Exploring the QCD phase diagram with three flavors of Möbius domain wall fermions

Yu Zhang

(RIKEN R-CCS)

In collaboration with

Y. Aoki, S. Hashimoto, I. Kanamori, T. Kaneko, Y. Nakamura

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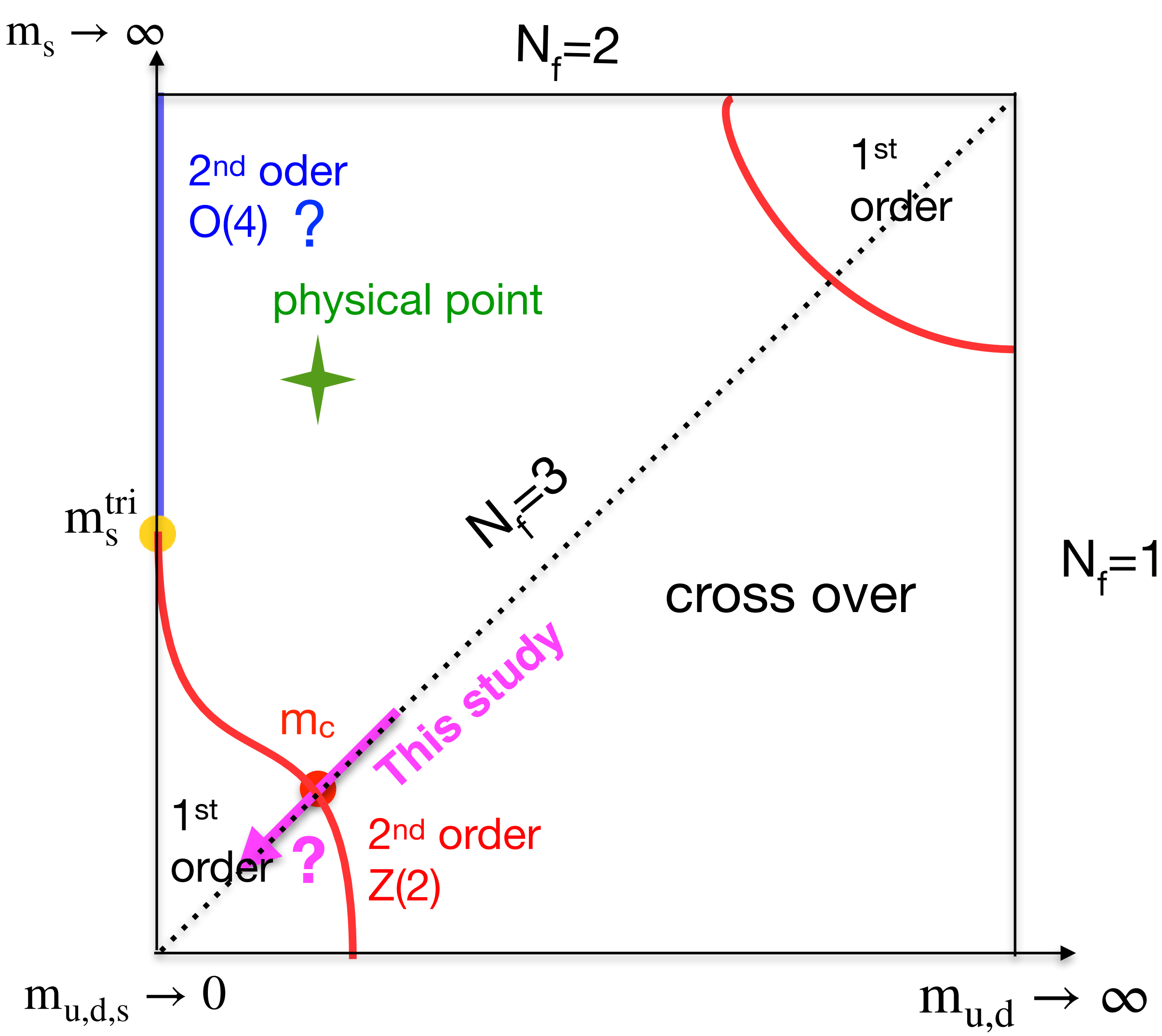
Outline

- Background & Motivation
- Previous lattice studies
- Lattice setup
- Results
- Summary & Outlook

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.**
Staggered,standard	4	290	Karsch et al. (2001)
Staggered,standard	6	150	de Forcrand et al. (2007)
Staggered, HISQ	6	$\lesssim 50$	Bazavov et al. (2017)
Staggered, stout	4-6	$0?$	Varnhost (2014)
Staggered, HISQ	8	$\lesssim 80$	Dini et al. (2022)
Wilson, standard	4	$\lesssim 670$	Iwasaki et al. (1996)
Wilson-Clover	6-10	$\lesssim 170$	Jin et al. (2017)
Wilson-Clover	6-12	$\lesssim 110$	Kuramashi et al. (2020)

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

1st order region shrinks as $a \to 0$ or even disappear
with both staggered and Wilson fermions

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

- N_f=3 Mobius Domain Wall Fermion
- Tree-level Symanzik improved gauge action and stout smearing 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_s=24, N_t=48, L_s=16: $0.02 \leq am_q \leq 0.045$, $am_{\text{res}}(\text{estimated}) \approx 0.006$

☆ T > 0:

N_t=12 (T=120.8(1.8) MeV), L_s=16: N_s=36, $-0.005 \leq am_q \leq 0.001$

N_s=24, $-0.006 \leq am_q \leq 0.1$

L_s=32: N_s=24, $-0.001 \leq am_q \leq 0.003$

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

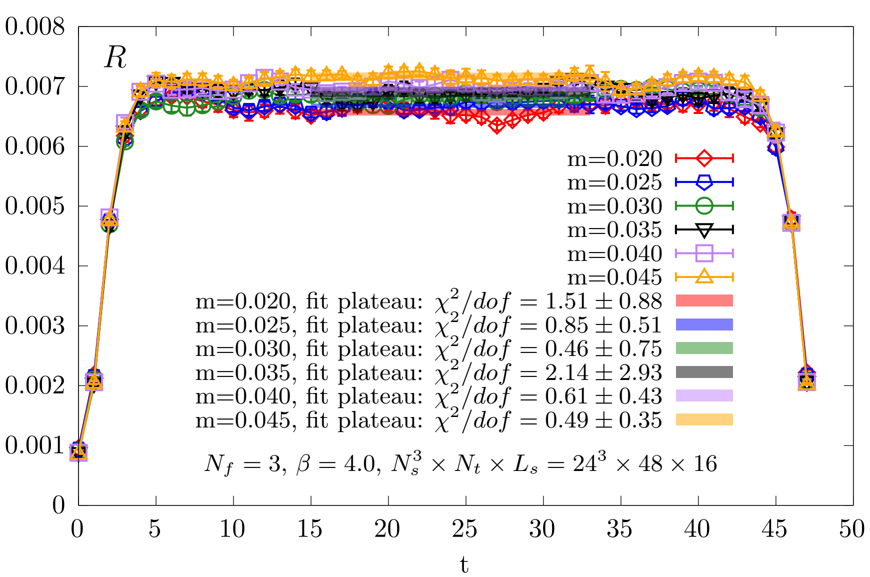
Residual chiral symmetry breaking

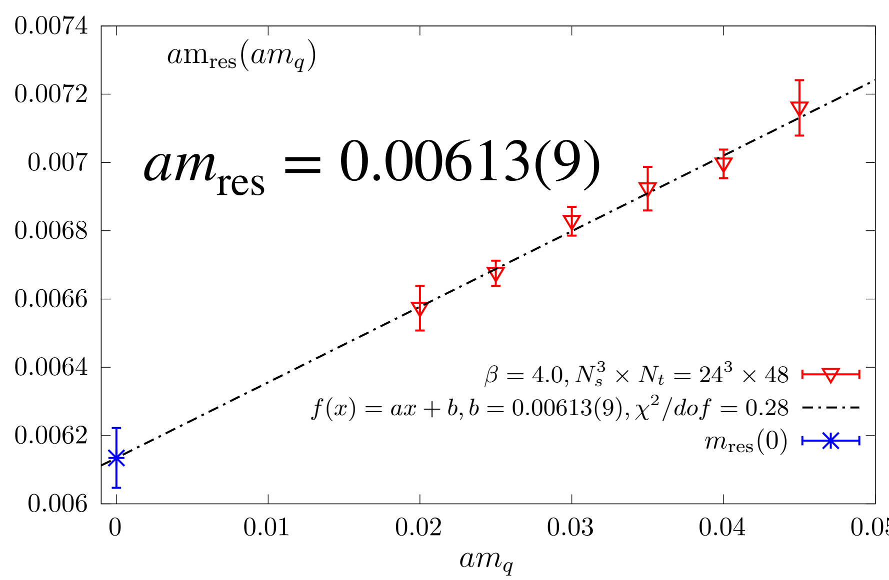
- For finite Ls chiral symmetry is broken, its leading contribution is equivalent to an additive renormalization to the input quark mass m_q, which knows as m_{res}, so the total quark mass becomes $m_q + m_{\text{res}}$

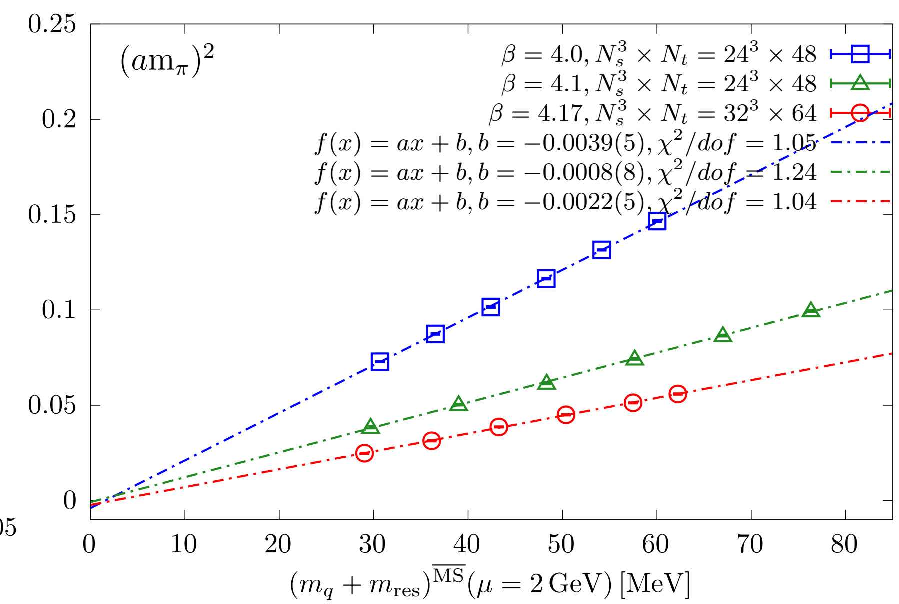
- Measure the ratio of midpoint correlator to the pion correlator evaluated at large distance

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

Intercept zero within error at $m_q = -m_{\text{res}}$







- $\langle \bar\psi\psi \rangle|_{DWF} \sim C\dfrac{m_q + x m_{res}}{a^2} + \langle \bar\psi\psi \rangle|_{\text{cont.}} + \ldots,$ x is not known , expected $x = \mathcal{O}(1)$

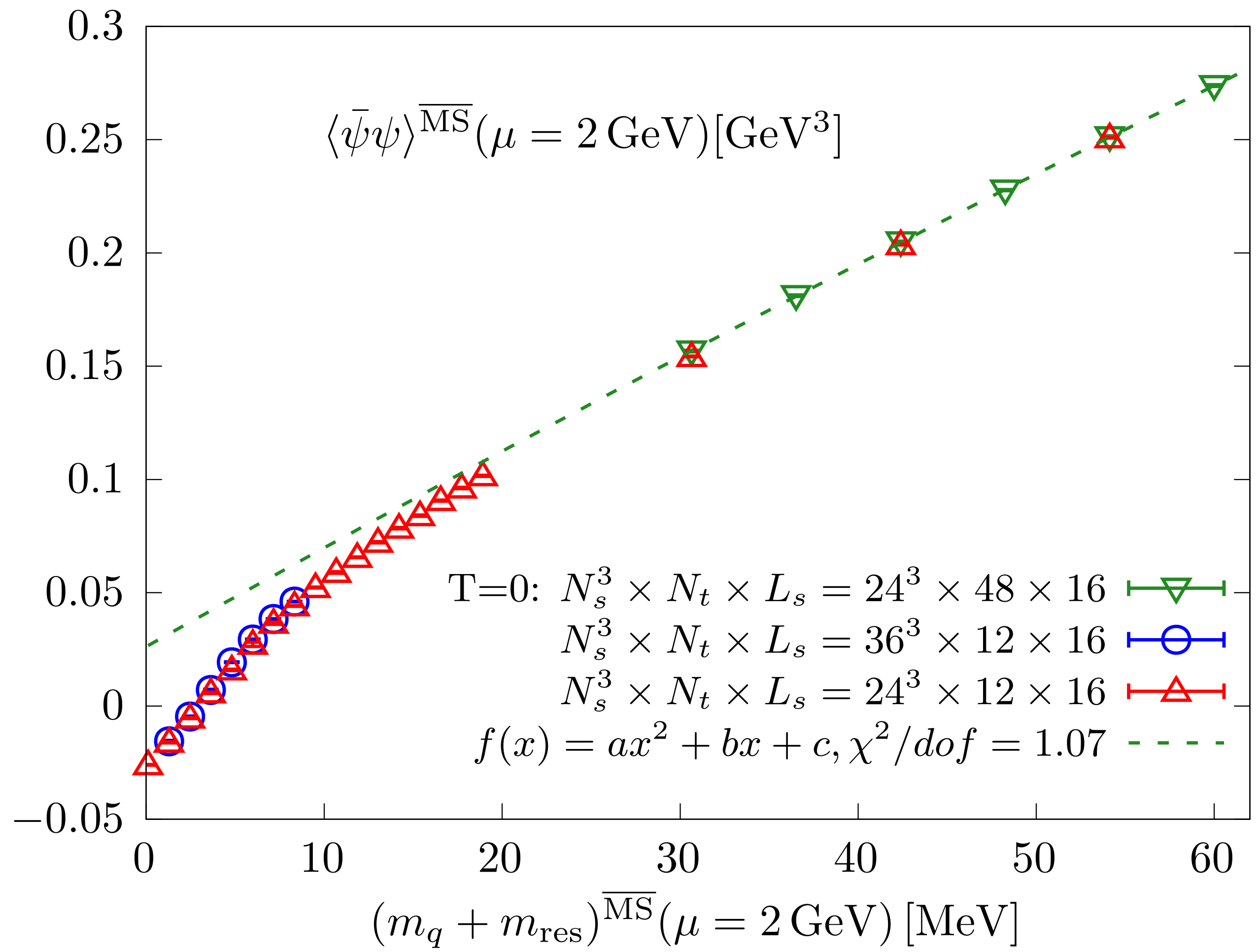
Additive divergence remains if one extrapolates to $m = m_q + m_{res} = 0$:

➡ $\lim_{m\to 0}\lim_{V\to 0} \langle \bar\psi\psi \rangle|_{DWF} \sim \langle \bar\psi\psi \rangle|_{\text{cont.}} + C(x-1)\dfrac{m_{res}}{a^2}\ldots$

[S. Sharpe, arXiv: 0706.0218]

Chiral condensate at T~121 MeV

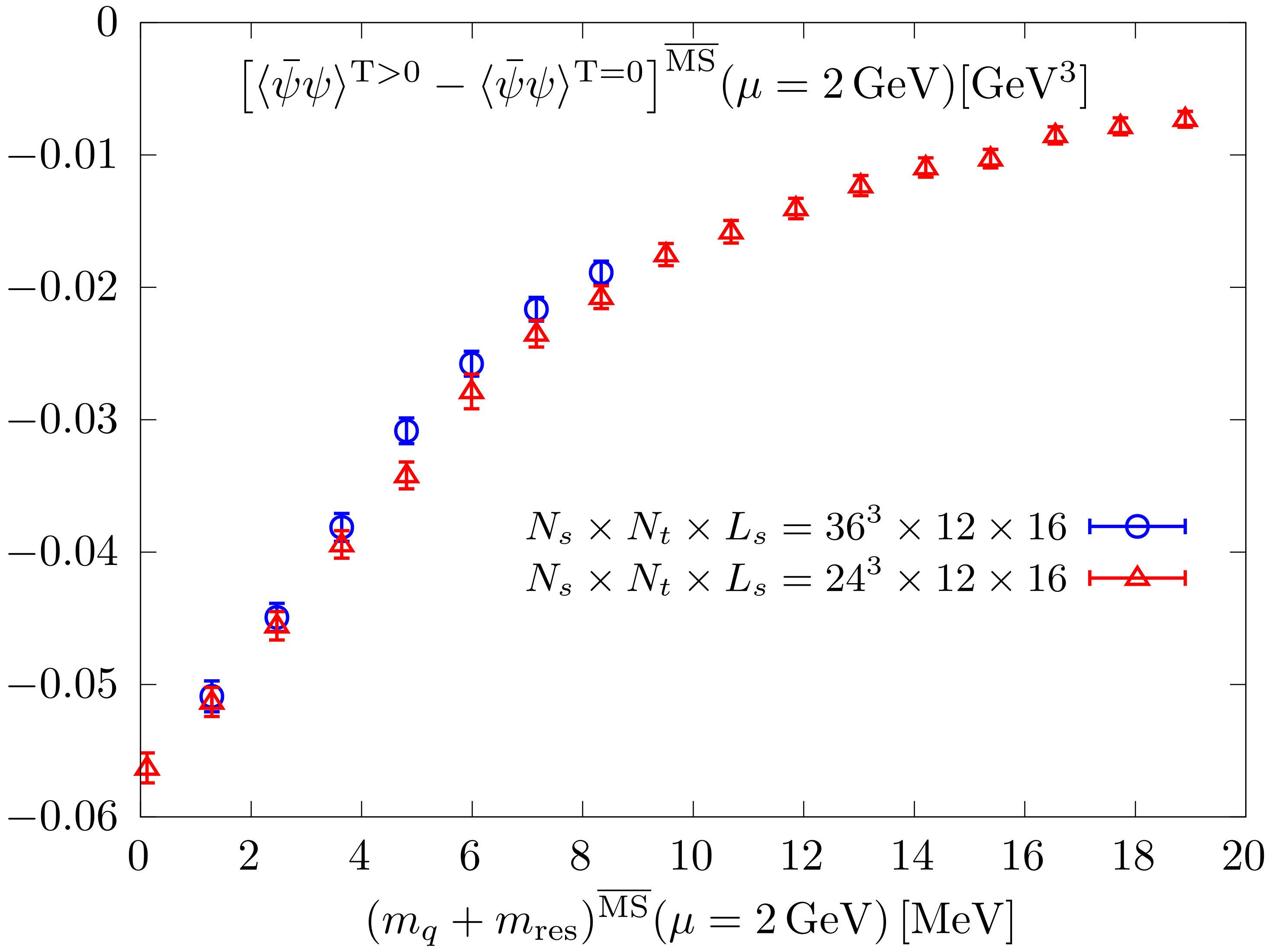
Order parameter for χ_{SB}: $\langle \bar{\psi}\psi \rangle = \dfrac{N_f}{N_s^3 N_t} \mathrm{Tr} \langle M^{-1} \rangle$



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

Chiral condensate at T~121 MeV

Additively and multiplicatively renormalized order parameter

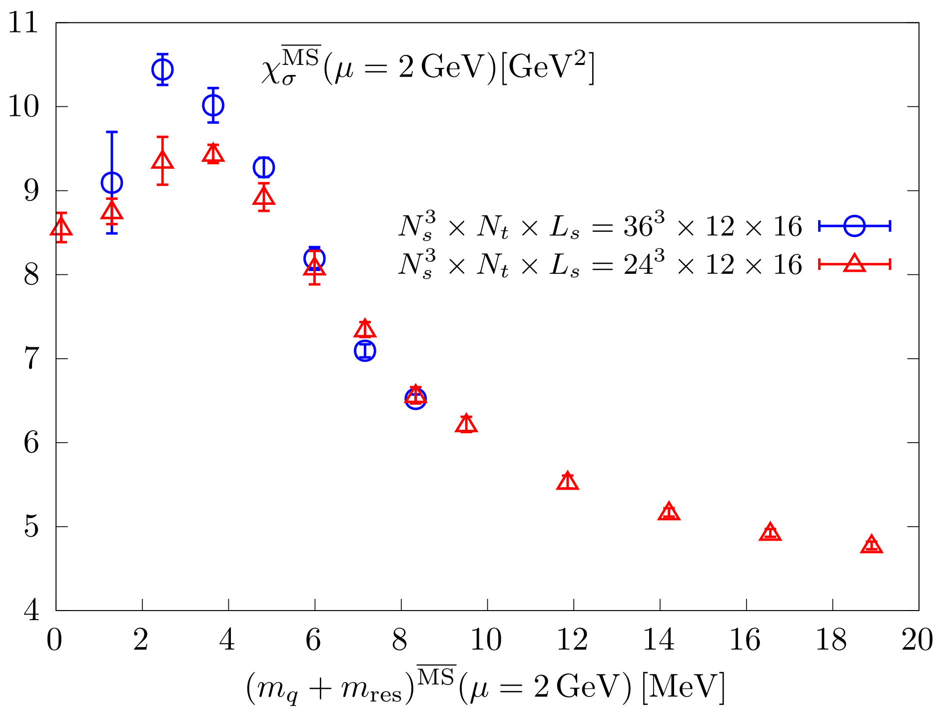


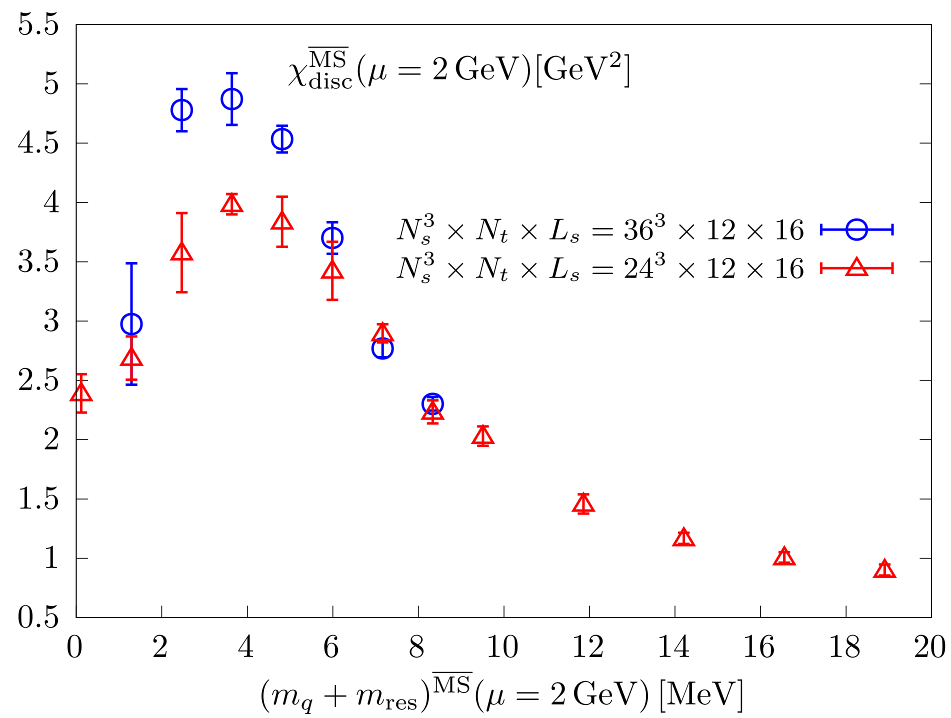
Finite size dependence is visible around $(m_q + m_{\mathrm{res}})^{\overline{\mathrm{MS}}} \sim 4 - 9\,\mathrm{MeV}$

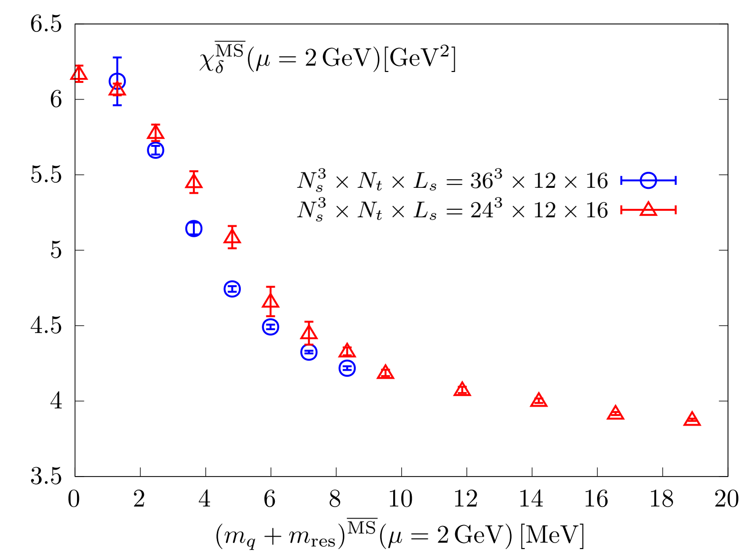
Chiral susceptibility at T~121 MeV

$$\chi_\sigma = \frac{T}{V}\frac{\partial^2 \ln Z}{\partial m^2} = \chi_{\rm disc} + \chi_{\rm con},\ \ \chi_{\rm disc} = \frac{N_f^2}{N_s^3 N_t}\left[\left\langle\left(\mathrm{Tr}\,M^{-1}\right)^2\right\rangle - \left\langle\mathrm{Tr}\,M^{-1}\right\rangle^2\right],\ \ \chi_{\rm con} = -\frac{N_f}{N_s^3 N_t}\langle \mathrm{Tr}\,M^{-2}\rangle$$

Renormalize susceptibility to $\overline{\rm MS}(\mu = 2\,{\rm GeV})$ with $(Z_m^{\overline{\rm MS}})^{-2}$ to remove the multiplicative divergence







- **The change in peak height & position for $\chi_{\rm disc}$ and χ_σ is not as large as anticipated from the first order transition (see next slide)**
  - ➡ **Consistent with the crossover rather than true phase transition**

For crossover transition, the peak height of susceptibility would be volume independent for large volumes, currently $48^3 \times 12$ simulation is underway

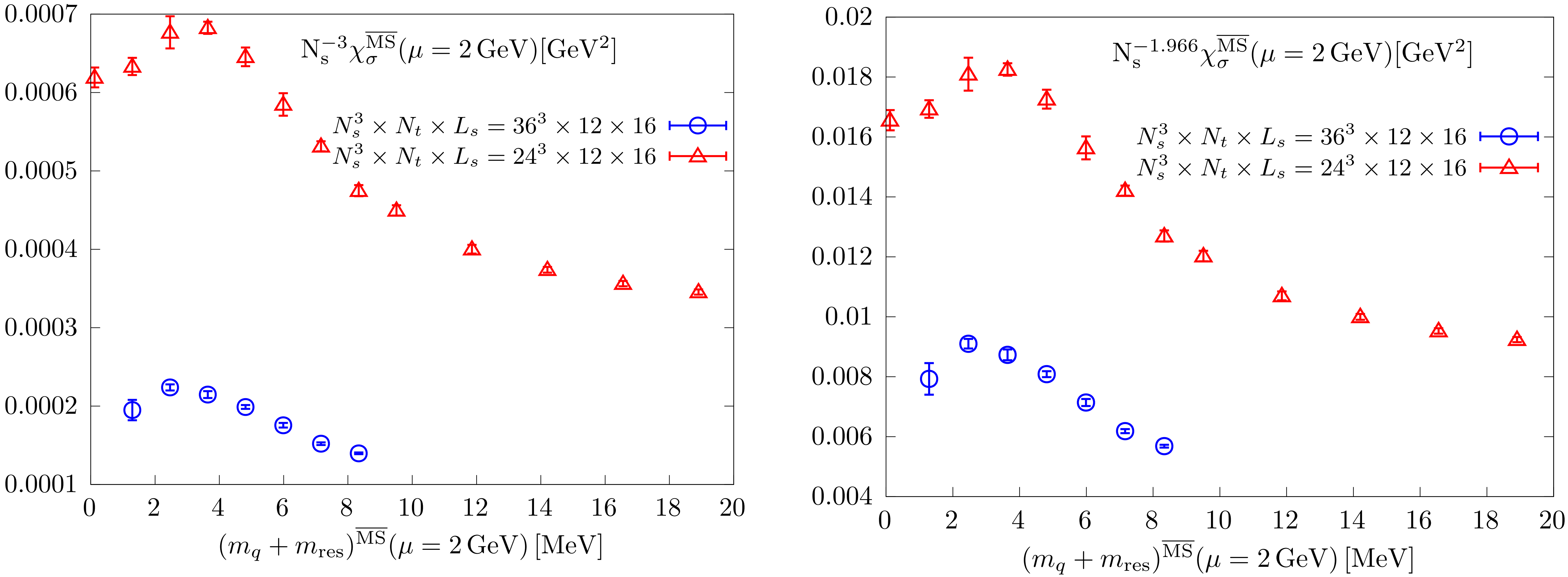
- **The transition mass point determined from $\chi_{\rm disc}$ and χ_σ is around 3.6 MeV & 2.5 MeV in the $\overline{\rm MS}$ scheme at a scale of μ=2 GeV, they coincide in the chiral phase transition temperature**

Finite size scaling: susceptibility χ_σ at T~121 MeV

Finite size scaling function for the susceptibility at critical point:

$$\chi_\sigma^{\max}(N_s) \sim \begin{cases} N_s^3, & \text{first order phase transition} \\ N_s^{1.966} & \text{Z(2) second order phase transition} \end{cases}$$

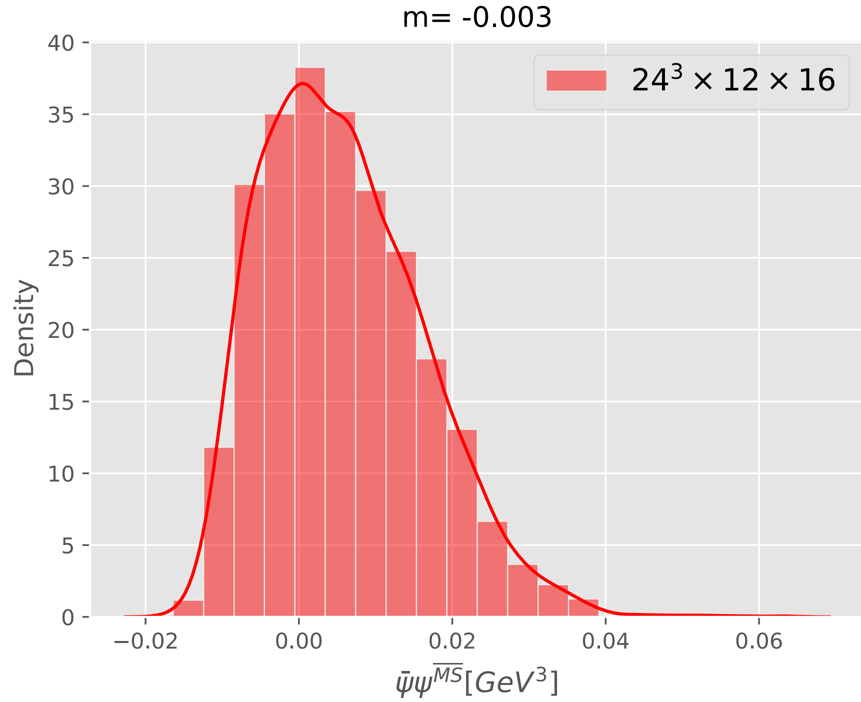
finite-size scaled susceptibility



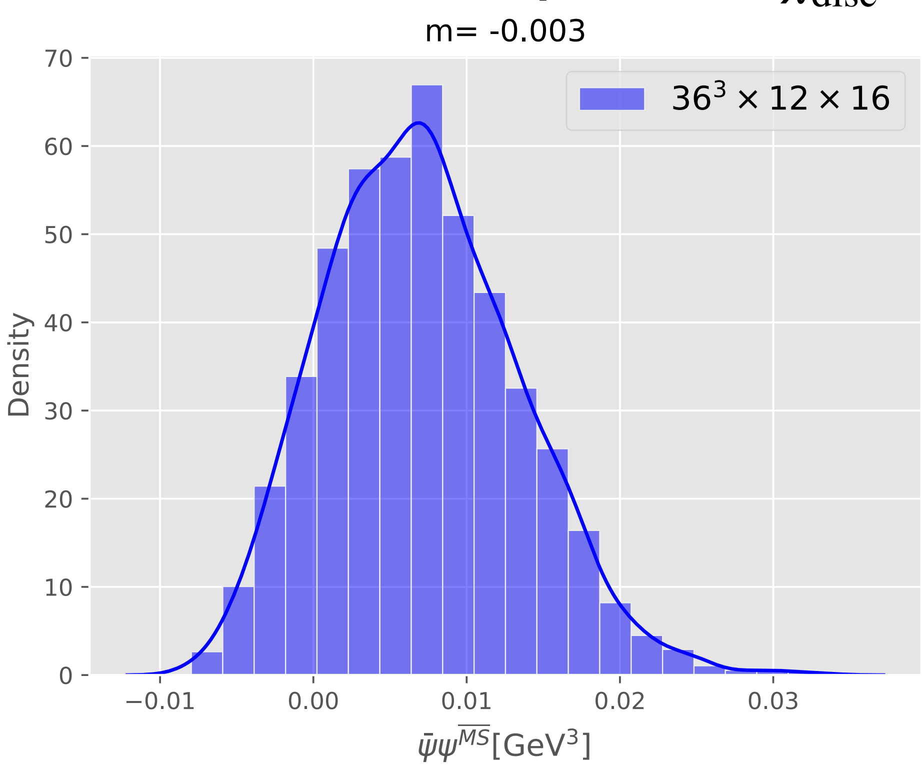
The peak height of chiral susceptibility does not scale like a first order and Z(2) second order phase transition

The histogram of chiral condensate at T~121 MeV

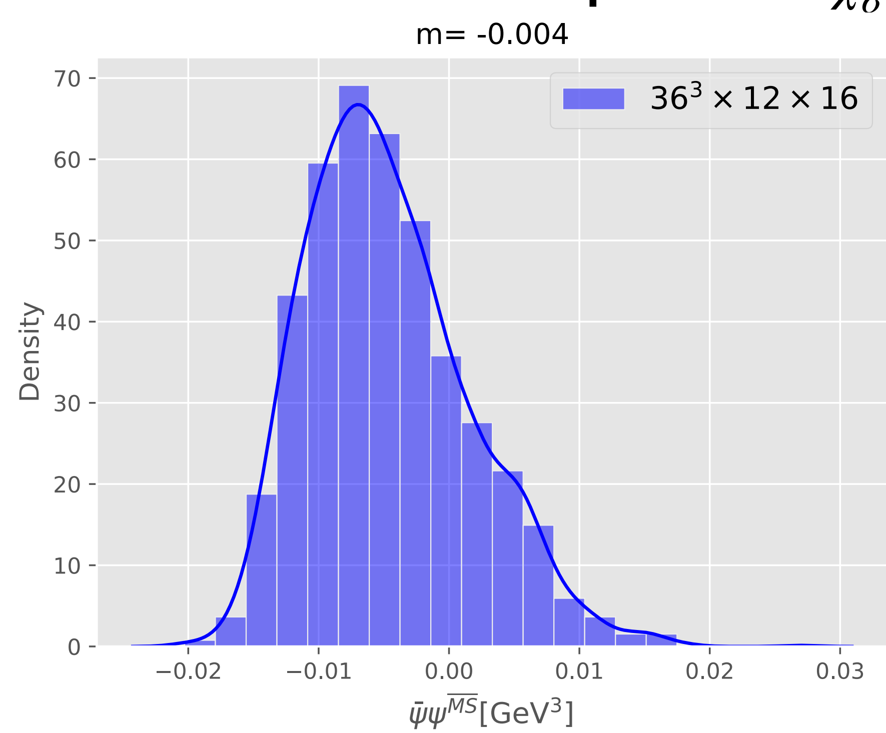
The normalized histogram at transition mass point determined from $\chi_{\rm disc}$ and χ_σ →



At transition mass point from $\chi_{\rm disc}$



At transition mass point from χ_σ

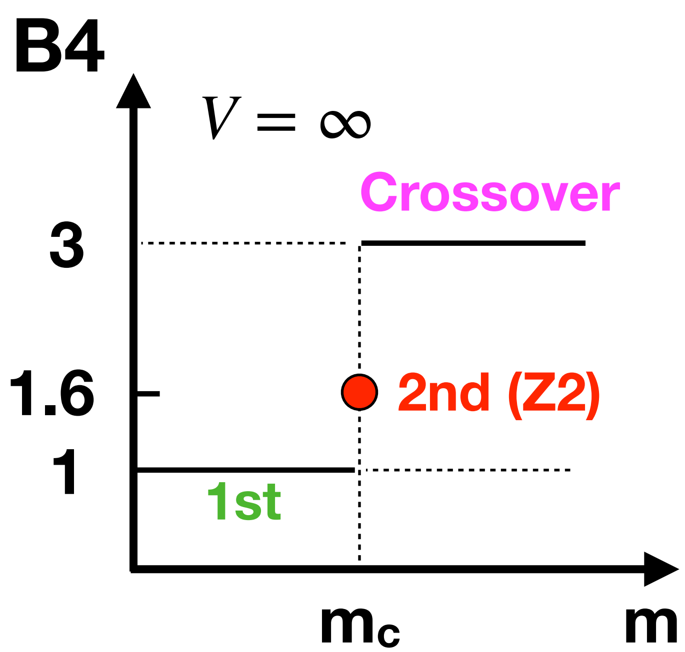


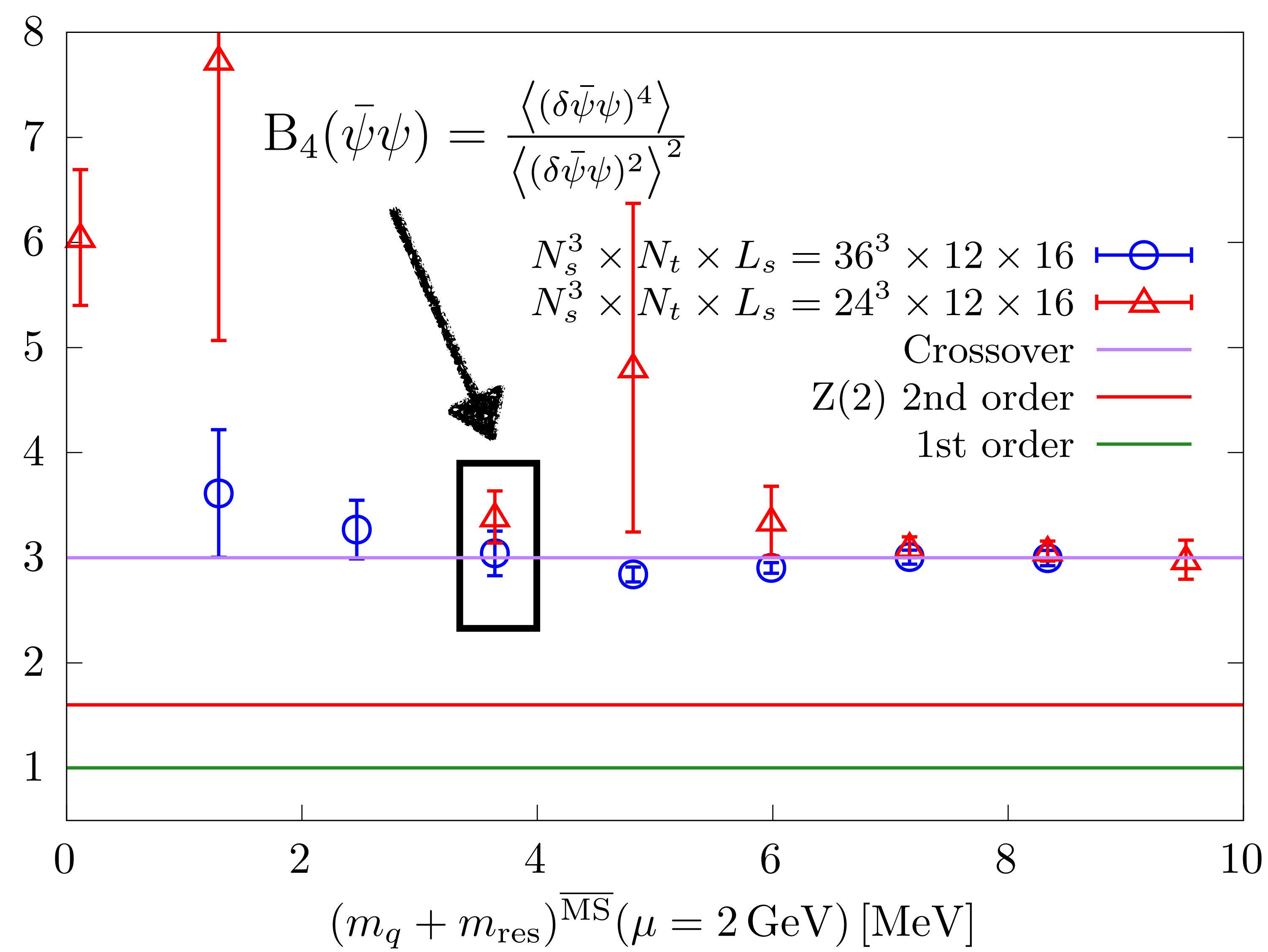
Behaves like gaussian distribution

no evidence that a double peak structure would appear as volume increases

Binder cumulant of chiral condensate at T~121 MeV

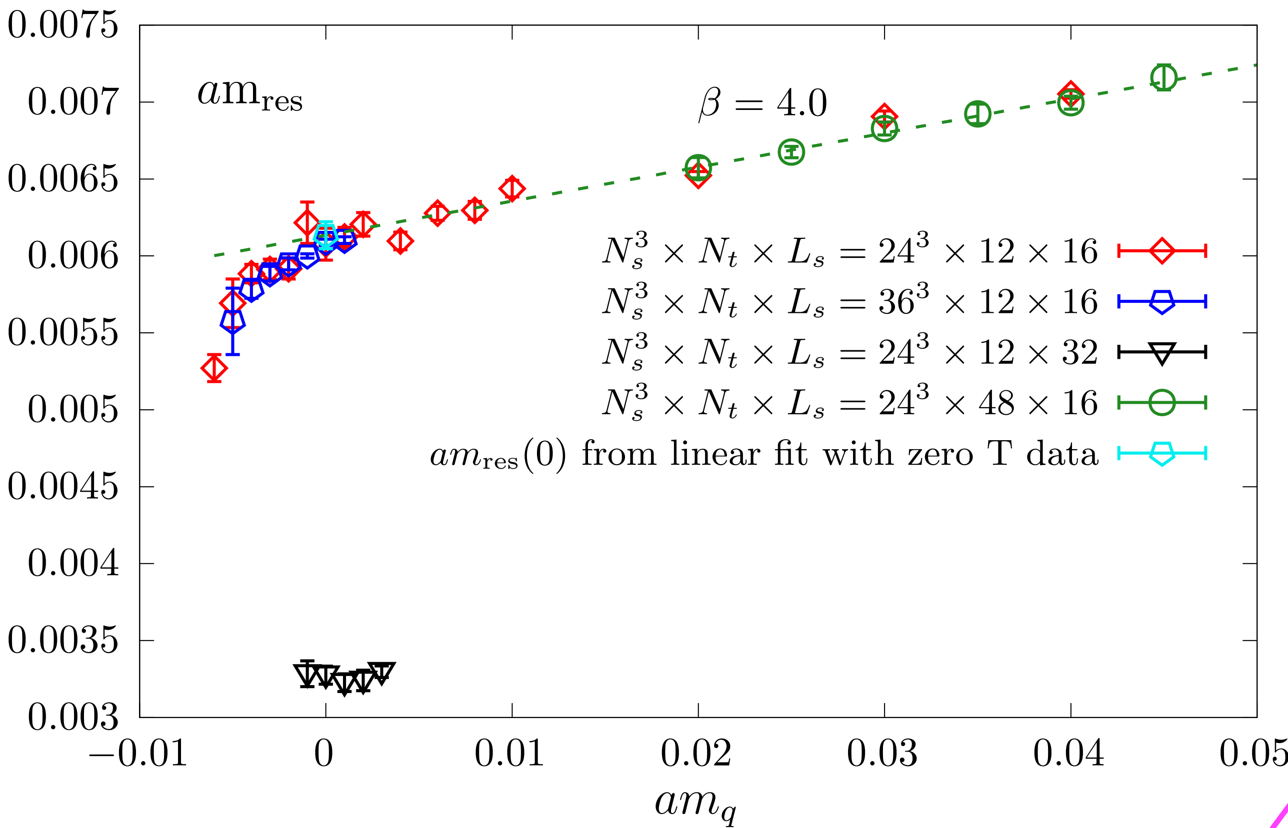
$$B_4(\bar\psi\psi) = \frac{\langle(\delta\bar\psi\psi)^4\rangle}{\langle(\delta\bar\psi\psi)^2\rangle^2}, \quad \delta\bar\psi\psi = \bar\psi\psi - \langle\bar\psi\psi\rangle$$

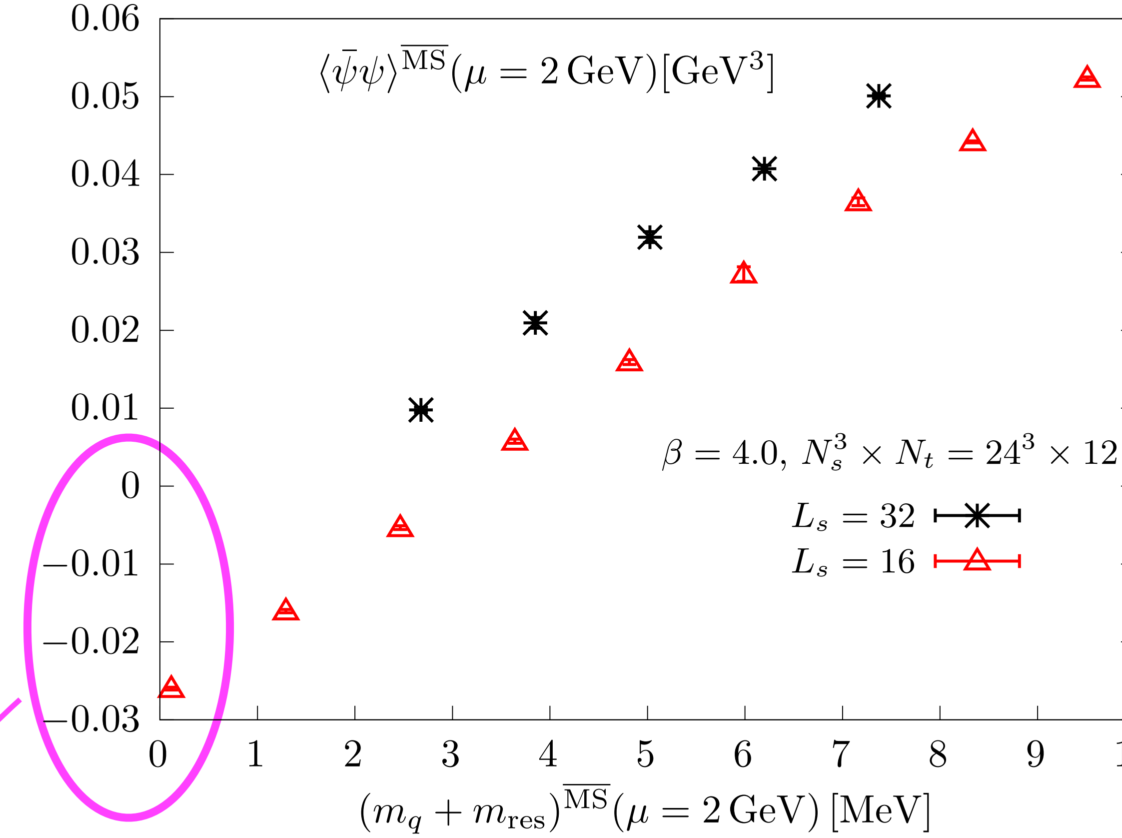




Suggests a crossover transition

Residual mass and Chiral condensate at varying Ls





- $am_{\rm res}$ computed at fixed $\beta = 4.0$ for both zero & finite T are consistent
- Adjust input quark mass for Ls=32 so that $a(m_q + m_{\rm res})$ is similar with Ls=16
- $am_{\rm res}$ reduced almost half for Ls=32, 1/Ls dependence dominates the contribution

$$\langle\bar\psi\psi\rangle|_{DWF} \sim C\left(\frac{(x-1)m_{res}}{a^2} + \frac{m_q + m_{res}}{a^2}\right) + \langle\bar\psi\psi\rangle|_{cont.} + \ldots,$$

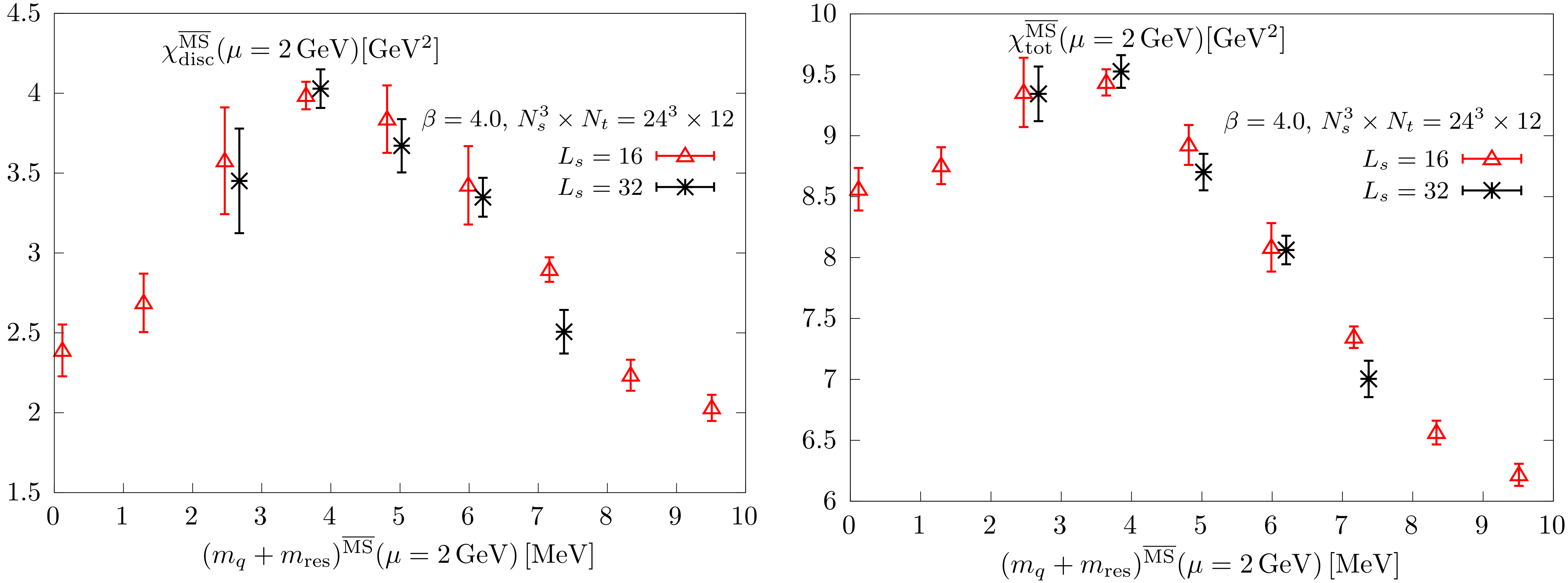
[S. Sharpe, arXiv: 0706.0218]

The result has contamination due to the lack of exact chiral symmetry after taking chiral limit

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

- Residual chiral symmetry breaking effect is smaller for Ls=32

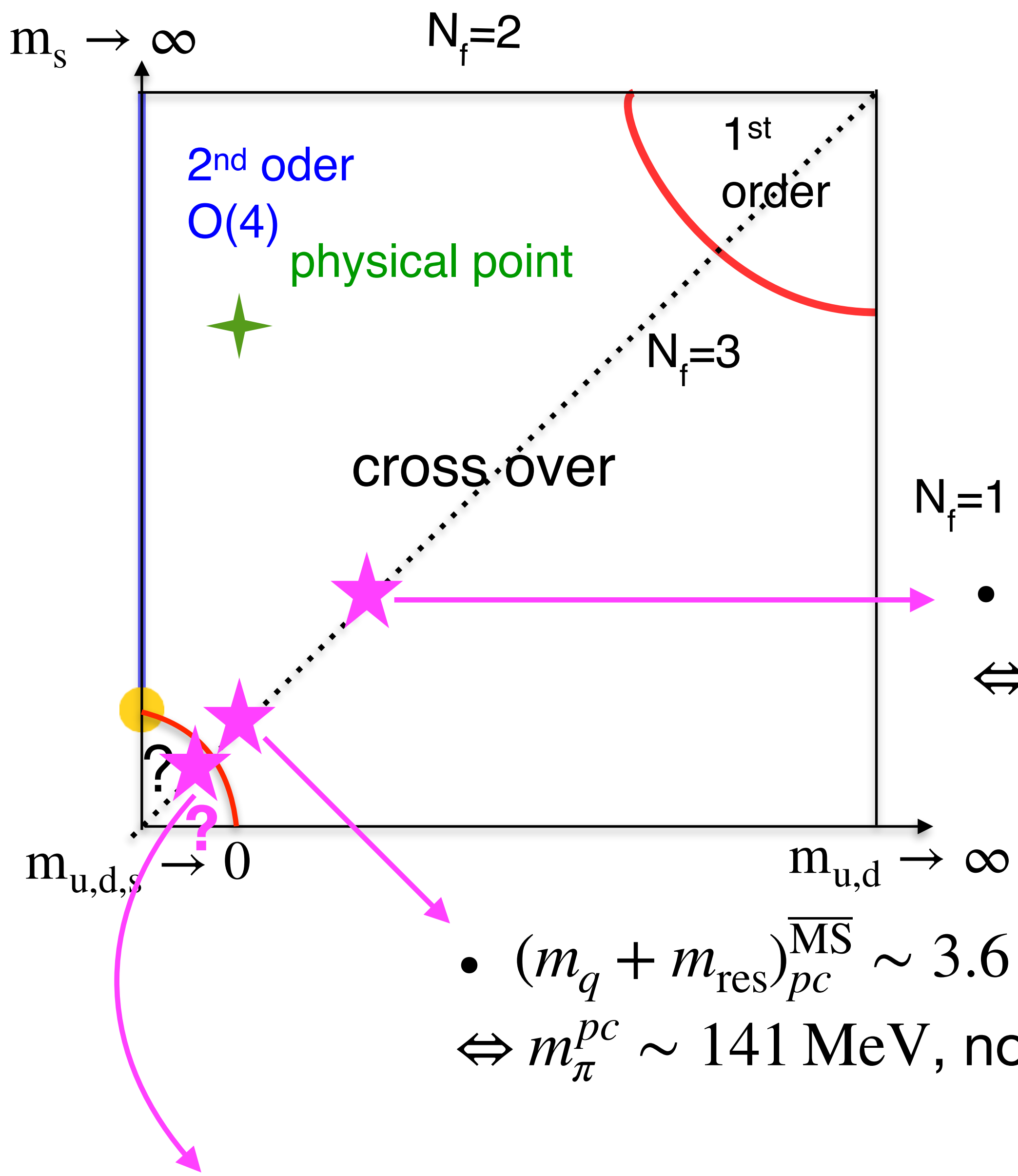
Chiral susceptibility at varying Ls



- For two lattices with the approximate same total quark mass, we observe the consistent results in the susceptibility, the transition mass point is similar

  ⇒ The choice of our negative input quark mass for Ls=16 is safe
- Susceptibility seems to be function of total light quark mass $m_q + m_{\rm res}$

Summary and outlook



- $(m_q + m_{\rm res})^{\overline{\rm MS}}_{pc} \sim 42\,{\rm MeV}, {\rm T} \sim 181{\rm MeV}\ (N_t = 8, {\rm MDWF})$
$\Leftrightarrow m_\pi^{pc} \sim 480\,{\rm MeV}$, no phase transition

[Y. Zhang lattice 2022]

- $(m_q + m_{\rm res})^{\overline{\rm MS}}_{pc} \sim 3.6\,{\rm MeV}, {\rm T} \sim 121{\rm MeV}\ (N_t = 12, {\rm MDWF})$
$\Leftrightarrow m_\pi^{pc} \sim 141\,{\rm MeV}$, no phase transition

- ${\rm T} \sim 104\,{\rm MeV}\ (N_t = 14, {\rm MDWF})$, lighter quark mass simulation is underway

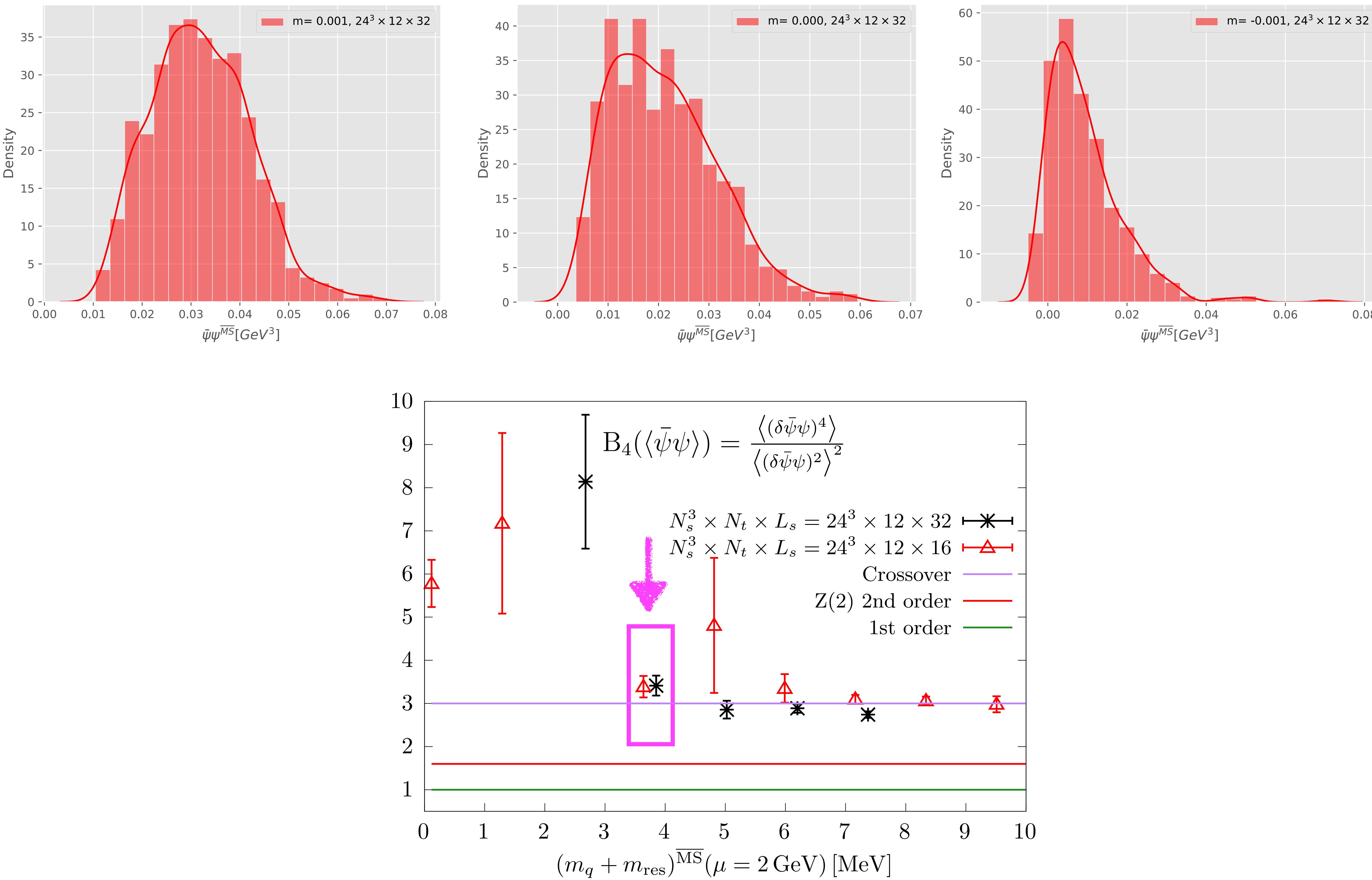
Acknowledgements

- Codes
  - HMC
    - Grid (implementation for A64FX: thanks to the Regensburg group)
  - Measurements
    - Bridge++
    - Hadrons / Grid

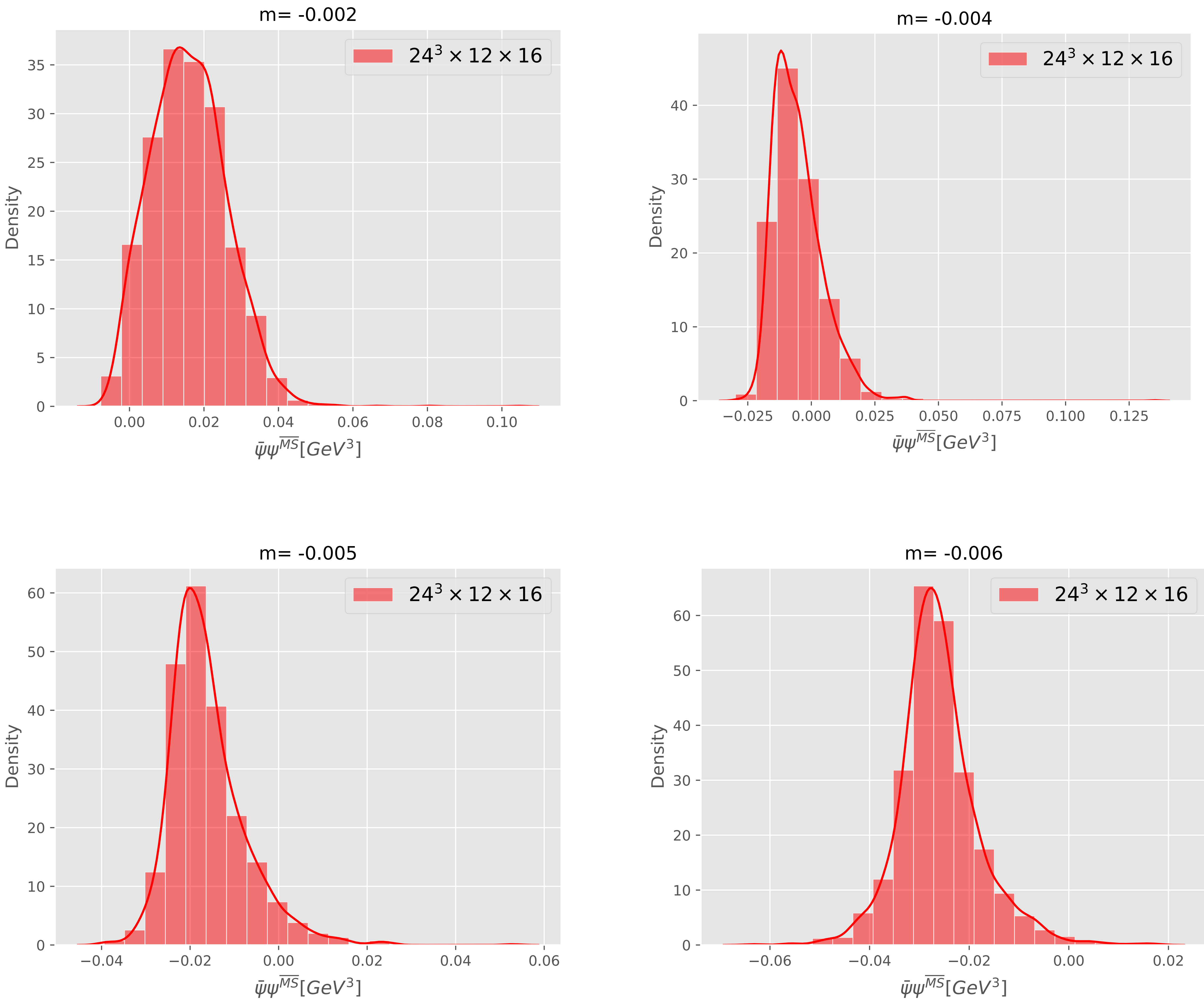
- Computers
  - Supercomputer Fugaku provided by the RIKEN Center for Computational Science through HPCI project #hp210032 and Usability Research ra000001.
  - Wisteria/BDEC-01 Oddysey at Univ. Tokyo/JCAHPC through HPCI project #hp220108 Ito supercomputer at Kyushu University through HPCI project #hp190124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

- Grants
  - JSPS Kakenhi (20H01907)

Backup slide



m= 0.001, $24^3 \times 12 \times 32$
Density
$\bar{\psi}\psi^{\overline{MS}}[GeV^3]$
m= 0.000, $24^3 \times 12 \times 32$
Density
$\bar{\psi}\psi^{\overline{MS}}[GeV^3]$
m= -0.001, $24^3 \times 12 \times 32$
Density
$\bar{\psi}\psi^{\overline{MS}}[GeV^3]$
$\mathrm{B}_4(\langle\bar{\psi}\psi\rangle) = \frac{\left\langle(\delta\bar{\psi}\psi)^4\right\rangle}{\left\langle(\delta\bar{\psi}\psi)^2\right\rangle^2}$
$N_s^3 \times N_t \times L_s = 24^3 \times 12 \times 32$
$N_s^3 \times N_t \times L_s = 24^3 \times 12 \times 16$
Crossover
Z(2) 2nd order
1st order
$(m_q + m_{\rm res})^{\overline{\rm MS}}(\mu = 2\,{\rm GeV})$ [MeV]


m= -0.002
m= -0.004
m= -0.005
m= -0.006
$24^3 \times 12 \times 16$
$24^3 \times 12 \times 16$
$24^3 \times 12 \times 16$
$24^3 \times 12 \times 16$
Density
Density
Density
Density
$\bar{\psi}\psi^{\overline{MS}}[GeV^3]$
$\bar{\psi}\psi^{\overline{MS}}[GeV^3]$
$\bar{\psi}\psi^{\overline{MS}}[GeV^3]$
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