi et al. (2020)
HISQ	8	$\lesssim 80$	Dini et al. (2022)

1st order region shrinks for both fermions as reduce a

$m_\pi^{Z_2}$ has strong cutoff and discretization scheme dependence

Evidence for continuum chiral limit to feature 2nd order phase transition with staggered fermion [Cuteri et al.(2021)]

Our aim is to investigate $N_f = 3$ QCD phase structure with Mobius Domain Wall Fermion

Why MDWF

- Exact chiral symmetry at finite a for infinite Ls
- Reduced χ_{SB} parameterized by residual mass when Ls is finite

Lattice Setup for $N_f = 3$

- N_f=3 Mobius Domain Wall Fermion with L_s=16
- Symanzik gauge action at β = 4.0 (a=0.1361(20) fm)
- Using Wilson flow t_0 to set the scale and matching with N_f=2+1 physical point
  $\sqrt{t_0}^{phys} = 0.1465(21)(13)$ fm [S.Borsanyi et al., JHEP 2012]

☆T > 0:

- ☑ N_t=8 (T=181.1(2.6) MeV): N_s=16, $0 \leq m_l \leq 0.2$
  N_s=24, $0 \leq m_l \leq 0.14$
- ☑ N_t=12 (T=120.8(1.8) MeV): N_s=24, $-0.006 \leq m_l \leq 0.1$
  N_s=36, $-0.004 \leq m_l \leq 0.001$

☆T = 0:

N_s=24, N_t=48, $0.02 \leq m_l \leq 0.045$

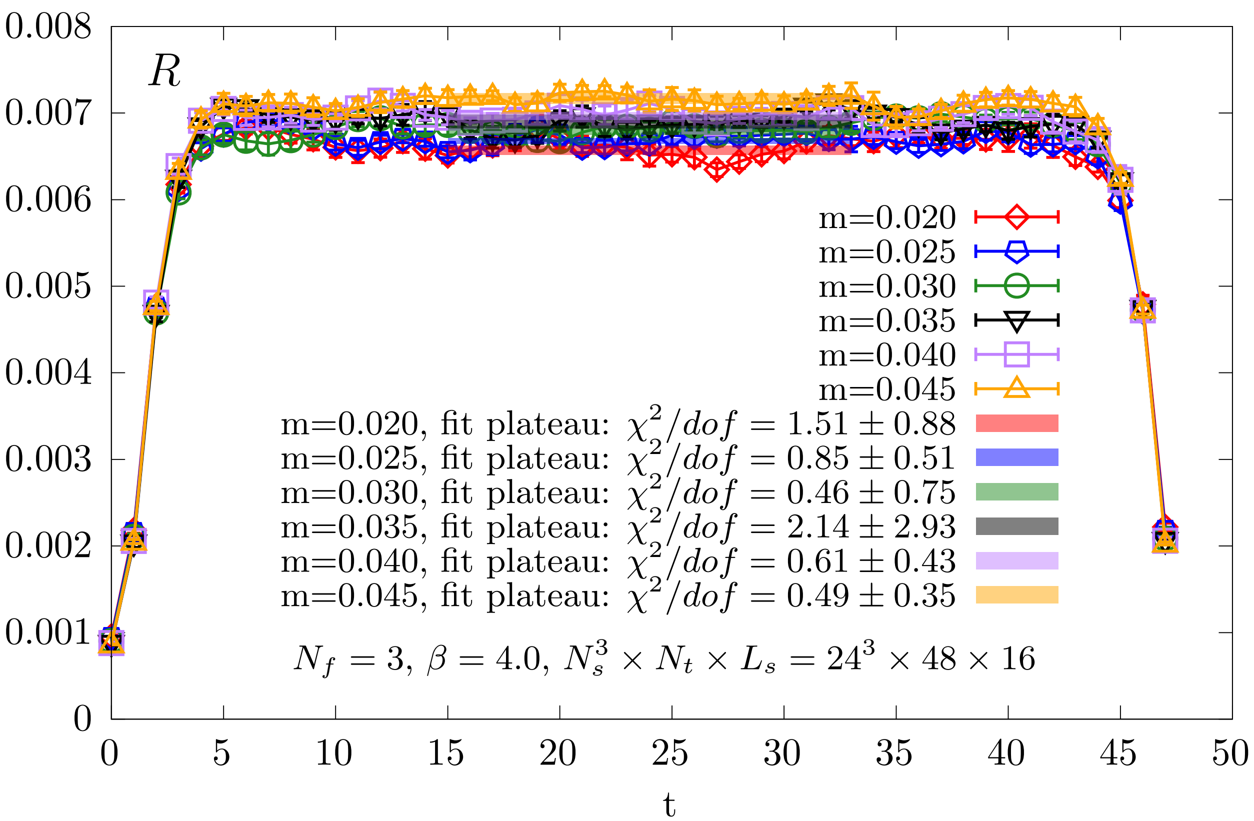
- Measured: residual mass, chiral condensate, disconnected chiral susceptibility & Binder cumulant
- Codes: Grid & Hardons
- Resources: Supercomputer Fugaku & Wisteria/BDEC-01 Oddysey

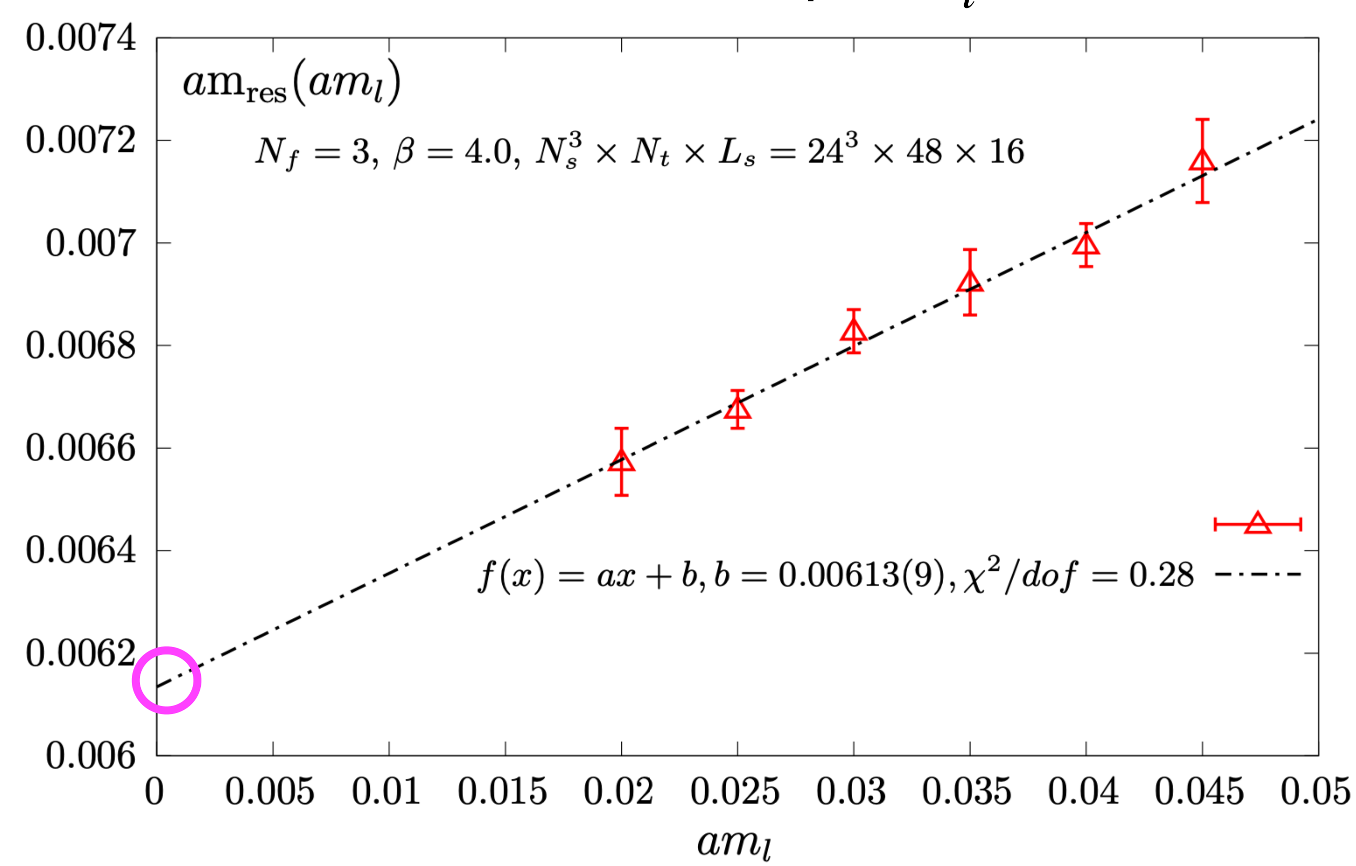
Residual chiral symmetry breaking

- For finite Ls chiral symmetry is broken, leading to an **additive renormalization of the quark mass** $m_l \to m_l + m_{\text{res}}$
- $m_{\text{res}} \to 0$ as $L_s \to \infty$**,** cost is high when increase Ls, practical simulation: Ls=16
- Measure the ratio of midpoint correlator to the pion correlator evaluated at large distance

$$m_{\text{res}} = R(t) = \frac{\left\langle \sum_{\vec{x}} J^a_{5q}(\vec{x}, t)\pi^a(\vec{0},0) \right\rangle}{\left\langle \sum_{\vec{x}} J^a_{5}(\vec{x}, t)\pi^a(\vec{0},0) \right\rangle}$$

Smallest input m_l is -0.006

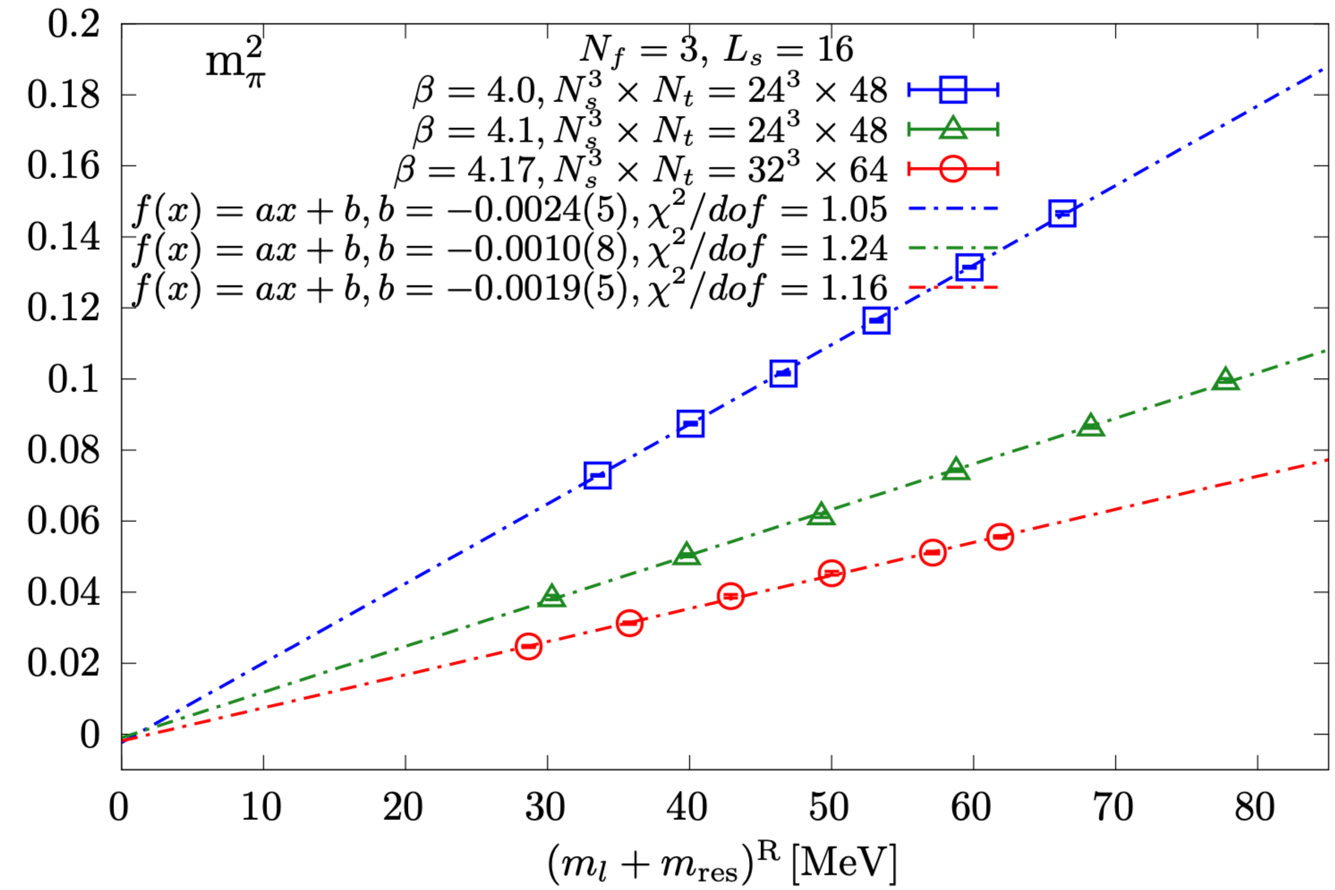




Residual chiral symmetry breaking on chiral condensate

- From low energy effective QCD $\mathscr{L}$, the effect of mixing between chiral walls for long-distance quantities will result in $m_l \to m_l + m_{\rm res}$. e.g. $m_\pi^2 \propto m_l + m_{\rm res}$

- For quantities whose sensitivity to χ_{SB} effects extends up to the cutoff scale, the above argument doesn't go through. e.g.$\langle \bar{\psi}\psi \rangle$



$$\langle \bar{\psi}\psi \rangle |_{DWF} \sim \frac{m_l + x m_{res}}{a^2} + \langle \bar{\psi}\psi \rangle |_{\rm cont.} + \ldots$$

x is not known , expected $x = \mathcal{O}(1)$

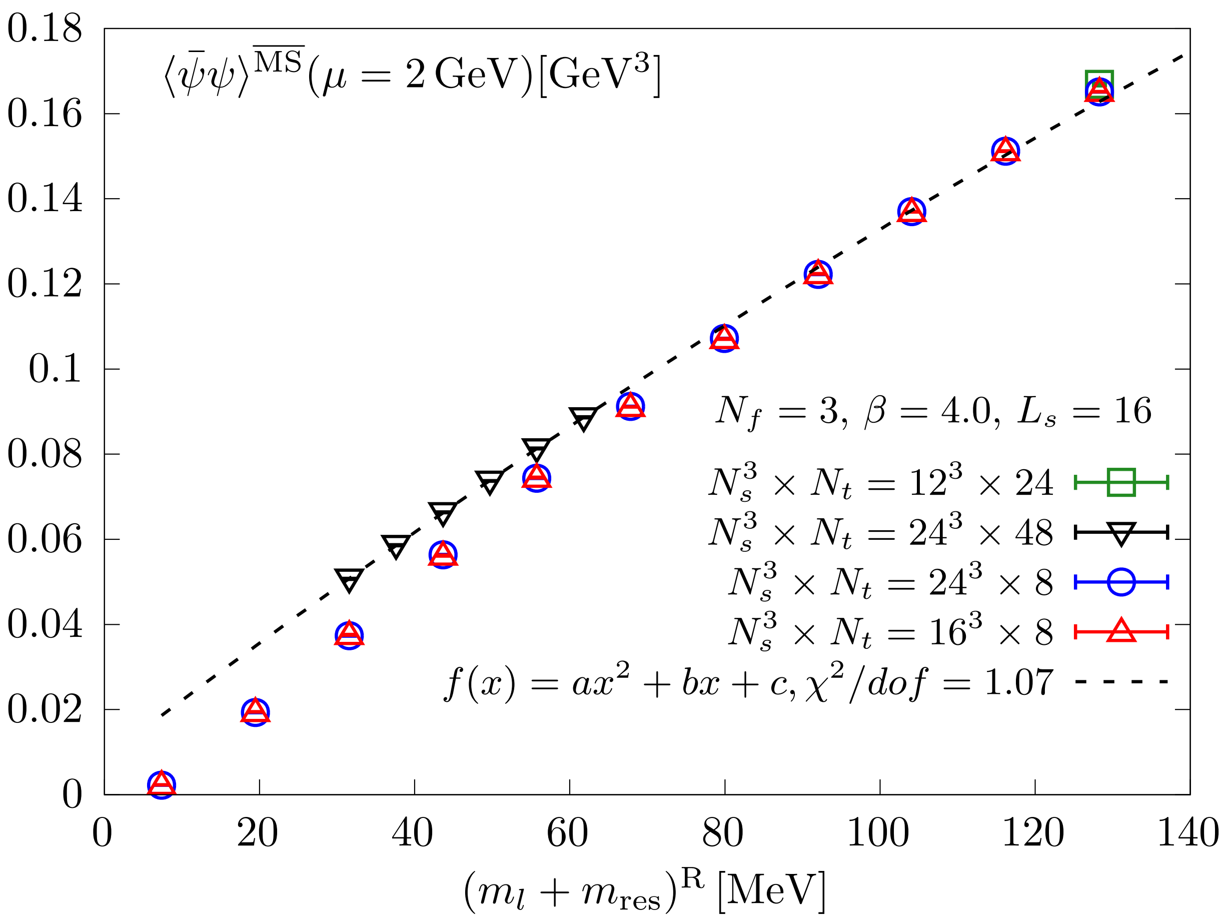
[S. Sharpe, arXiv: 0706.0218]

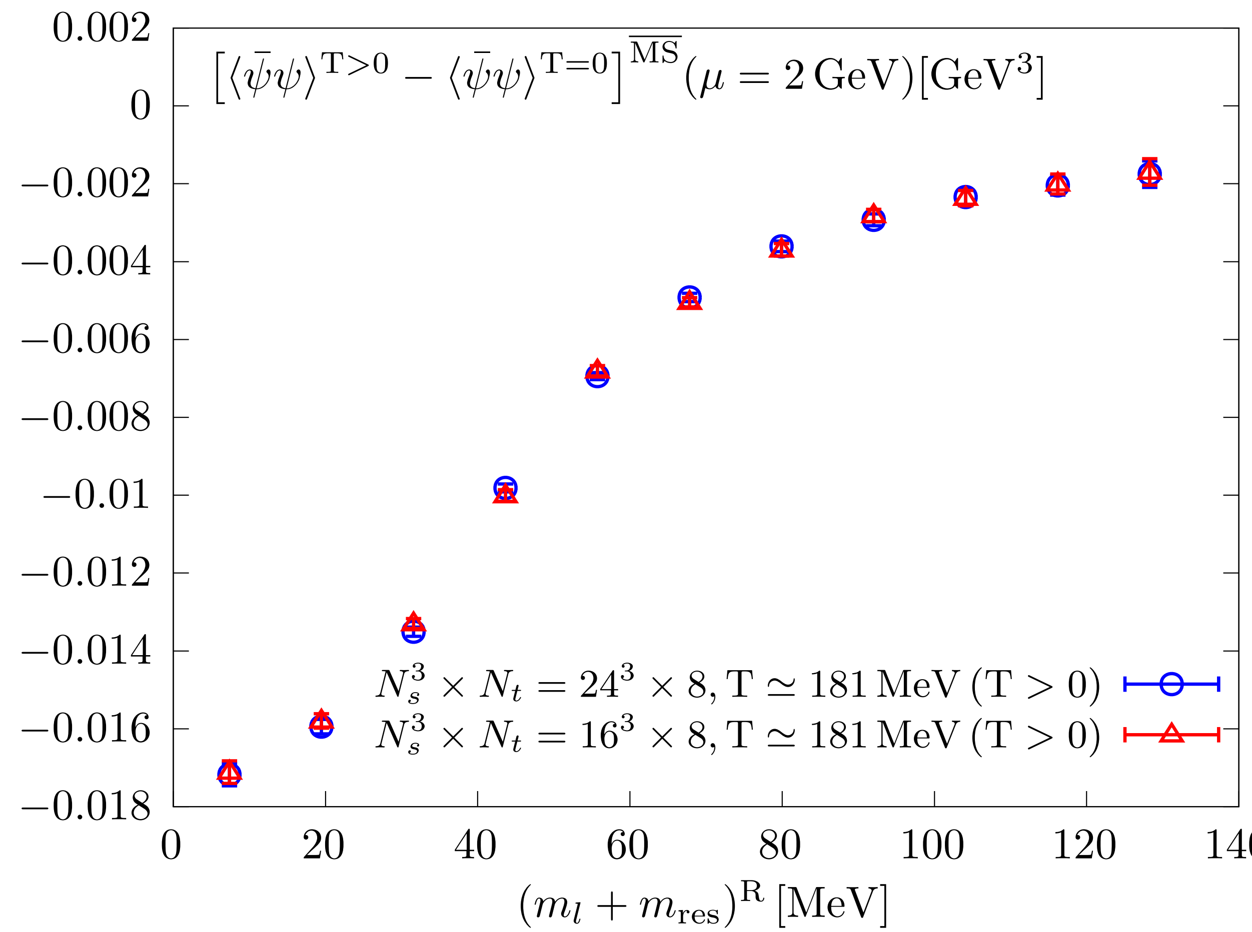
Additive divergence remains if one extrapolates to $m_q = m_l + m_{res} = 0$

$$\Rightarrow \lim_{m_q \to 0} \lim_{L \to 0} \langle \bar{\psi}\psi \rangle |_{DWF} \sim \langle \bar{\psi}\psi \rangle |_{\rm cont.} + (x-1)\frac{m_{res}}{a^2} \ldots$$

Chiral condensate at T= 181.1(2.6) MeV

Order parameter for χ_{SB}: $\langle \bar{\psi}\psi \rangle = \frac{1}{N_s^3 N_t} \mathrm{Tr} \langle M^{-1} \rangle$





- Quark mass in $\overline{\mathrm{MS}}$ scheme: $m^{\overline{\mathrm{MS}}}(2\,\mathrm{GeV}) = Z_m^{\overline{\mathrm{MS}}}(2\,\mathrm{GeV}) a^{-1}(am)$
- Multiplicative renormalization: $\langle \bar{\psi}\psi \rangle^{\overline{\mathrm{MS}}}(2\,\mathrm{GeV}) = \frac{a^{-3}(a^3 \langle \bar{\psi}\psi \rangle)}{Z_m^{\overline{\mathrm{MS}}}(2\,\mathrm{GeV})}$
- Remove additive divergence $\frac{m_l + x m_{res}}{a^2}$ by $\langle \bar{\psi}\psi \rangle^{\mathrm{T}>0} - \langle \bar{\psi}\psi \rangle^{\mathrm{T}=0}$
- a crossover

[Y.Aoki Lattice 2022]

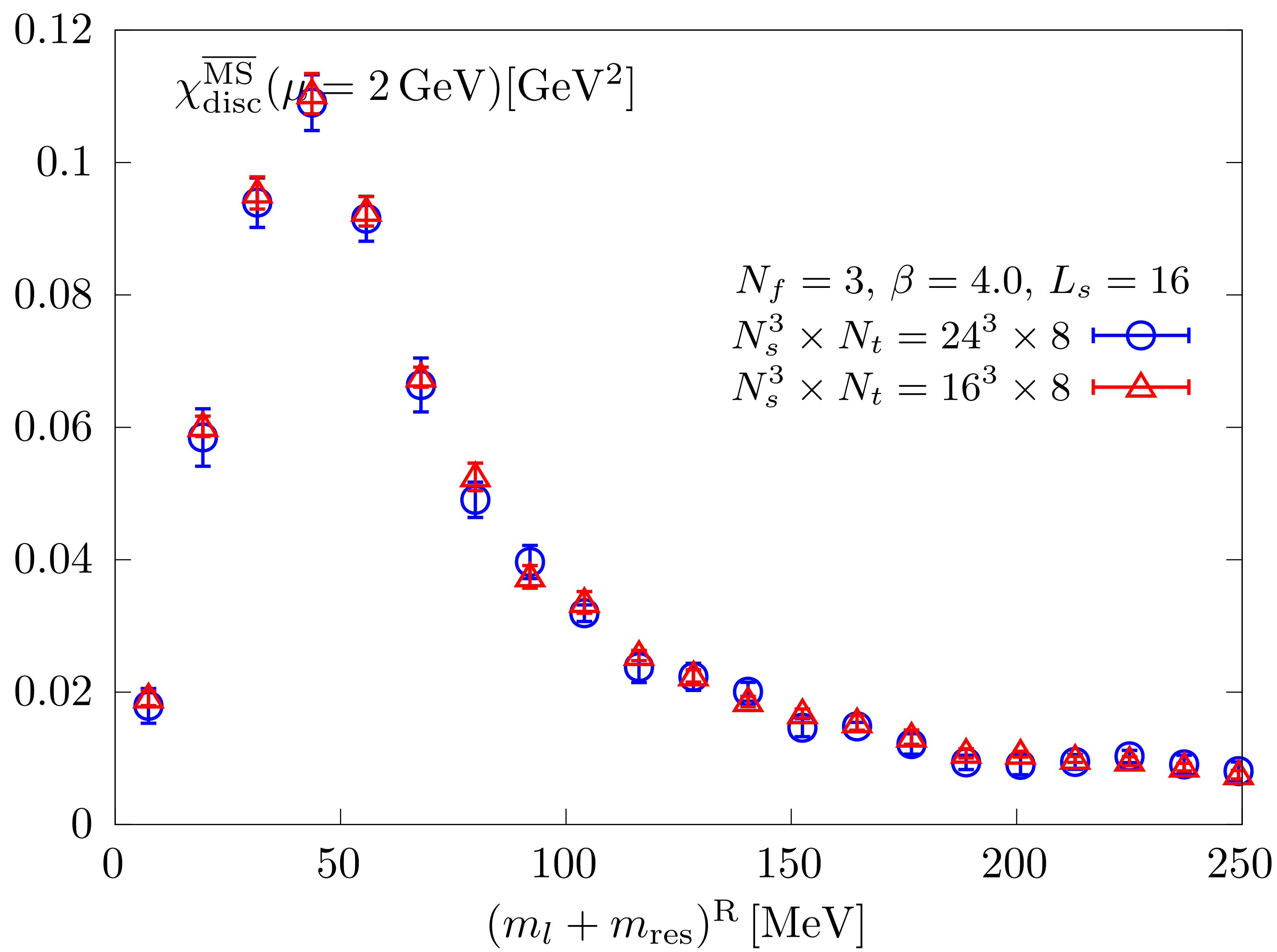
Disconnected chiral susceptibility at 181.1(2.6) MeV

$$\chi_{\rm disc} = \frac{1}{N_s^3 N_t}\left(\left\langle \left(\mathrm{Tr}\, M^{-1}\right)^2 \right\rangle - \left\langle \mathrm{Tr}\, M^{-1} \right\rangle^2\right)$$

Describes fluctuations of the chiral condensate & Peak at transition point

Renormalized to $\overline{\mathrm{MS}}(\mu = 2\,\mathrm{GeV})$ with $(Z_{\rm m}^{\overline{\rm MS}})^{-2}$ to remove the multiplicative divergence:

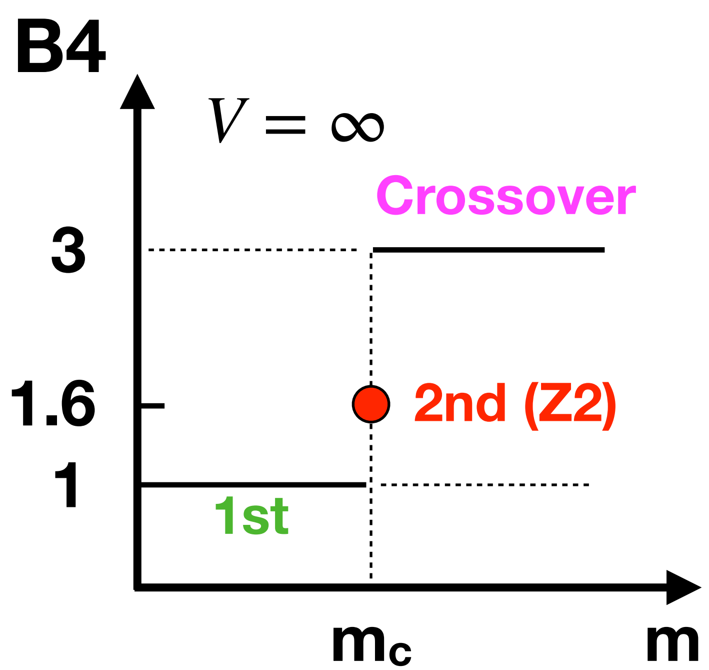
➡ $\chi_{\rm disc}^{\overline{\rm MS}}(\mu = 2\,\mathrm{GeV})[\mathrm{GeV}^2] = \left(\frac{1}{Z_m^{\overline{\rm MS}}}\right)^2 \chi_{\rm disc}^{\rm bare}\ (a^{-2}[\mathrm{GeV}^2])$

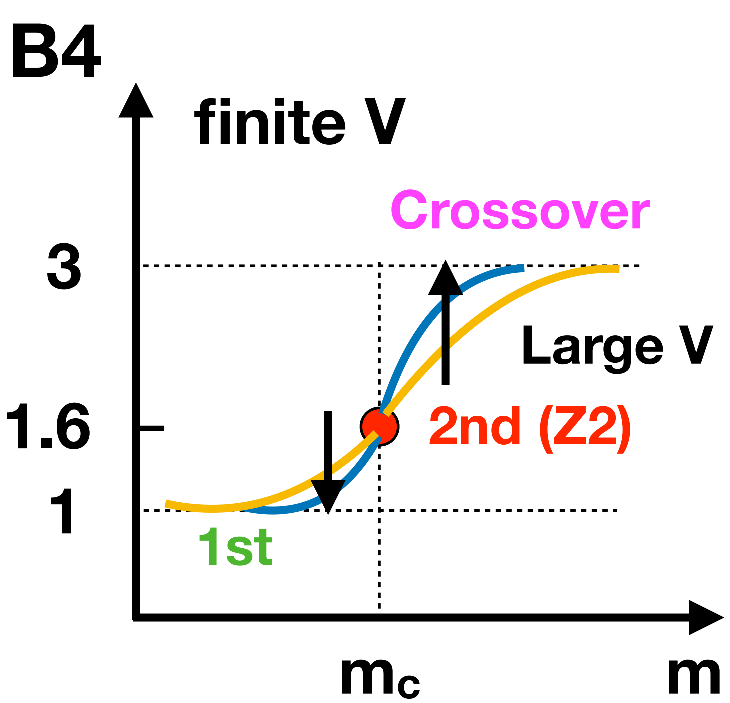


- **Pseudo critical mass is around 44 MeV**

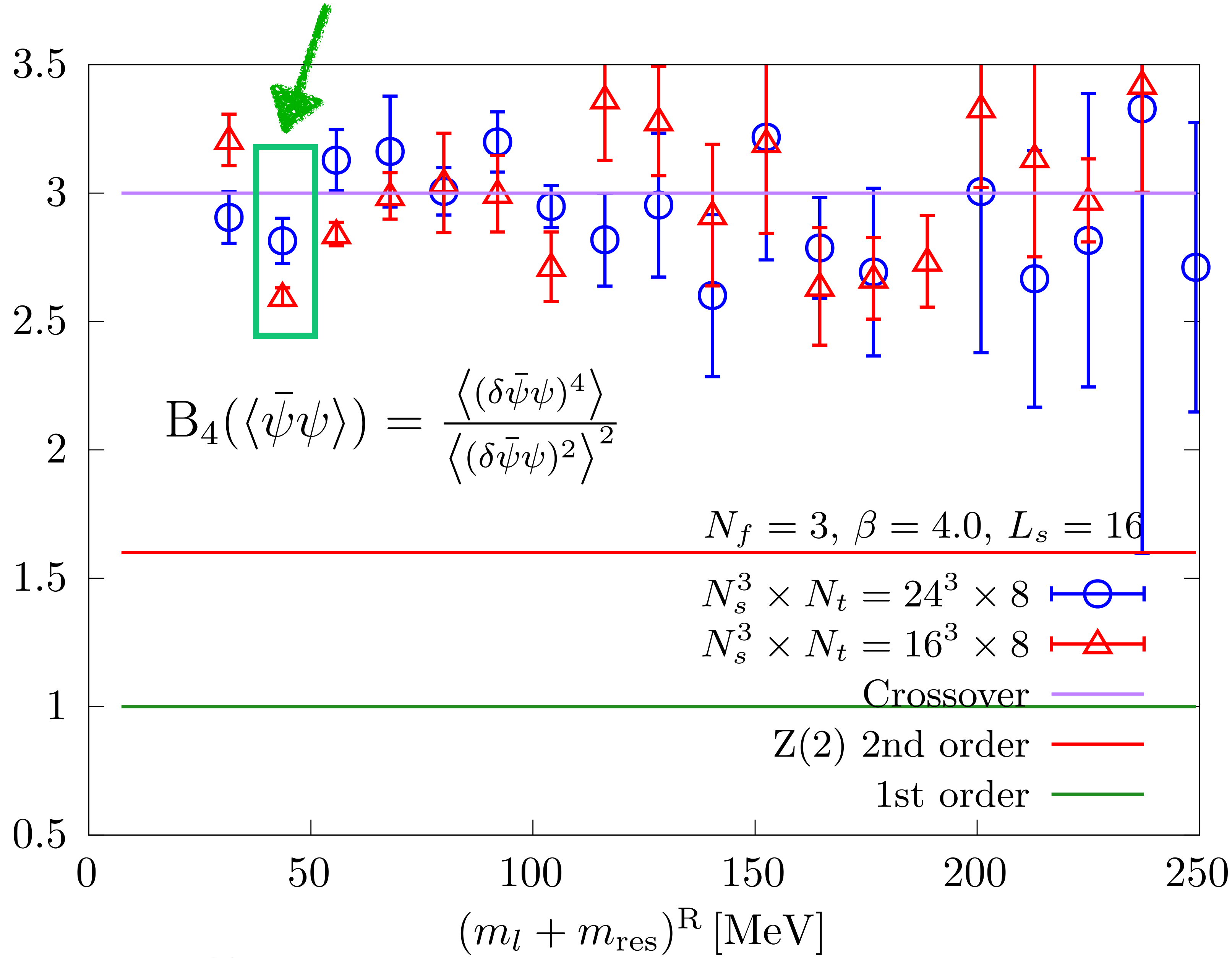
Binder cumulant of chiral condensate at 181.1(2.6) MeV

$$B_4(\bar\psi\psi) = \frac{\langle(\delta\bar\psi\psi)^4\rangle}{\langle(\delta\bar\psi\psi)^2\rangle^2}, \quad \delta\bar\psi\psi = \bar\psi\psi - \langle\bar\psi\psi\rangle$$



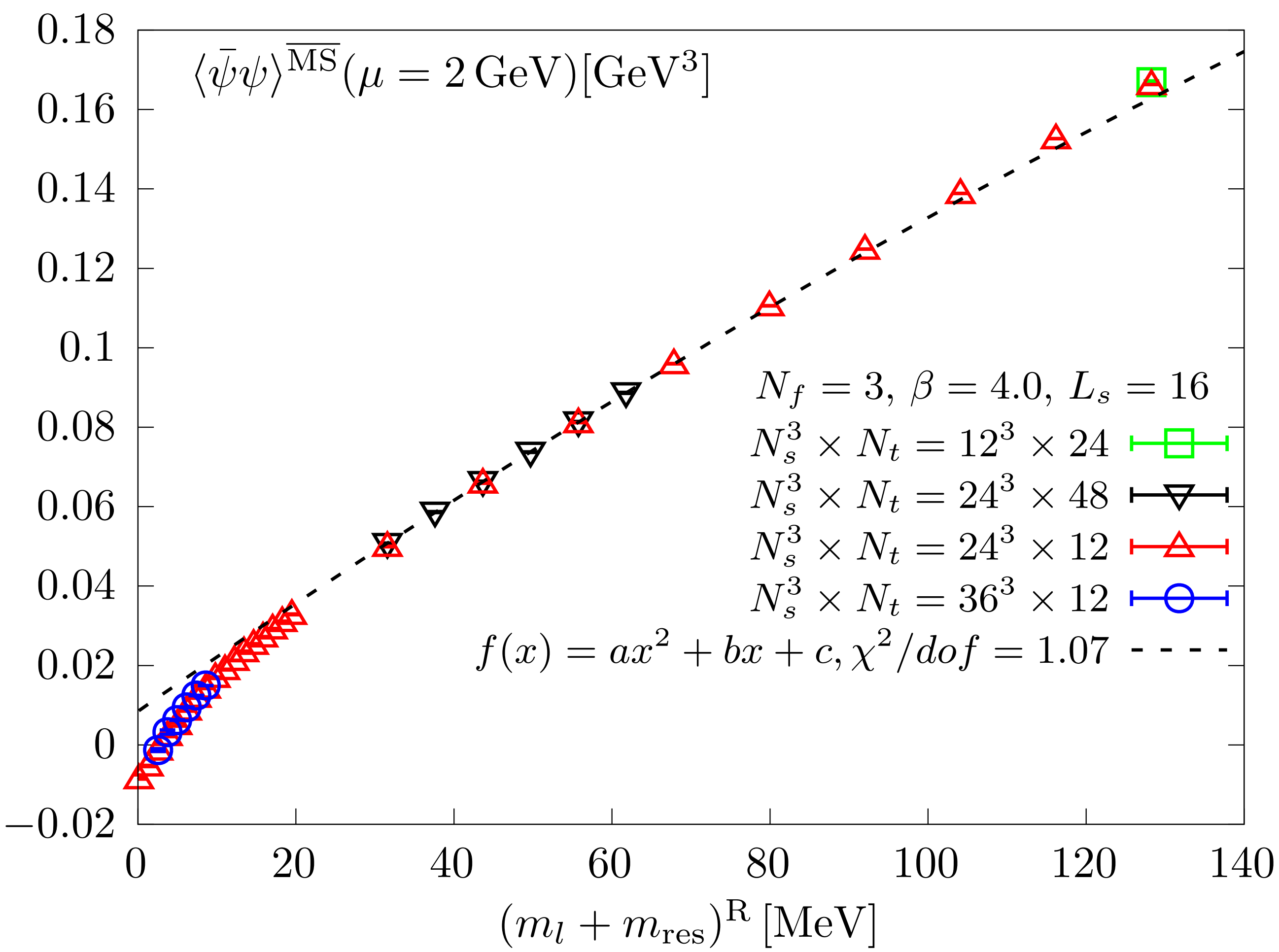


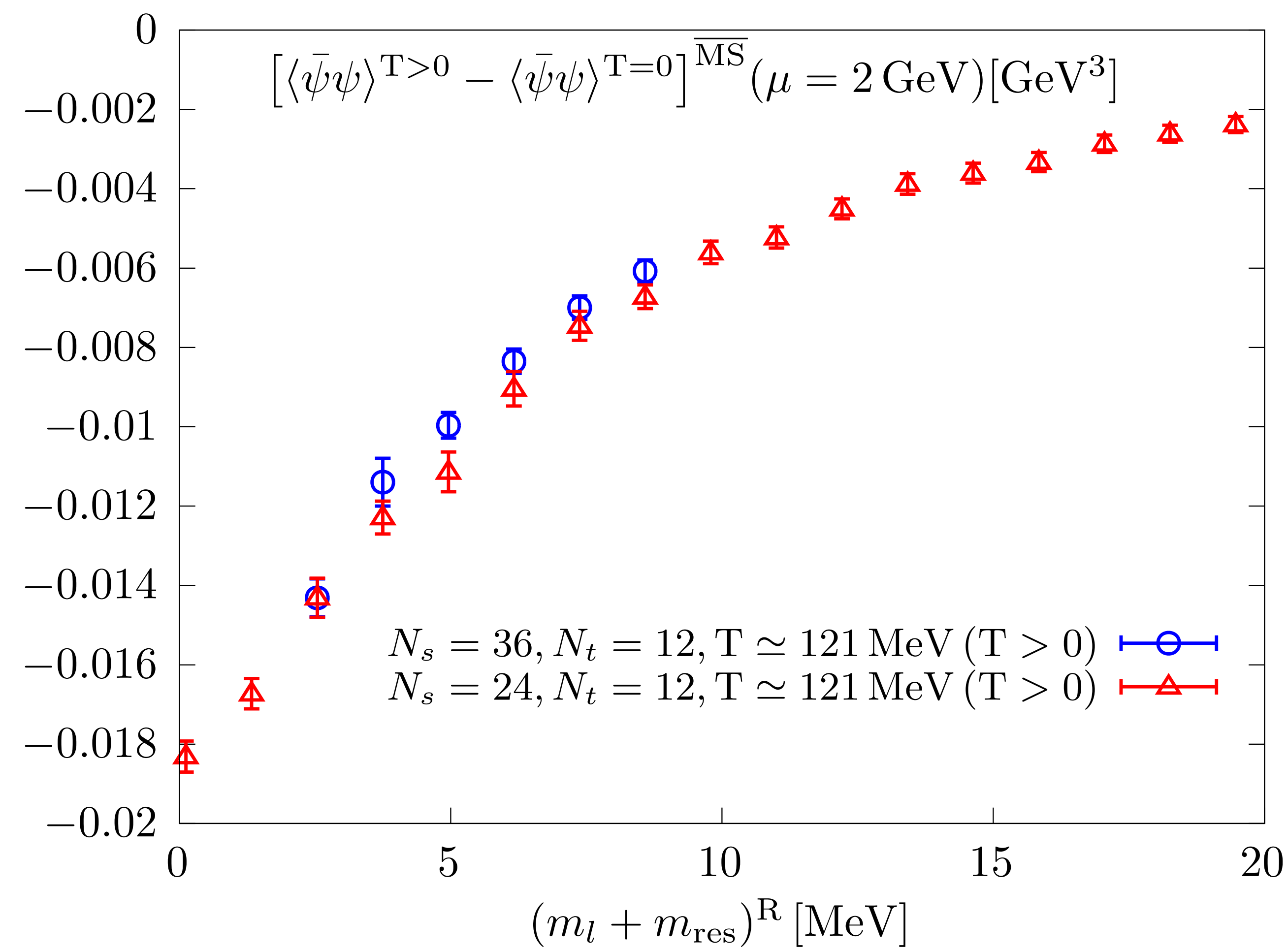
B4 at transition point seems to be a crossover in the thermodynamic limit.



[P. de Forcrand and O. Philipsen, JHEP 07]

Chiral condensate at T~120.8(1.8) MeV

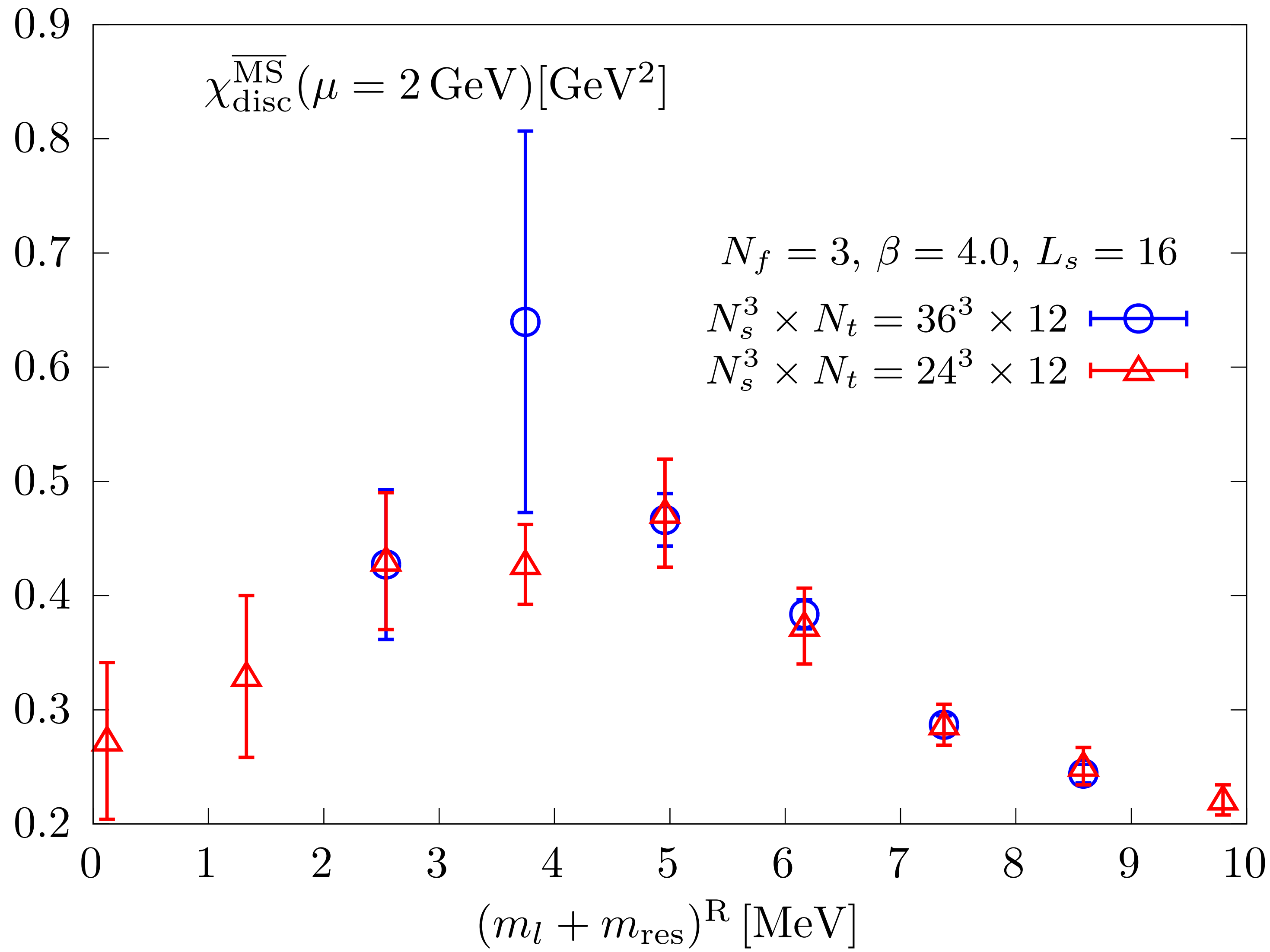




In the chiral limit, the negative result is due to the residual additive divergence

- **Additive & multiplicative divergence has been removed**

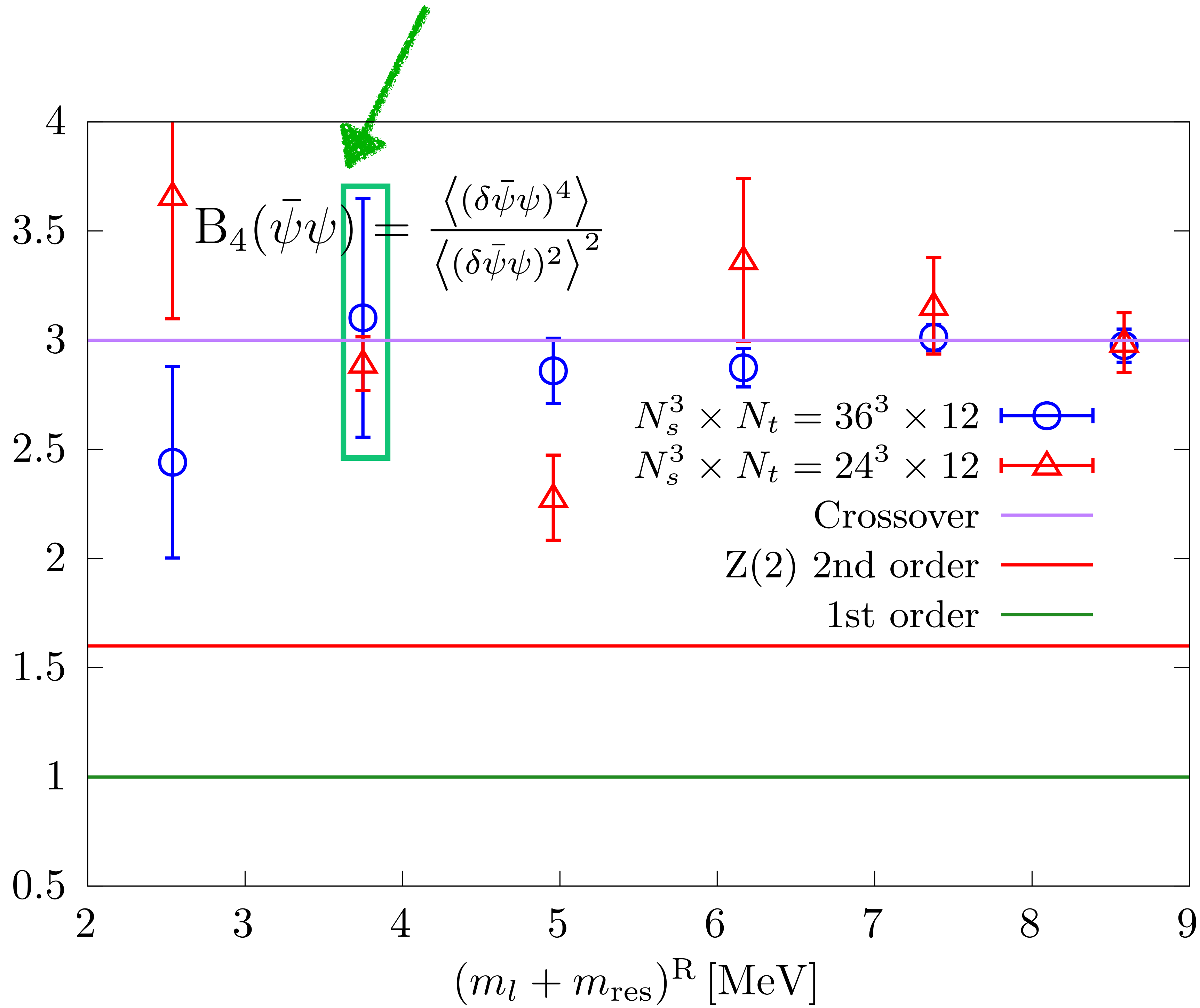
Disconnected chiral susceptibility at 120.8(1.8) MeV



Work in progress, need more statistics

- **Transition point is around 3.7 MeV**

Binder cumulant of chiral condensate at 120.8(1.8) MeV



- **Suggests a crossover phase transition**

Summary and outlook

Summary:

- ☑ For $\langle\bar{\psi}\psi\rangle$, the explicit χ_{SB} effect due to finite Ls is more complicated than a simple additive shift of the input quark mass by $m_{\rm res}$
- ☑ It is a crossover at T~181.1(2.6) MeV, pseudo critical quark mass is around 44 MeV
- ☑ Data suggest a crossover at T~120.8(1.8) MeV and pseudo critical quark mass is around 3.7 MeV

Outlook:

- ☐ Add more statistics for $36^3 \times 12$ and $24^3 \times 12$ lattices
- ☐ Perform simulation for 104 MeV which corresponds to N_t=14
- ☐ Investigate the Ls dependence to check whether our chiral symmetry is ok

Lattice Setup for $N_f = 2+1$

- N_f=2+1 Mobius Domain Wall Fermion with L_s=12
- Symanzik gauge action
- 0.08 < a < 0.14 fm, 121 MeV $\leq$ T $\leq$ 205 MeV

- $\boxed{m_s = m_s^{phys},\ m_l = 0.1 m_s,\ 24^3 \times 12,\ 4.0 < \beta < 4.17\ (a1)}$

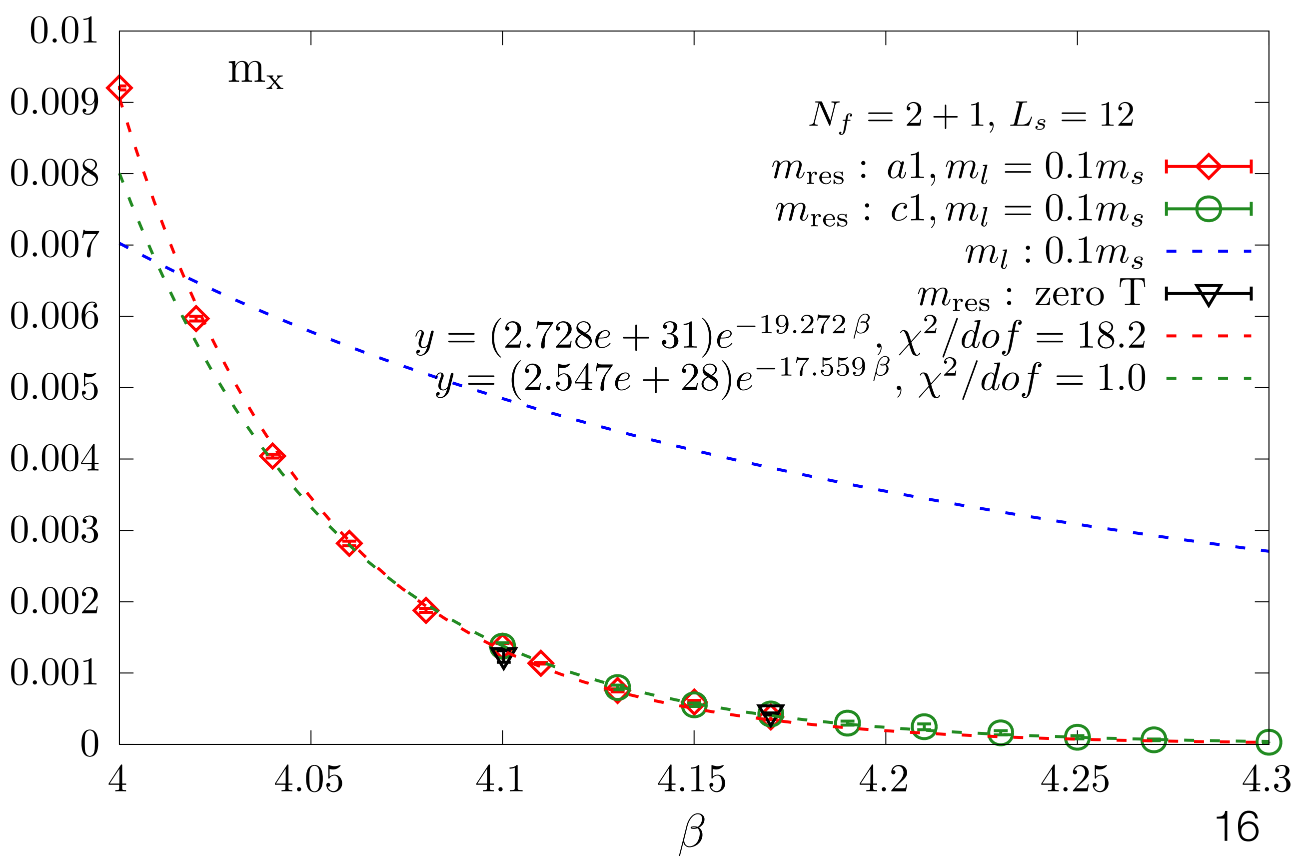
correct m_l by m_{res} for coarse lattice ($N_t = 12$)

- $\boxed{m_s + m_{res} = m_s^{phys}, m_l + m_{res} = 0.1(m_s + m_{res}), 24^3 \times 12, \ldots (d1)}$

$\ldots, 36^3 \times 12, \ldots (d2)$

$\ldots, 48^3 \times 12, \ldots (d3)$

- $\boxed{m_s = m_s^{phys},\ m_l = 0.1 m_s,\ 32^3 \times 16,\ 4.1 < \beta < 4.30\ (c1)}$ $\longrightarrow$ **use mass reweighing**

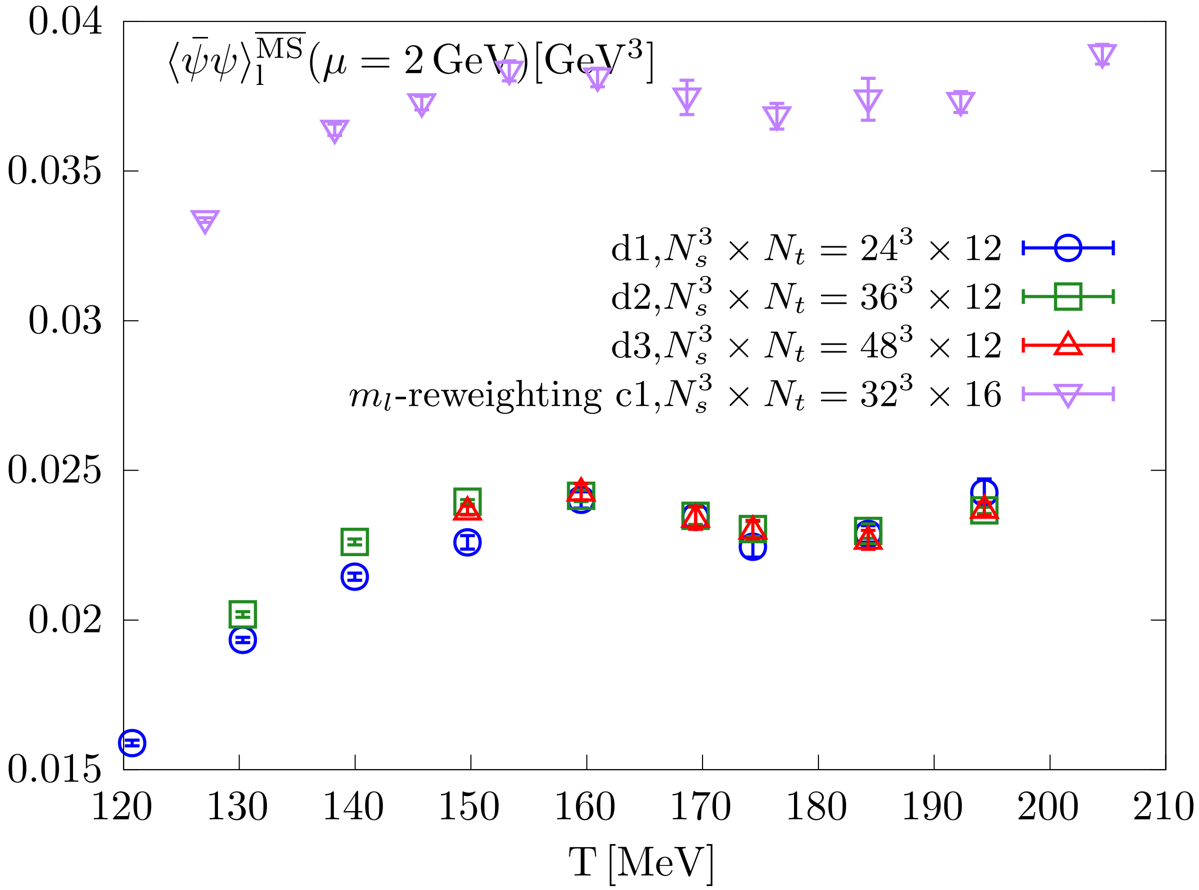


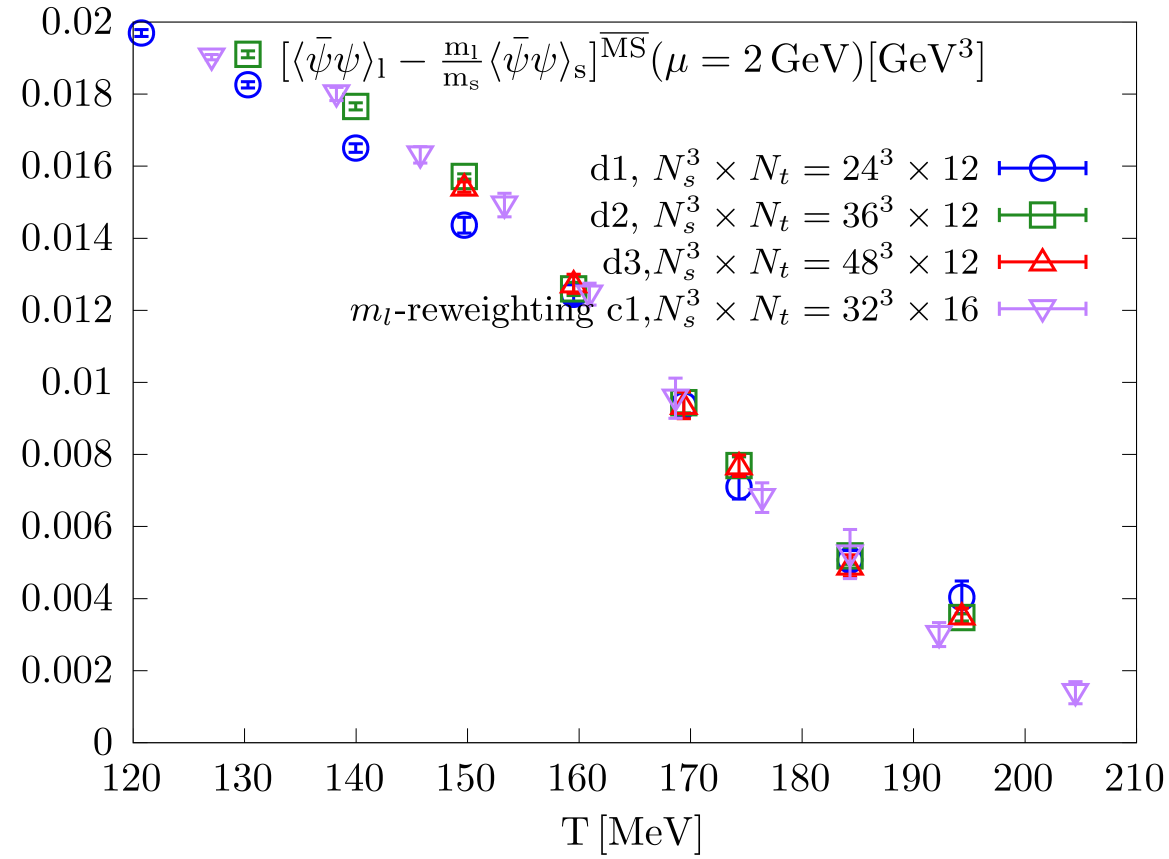
- m_{res} determined at $\beta = 4.1, 4.17$ at finite and zero T are consistent

- m_{res} increases exponentially with decreasing β, $m_{res} > m_l$ at $\beta = 4.0$

The temperature dependence of chiral condensate

$\langle\bar{\psi}\psi\rangle(T)$ signals chiral symmetry breaking and restoration





$$\langle\bar{\psi}\psi\rangle^{\mathrm{reweighting}} = \frac{\langle(\bar{\psi}\psi)w\rangle}{\langle w\rangle}$$

[See J. Goswami's poster for details]

$\langle\bar{\psi}\psi\rangle$ needs multiplicative & additive renormalization for $m \neq 0$

- Multiplicative renormalization: $\langle\bar{\psi}\psi\rangle^{\overline{\mathrm{MS}}}(2\mathrm{GeV}) = \dfrac{a^{-3}(a^3\langle\bar{\psi}\psi\rangle)}{Z_m^{\overline{\mathrm{MS}}}(2\mathrm{GeV})}$
- Subtract the leading additive divergence (~m_l/a^2): $[\langle\bar{\psi}\psi\rangle_l - m_l/m_s\langle\bar{\psi}\psi\rangle_s]$
- Neglect the residual contribution to $\langle\bar{\psi}\psi\rangle$: $\dfrac{x m_{\mathrm{res}}}{a^2}$, $x < 0.03$ [See Y. Aoki's poster for details]

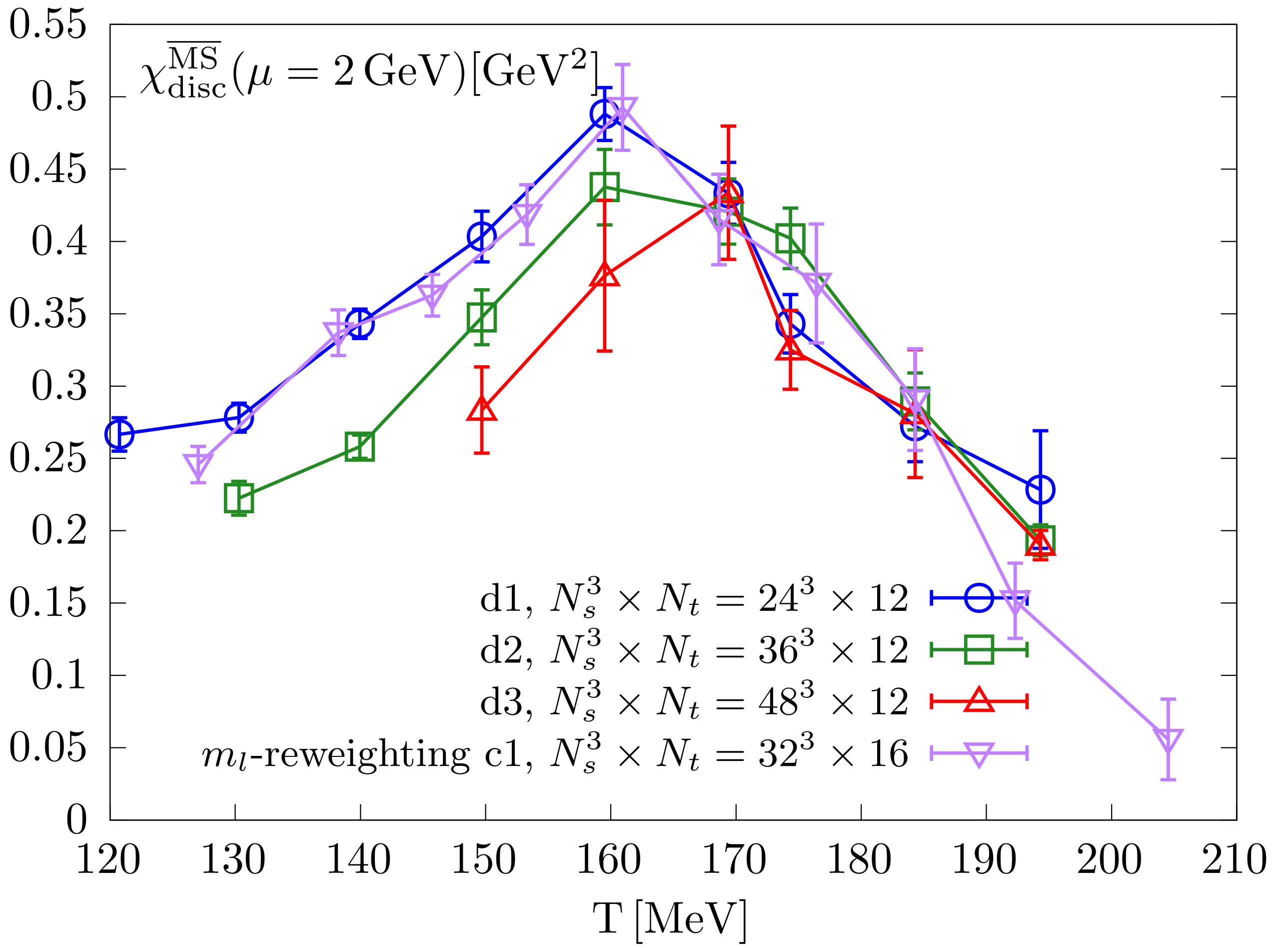
The temperature dependence of disconnected susceptibility

Describes fluctuations of the chiral condensate & Peak at transition point

$$\chi_{\rm disc} = N_s^3 N_t \left(\left\langle (\bar\psi\psi)^2 \right\rangle - \langle \bar\psi\psi \rangle^2 \right)$$

Renormalized to $\overline{\rm MS}(\mu = 2\,{\rm GeV})$ with $({\rm Z}_{\rm m}^{\overline{\rm MS}})^{-2}$: $\chi_{\rm disc}^{\overline{\rm MS}}(\mu = 2\,{\rm GeV})[{\rm GeV}^2] = \left(\frac{1}{Z_m^{\overline{\rm MS}}} \right)^2 \chi_{\rm disc}^{\rm bare} \; (a^{-2}[{\rm GeV}^2])$

$$\chi_{\rm disc}^{\rm reweighting} = N_s^3 N_t \left(\frac{\left\langle (\bar\psi\psi)^2 w \right\rangle}{\langle w \rangle} - \frac{\langle (\psi\bar\psi) w \rangle^2}{\langle w \rangle^2} \right)$$



- Small finite a effect: d1 & c1
- Small finite V effect at $T \gtrsim T_{pc}$ and large finite V effects at $T < T_{pc}$
- It's a crossover phase transition since no increase in the peak height of $\chi_{\rm disc}$ with increasing V is observed
- Peak position shifts to larger T as V is increased
- The transition T is around 160-175 MeV
- Work in progress, need more statistics for d3

Summary and outlook

Summary:

- T_{pc} is around 160-175 MeV for $m_l + m_{res} = 0.1 m_s^{phys}$
- Mass reweighing works for the fine lattice

Outlook:

- Need more statistics for $48^3 \times 12$ lattices with $m_l + m_{res} = 0.1 m_s^{phys}$
- Simulation for the physical quark mass
- m_{res} effect in the chiral condensate need to be better understand

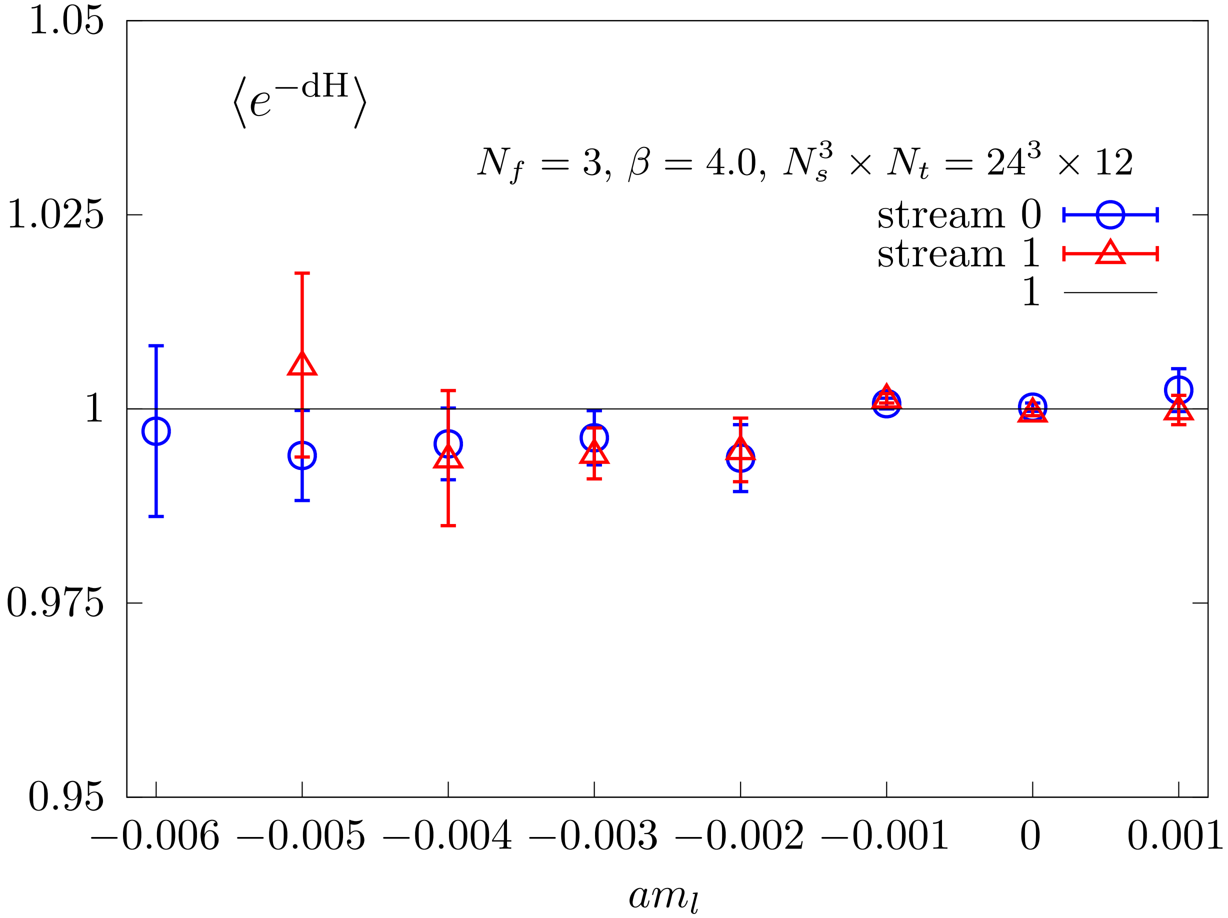
Acknowledgements

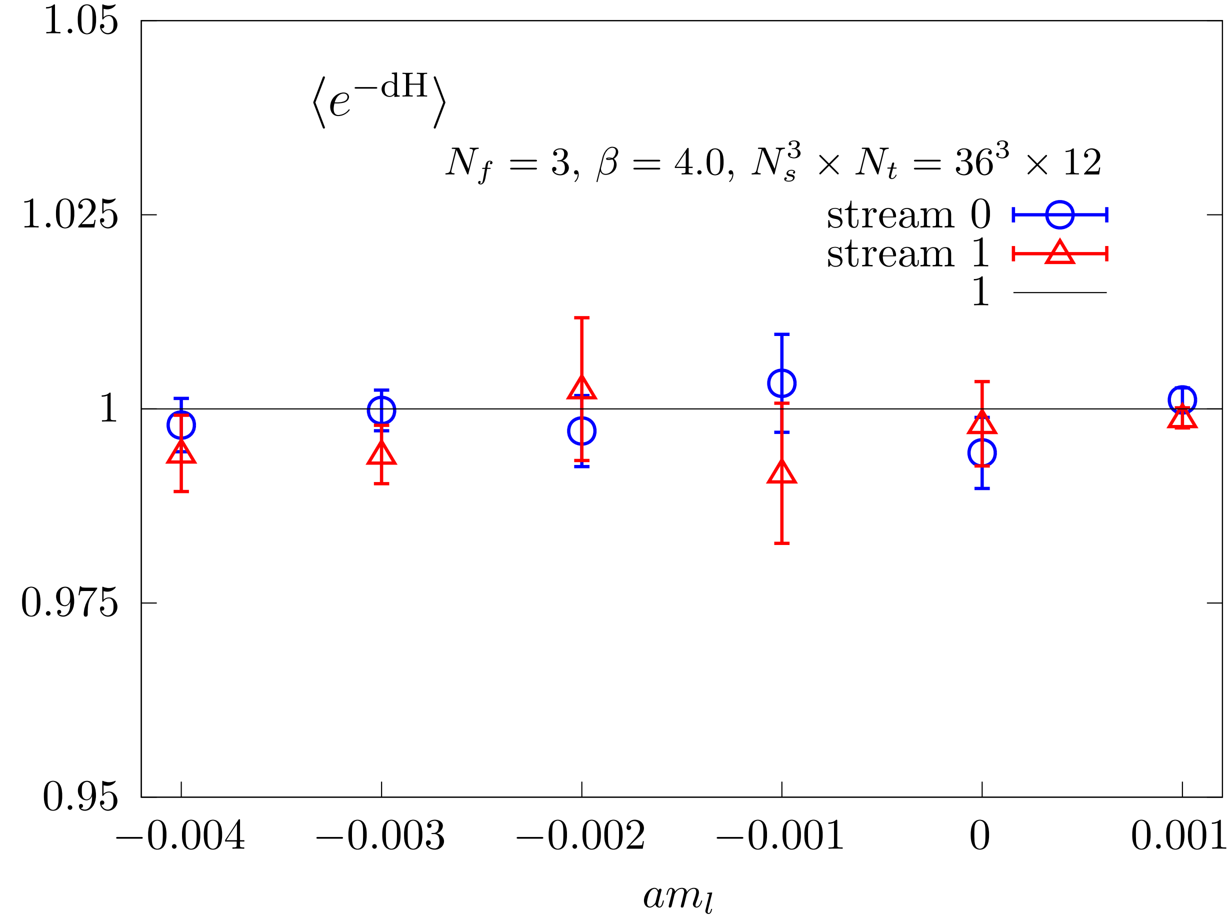
- Codes
  - HMC
    - Grid (Regensburg branch)
  - Measurements
    - Bridge++
    - Hadrons / Grid

- Computers
  - Supercomputer Fugaku provided by the RIKEN Center for Computational Science through HPCI project #hp210032 and Usability Research ra000001.
  - Wisteria/BDEC-01 Oddysey at Univ. Tokyo/JCAHPC through HPCI project #hp220108 Ito supercomputer at Kyushu University through HPCI project #hp190124 and hp200050
  - Hokusai BigWaterfall at RIKEN

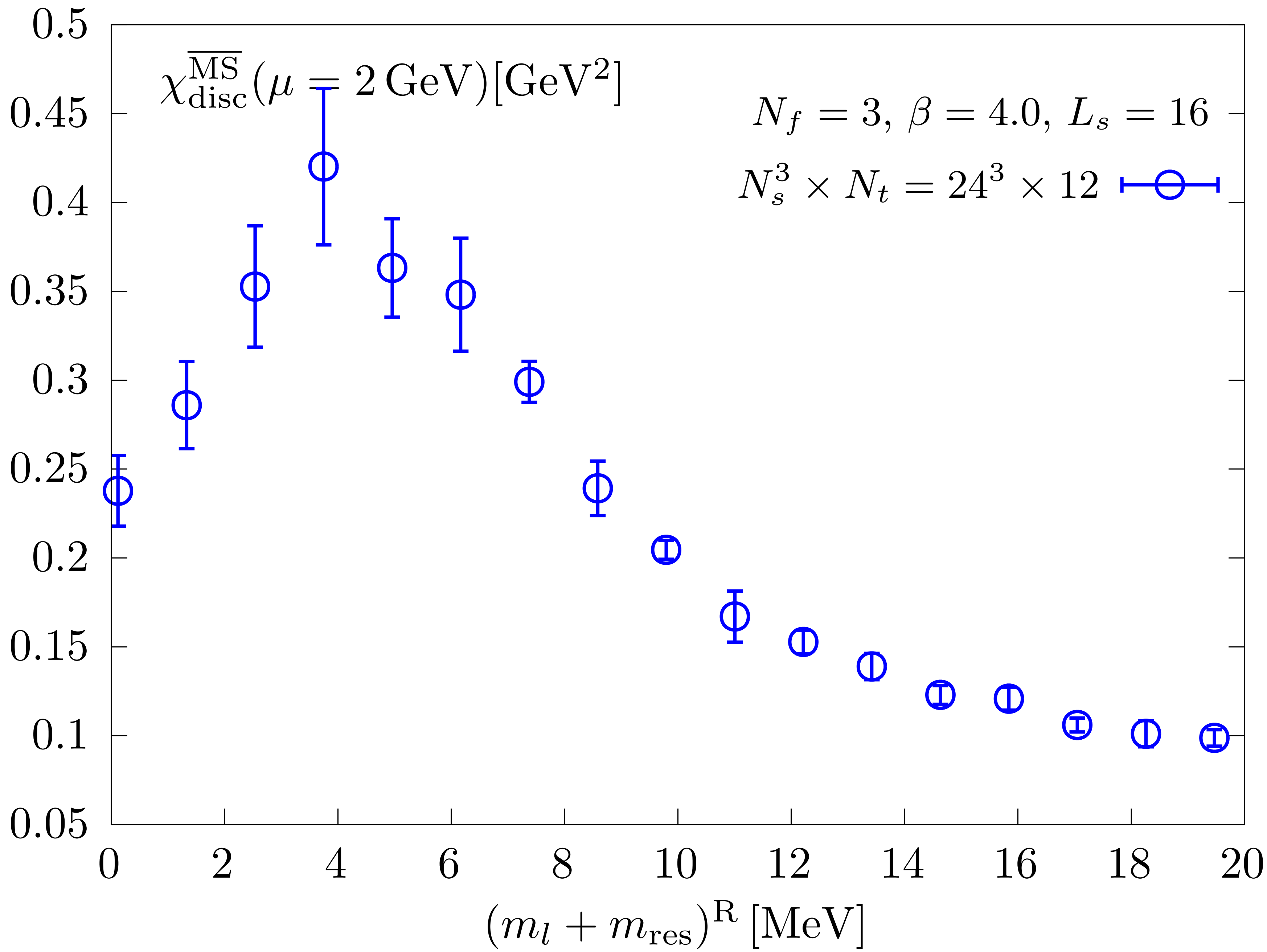
- Grants
  - JSPS Kakenhi (20H01907)

Backup


$\langle e^{-\mathrm{dH}} \rangle$
$N_f = 3,\ \beta = 4.0,\ N_s^3 \times N_t = 24^3 \times 12$
stream 0
stream 1
1
1.05
1.025
1
0.975
0.95
−0.006
−0.005
−0.004
−0.003
−0.002
−0.001
0
0.001
am_l


$\langle e^{-\mathrm{dH}} \rangle$
$N_f = 3,\ \beta = 4.0,\ N_s^3 \times N_t = 36^3 \times 12$
stream 0
stream 1
1
1.05
1.025
1
0.975
0.95
−0.004
−0.003
−0.002
−0.001
0
0.001
am_l

Disconnected chiral susceptibility at 120.8(1.8) MeV



- **Transition point is around 3.7 MeV**

Light Quark mass reweighing

We are usually not able to identify in advance the input bare quark mass that will correspond to a target renormalized mass, Quark mass reweighting allows us to fine tune the dynamic light quark mass to the nearby sea quark mass after an ensemble has been generated

The expectation value of O on ensembles with light sea quark mass m_2 can be calculated from an ensemble generated with sea quark mass m_1 as:

$$\langle O\rangle_2 = \frac{1}{Z_2}\int DU\, O\, e^{-S_g} \frac{\det\{D^\dagger(m_2)D(m_2)\}}{\det\{D^\dagger(1.0)D(1.0)\}} \frac{\sqrt{\det\{D^\dagger(m_s)D(m_s)\}}}{\sqrt{\det\{D^\dagger(1.0)D(1.0)\}}}. \tag{1}$$

$$\begin{aligned} &\langle O\rangle_2 \qquad (2)\\ &= \frac{Z_1}{Z_2}\cdot\frac{1}{Z_1}\int DU \left[O\, \frac{\det\{D^\dagger(m_2)D(m_2)\}}{\det\{D^\dagger(m_1)D(m_1)\}}\right] e^{-S_g} \frac{\det\{D^\dagger(m_1)D(m_1)\}}{\det\{D^\dagger(1.0)D(1.0)\}} \frac{\sqrt{\det\{D^\dagger(m_s)D(m_s)\}}}{\sqrt{\det\{D^\dagger(1.0)D(1.0)\}}}\\ &= \frac{\langle O\, w(m_1,m_2)\rangle_1}{\langle w(m_1,m_2)\rangle_1}. \qquad (3)\end{aligned}$$

$$w(U;m_1,m_2) = \frac{\det\{D^\dagger(U,m_2)D(U,m_2)\}}{\det\{D^\dagger(U,m_1)D(U,m_1)\}} \tag{4}$$

- Performe a similar process to write the ratio Z_1/Z_2 as $\langle w(m_1,m_2)\rangle_1$
- Reweighting a conf. from m_1 to m_2 requires the evaluation of $w(U;m_1,m_2)$ for each conf.