Characterizing Strongly Interacting Matter at Finite Temperature: (2+1) Flavor QCD with Möbius Domain Wall Fermions

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Acknowledgments

Computer resources: supercomputer Fugaku (hp200130, hp210165, hp220174, ra000001).
MEXT as “Program for Promoting Researches on the Supercomputer Fugaku” (Simulation for basic science: from fundamental laws of particles to creation of nuclei, JPMXP1020200105, シミュレーションでせまる基礎科学：量子新時代へのアプローチ課題番号, JPMXP1020230411) and JICFuS.
JPS KAKENHI(JP20K0396, I. K).

Ongoing work and code bases

Lattice2023 finite temperature talks using Möbius Domain Wall Fermions (JLQCD collaboration)

(1) **H. Fukaya: chiral susceptibility in phase transition of $N_f = 2$ and $2+1$ QCD**

(2) **J. Goswami : Quark number susceptibility**

(3) ***K. Suzuki : axial U(1) anomaly***

(4) ***D. Ward : meson screening mass and symmetries***

(5) **Y. Zhang : 3-flavor QCD phase transition**

Configuration generation: Grid(https://github.com/paboyle/Grid)

Measurements : Hadrons (https://github.com/aportelli/Hadrons)

Bridge++ version 2.0.1(https://bridge.kek.jp/Lattice-code/)

Data Analysis : https://github.com/LatticeQCD/LatticeToolbox

Outline

- **Simulation details and tuning of the input quark masses**

- **Pseudo-critical temperature from χ_{disc} for (2+1)-flavor Möbius Domain wall fermions (MDWF).**

- **Quark number susceptibility.**

- **Conserved charge fluctuations.**

Möbius Domain wall fermions (MDWF) and simulation details

We use, Symanzik + Möbius Domainwall fermion (on stout smear)
In our calculations.
"Almost" chiral fermions for finite L_s.

Line of Constant Physics 2022 : fixed $m_l/m_s = 0.1$,
$m_s(\beta)$ obtained from zero temperature data and tune to its physical values.

Lattice sizes :

$$N_\sigma^3 \times N_\tau = 32^3 \times 16,\ 24^3 \times 12\ ,\ 36^3 \times 12,\ 48^3 \times 12$$

Challenge : m_{res} become larger for smaller β . How to control the m_{res} effect ??

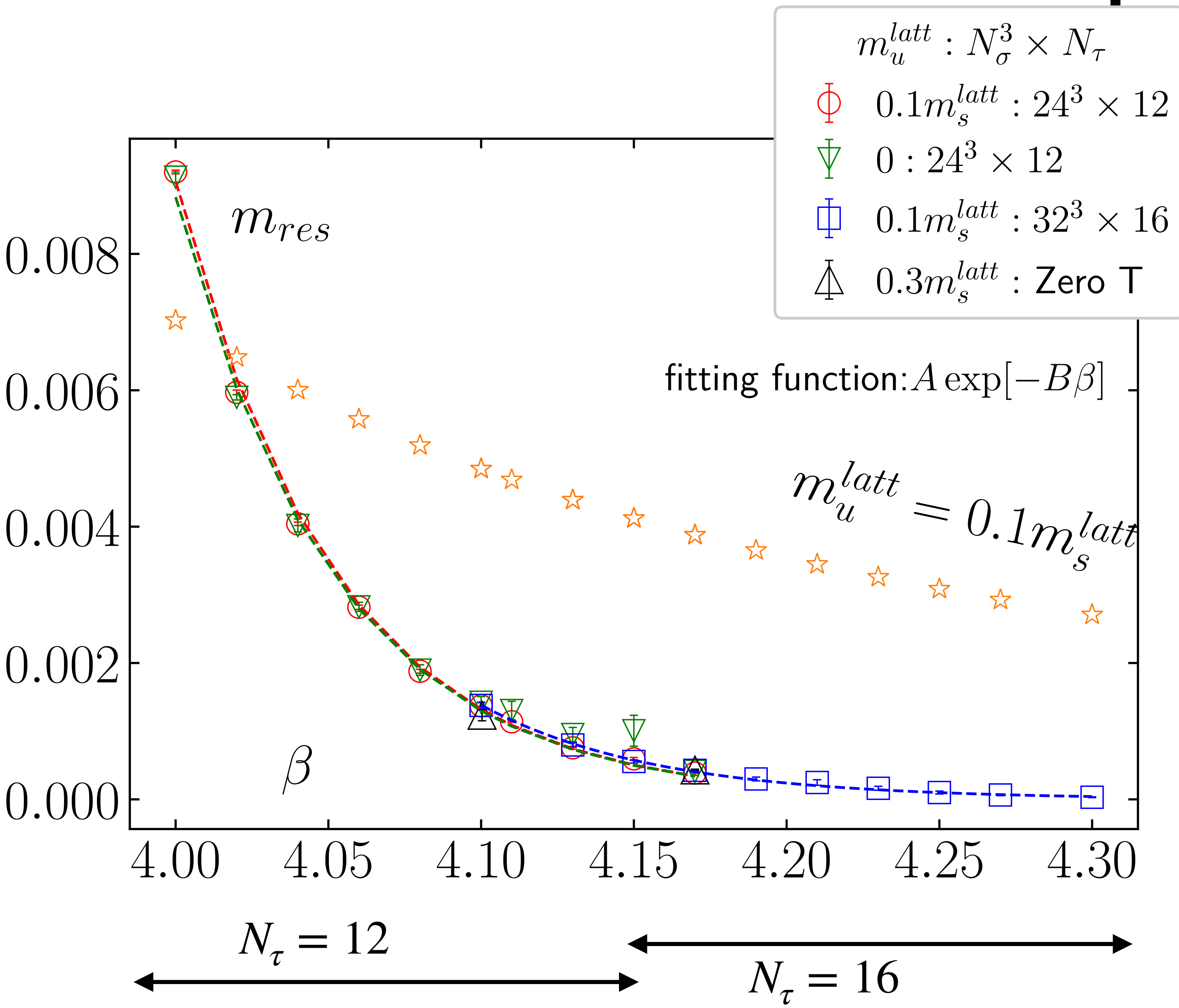
Supplemental Material:

Brian Colquhoun et al (JLQCD coll.), Phys. Rev. D 106, 054502

Y. Aoki, I. Kanamori, Lattice2022

Richard C. Brower, arXiv:1206.521

Tuning of the bare input quark masses on the line of constant physics (LCP)



Tuning of bare input quark masses (m_f^{input}) in the Domain Wall action:

$$m_f^{latt} = m_f^{input} + m_{res} \;,\; f = \{u, d, s\}$$

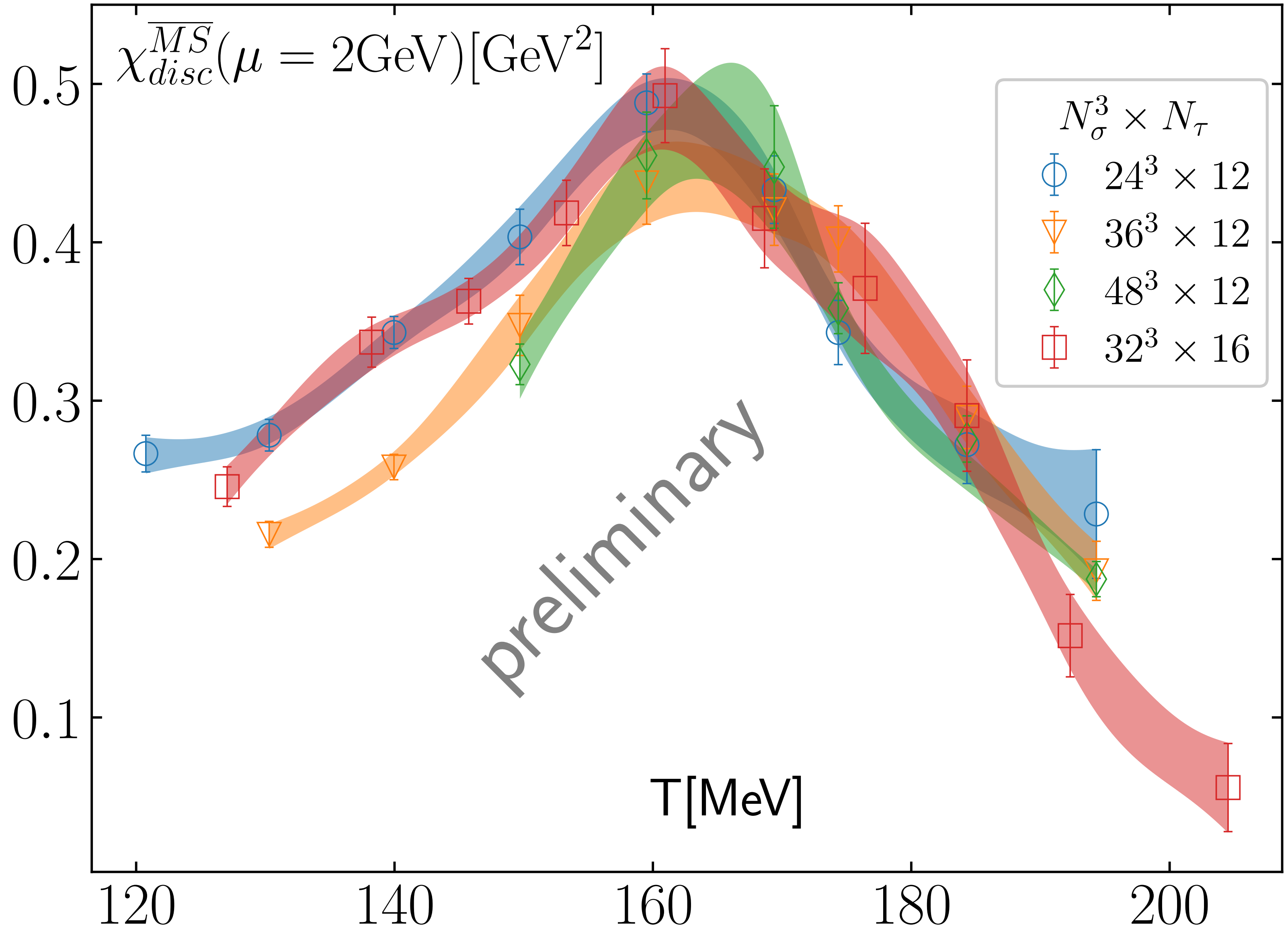
Y. Aoki et al, *PoS* LATTICE2021 (2022) 609

$$\frac{m_u^{latt}}{m_s^{latt}} = \frac{m_u^{input} + m_{res}}{m_s^{input} + m_{res}} = 0.1$$

For, $N_\tau = 12$, $m_u^{latt} \leq m_{res}$. We tune the m_u^{input} in the LCP.

For, $N_\tau = 16$, $m_u^{latt} > m_{res}$, we perform mass reweighting.

Pseudo-critical temperature



- **We determine the T_{pc} by determining the maxima of the χ_{disc}.**
- **The error on the T_{pc} determined through gaussian bootstrap method.**
- **The peak of χ_{disc} doesn't show any volume dependence which is consistent with a crossover transition.**

  $T_{pc}(N_\tau^3/N_\sigma^3 \to 0) = 165(2)$ MeV

Quark number susceptibility with Domain wall fermions

$$Z = \int DU \prod_{f=u,d,s} detM(m_f)\exp[-S_g], \qquad \det M(m_f, \hat{\mu}_f) = \left[\frac{\det D(m_f, \hat{\mu}_f)^{DWF}}{\det D(m_{PV}, \hat{\mu}_f)^{DWF}}\right]$$

$$U_4(x) \to \exp(\hat{\mu}_f)U_4(x),\ U_4^{\dagger}(x) \to \exp(-\hat{\mu}_f)U_4^{\dagger}(x),$$ J. Bloch and T. Wettig, Phys. Rev. Lett. 97, 012003 (2006)

$\hat{\mu}_f = \mu_f/T$, where , μ_f is the quark chemical potential.

The diagonal and off-diagonal quark number susceptibilities can be written as,

$$\chi_2^f = \frac{N_\tau}{N_\sigma^3}\frac{\partial^2 \ln Z}{\partial \hat{\mu}_f^2} = \frac{N_\tau}{N_\sigma^3}\left[\left\langle \frac{\partial^2}{\partial \mu_f^2}\ln\det M \right\rangle + \left\langle \left(\frac{\partial}{\partial \mu_f}\ln\det M\right)^2 \right\rangle\right]$$

$$= \frac{N_\tau}{N_\sigma^3}\langle D_2^f\rangle + \langle (D_1^f)^2\rangle,\ f = \{u,d,s\}$$

M. Cheng et al, Phys.Rev.D81:054510,2010 ; P. Hegde et al, PoS LATTICE2008:187,2008

$$\chi_{11}^{fg} = \frac{N_\tau}{N_\sigma^3}\frac{\partial^2 \ln Z}{\partial \hat{\mu}_f \partial \hat{\mu}_g} = \langle D_1^f D_1^g\rangle,\ f \neq g,\ f,g = \{u,d,s\}$$

$(D_1^f)^2$ and $D_1^f D_1^g$ are the most noisy part in our calculation

Stochastic trace estimation

Matrix size : $12V_5 \times 12V_5$

$V_5 = N_\sigma^3 \times N_\tau \times L_s$

Error reduction in stochastic trace estimators ??

Each trace needs proper subtraction from the unphysical degrees of freedom

$$D_1^f = \mathrm{Tr}\left[D(m_f)^{-1}\frac{dD(m_f)}{d\hat{\mu}_f} - D(m_{pv})^{-1}\frac{dD(m_{pv})}{d\hat{\mu}_f}\right]$$

$$D_1^f = \frac{1}{N_n}\sum_j^{N_n}\left[\eta_j^\dagger D(m_f)^{-1}\frac{dD(m_f)}{d\hat{\mu}_f}\eta_j - \eta_j^\dagger D(m_{pv})^{-1}\frac{dD(m_{pv})}{d\hat{\mu}_f}\eta_j\right]$$

η_j **is the gaussian random noise.**

Stochastic error reduction using dilution vectors :

$$D_1^f = \frac{1}{N_n}\sum_j^{N_n}\left[\sum_{a=1}^{N_p}\eta_{aj}^\dagger D(m_f)^{-1}\frac{dD(m_f)}{d\mu_f}\eta_{aj} - \sum_{a=1}^{N_p}\eta_{aj}^\dagger D(m_{pv})^{-1}\frac{dD(m_{pv})}{d\mu_f}\eta_{aj}\right]$$

η_{aj} **is the diluted gaussian random noise.**

$(D_1^f)^2$ we need to employ the unbiased estimator method.

We present calculations of qns and charge fluctuations for the lattice size,

$$N_\sigma^3 \times N_\tau \times L_s = 24^3 \times 12 \times 12$$

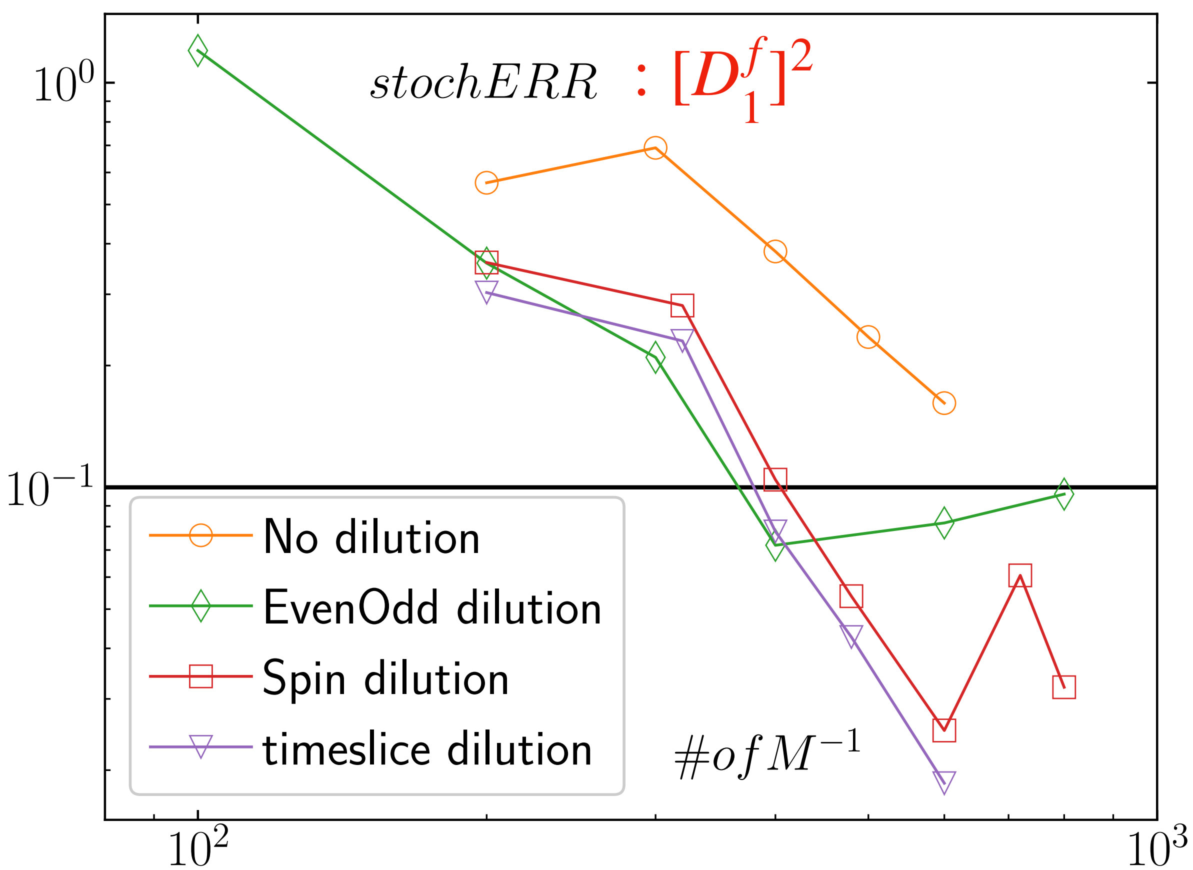
Stochastic error reduction

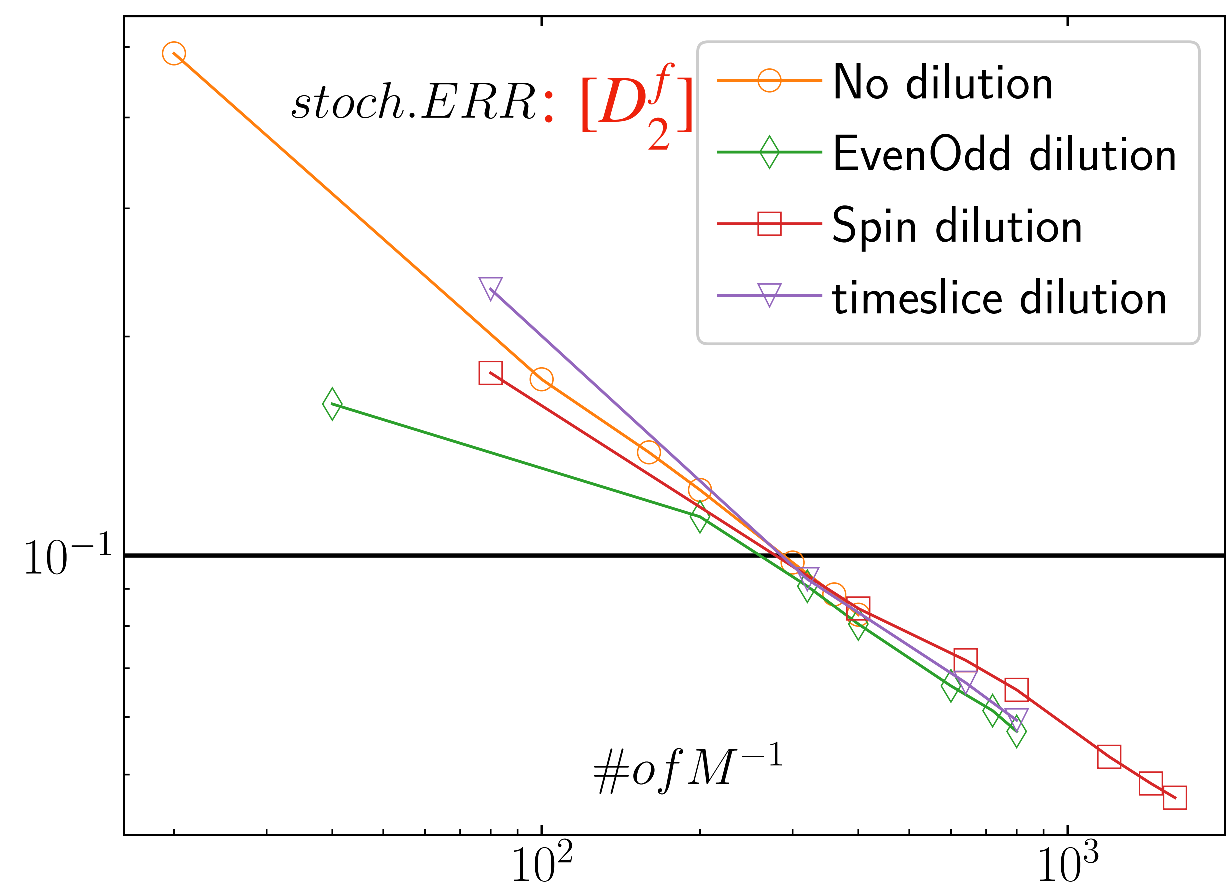
We examine three dilution methods:

(i) Even Odd dilution : splitting the η_j into two parts, in even and Odd lattice sites.

(ii) Spin dilution : splitting the η_j into four spinor components.

(iii) Timeslice dilution : splitting the η_j into four parts, using $(N_\tau \mod 4)$.

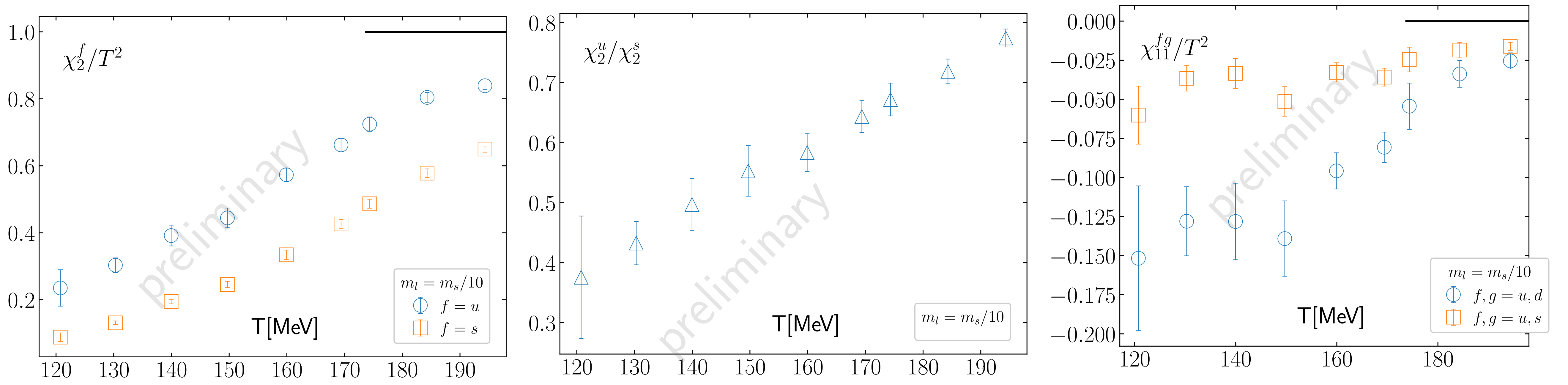




Spin and timeslice dilution : Efficient for $(D_1^f)^2$, $2-3$ times error reduction.

EvenOdd dilution : Efficient for (D_2^f).

Quark number susceptibility



Spin dilution method and 150 gaussian random noises for $(D_1^f)^2$.

Even-Odd dilution and 100 gaussian random noises for D_2^f.

χ_2^f's are smaller at low temperatures and grow larger in the vicinity of the T_{pc}. Remain significantly smaller than the Ideal gas limit (solid black line).

χ_2^u/χ_2^s indicates a reduction in the mass difference between u, s quarks at high temperatures.

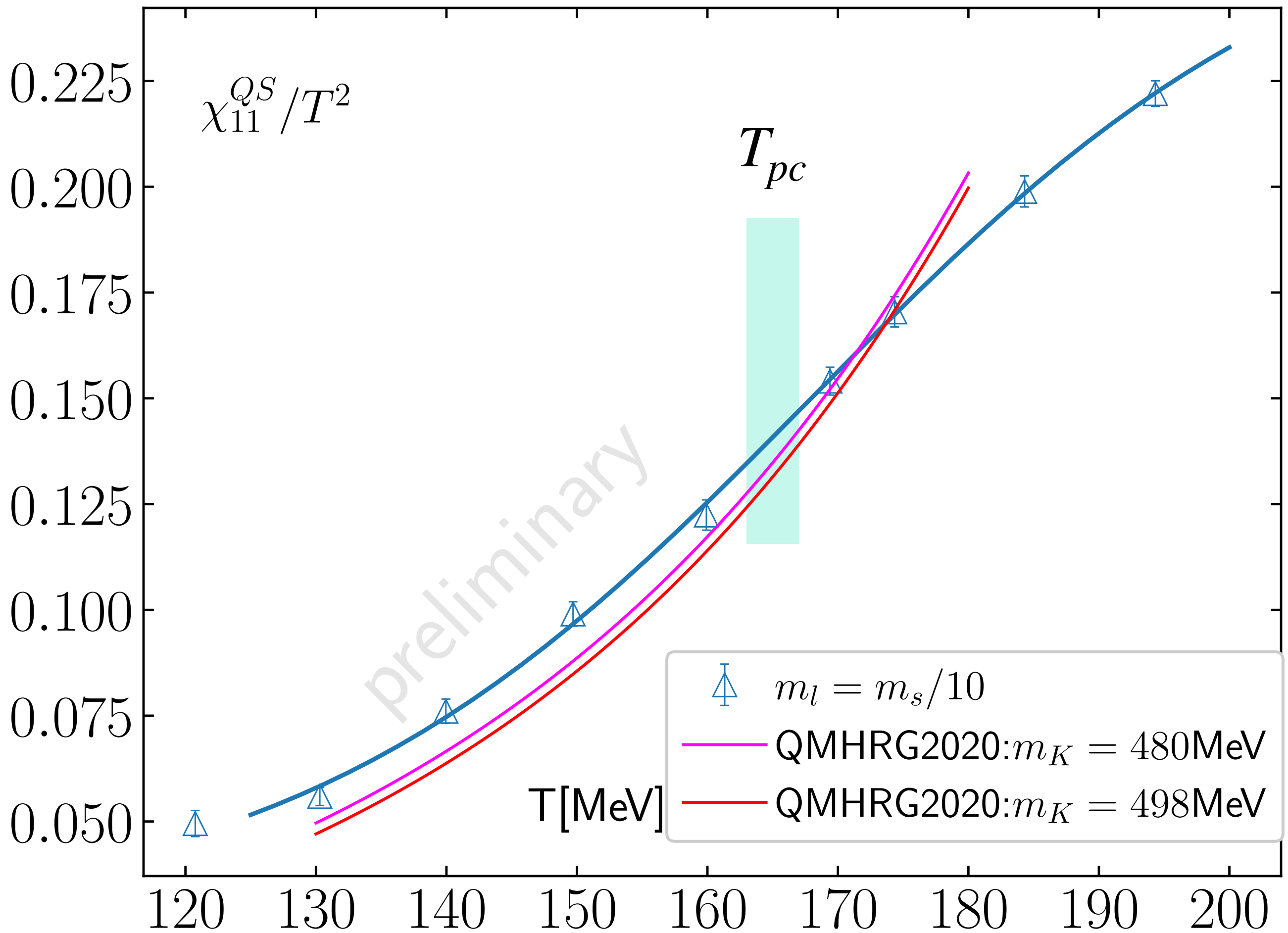
In high T PT: $\chi_2^f \sim \chi_2^{f,ideal} + O(g^2)$, $\chi_{11}^{fg} \sim O(g^6 lng)$

A. Vuorinen, PRD68, 054017 (2003)

S. Borsanyi et al, JHEP 1201 (2012) 138

Conserved charge fluctuations : electric charge-strangeness correlations

$$\chi_{11}^{QS} = \frac{1}{3}(\chi_2^s - \chi_{11}^{us})$$



Low temperatures, χ_{11}^{QS} is dominated by the ground state kaons and $K*$.

At $T \sim 120$ MeV, our estimated kaon mass is 480 MeV.

Good agreement between QCD data and the HRG curve for $T < T_{pc}$.

Differences in QCD vs HRG : can be due to $K*$.

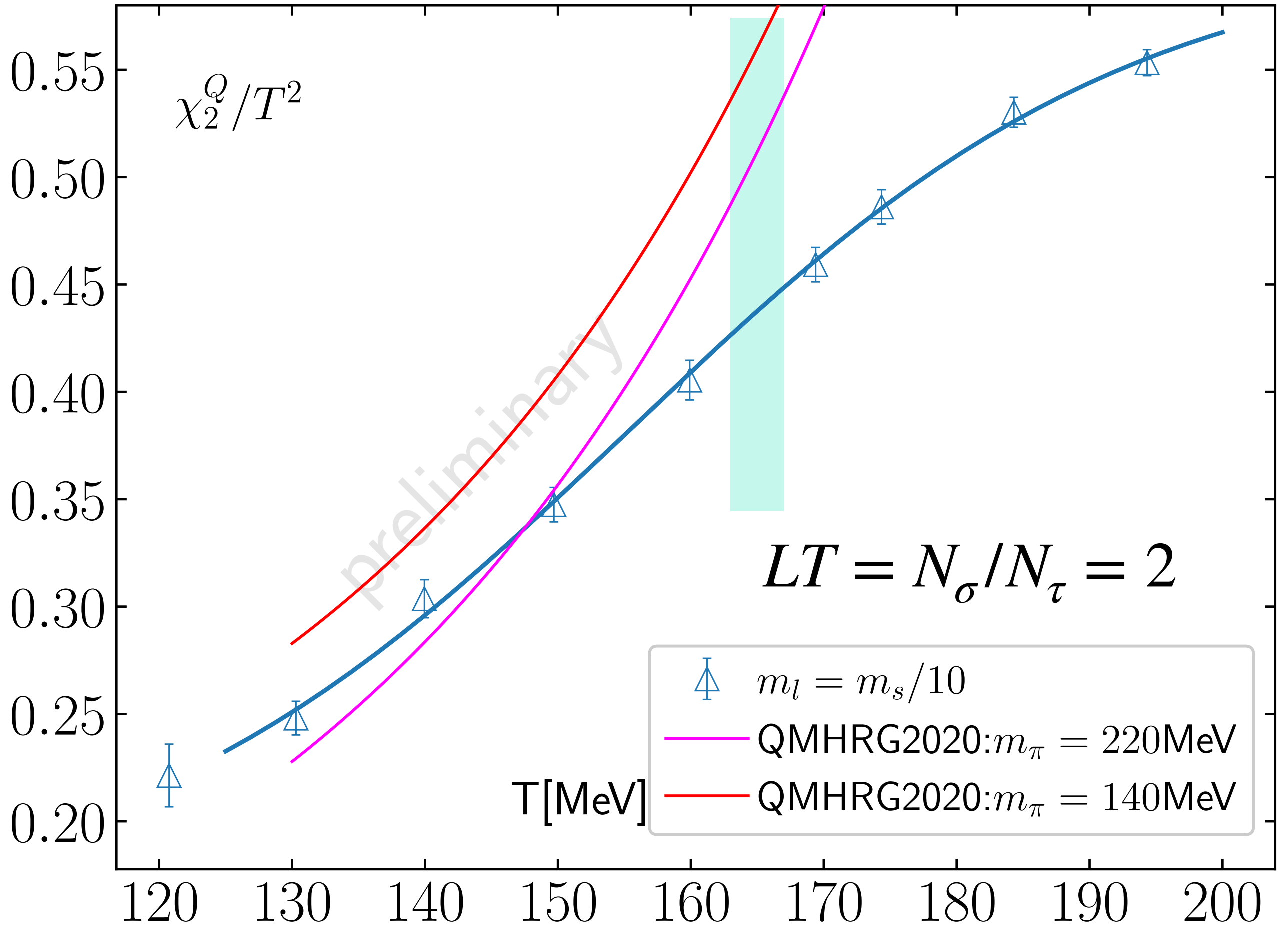
We plan to use $N_\tau = 16$ to understand the m_{res} correction on the input quark masses in the LCP and cut-off dependence on this observable at low temperatures.

QMHRG2020 : D. Bollweg el al, *Phys.Rev.D* 104 (2021) 7, 074512

R. Bellwied et al, Phys. Rev. D 92, 114505 (2015)
D. Bollweg el al, *Phys.Rev.D* 104 (2021) 7, 074512

Conserved charge fluctuations : electric charge cumulant

$$\chi_2^Q = \frac{1}{9}(5\chi_2^u + \chi_2^s - 4\chi_{11}^{ud} - 2\chi_{11}^{us})$$



At low temperatures, χ_2^Q is dominated by pions.
Our estimated pion mass for slightly heavy light quarks ($m_l = 0.1m_s$) is 220 MeV.

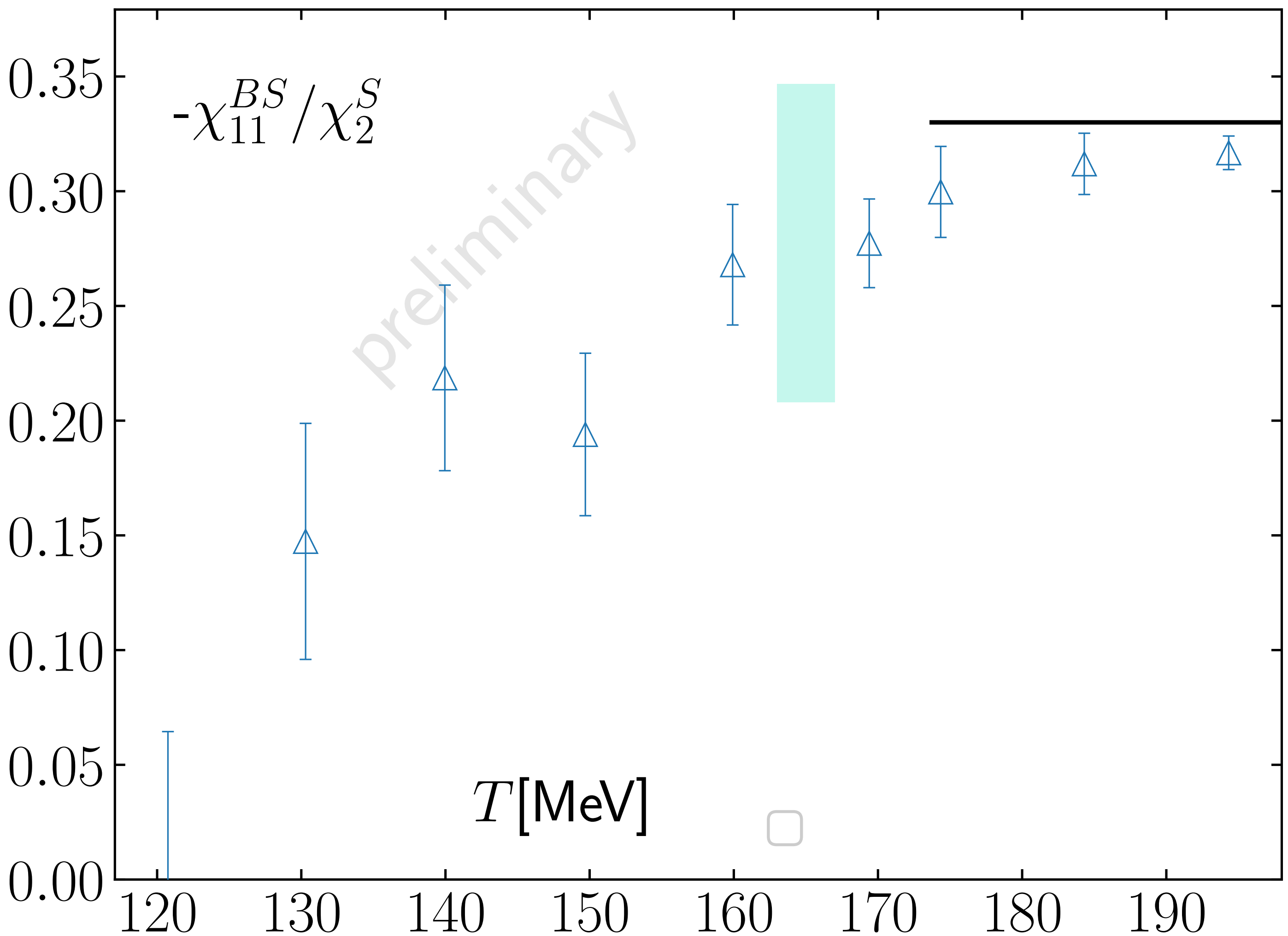
Unlike calculations with staggered fermions, we see a good agreement with hadron resonance gas (HRG) with χ_2^Q at low temperatures at $N_\tau = 12$.

However, close to the T_{pc} the deviations seems to be robust.

D. Bollweg el al, *Phys.Rev.D* 104 (2021) 7, 074512

Conserved charge fluctuations : Baryon Strangeness correlation

$$-\chi_{11}^{BS}/\chi_2^S = \frac{1}{3}(\chi_2^s + 2\chi_{11}^{us})/\chi_2^s = \frac{1}{3} + 2\chi_{11}^{us}/3\chi_2^s$$



At high temperature, ratio of BS correlation to the χ_2^S approaches to the free gas limit faster compare to other observables.

$\chi_{11}^{us} \to 0$, uncorrelated quark gas.

In high T PT: $\chi_{11}^{us} \sim O(g^6 lng)$

V. Koch et al, Phys.Rev.Lett.95:182301,2005

Summary and future work

- We present results on the thermodynamics of strongly interacting matter using (2+1) Flavor QCD with a chiral fermion formalism, specifically Möbius Domain Wall Fermions.

- For benchmarking and understanding all the systematics of Möbius Domain Wall Fermions, we consider $m_l = m_s/10$ on the line of constant physics.

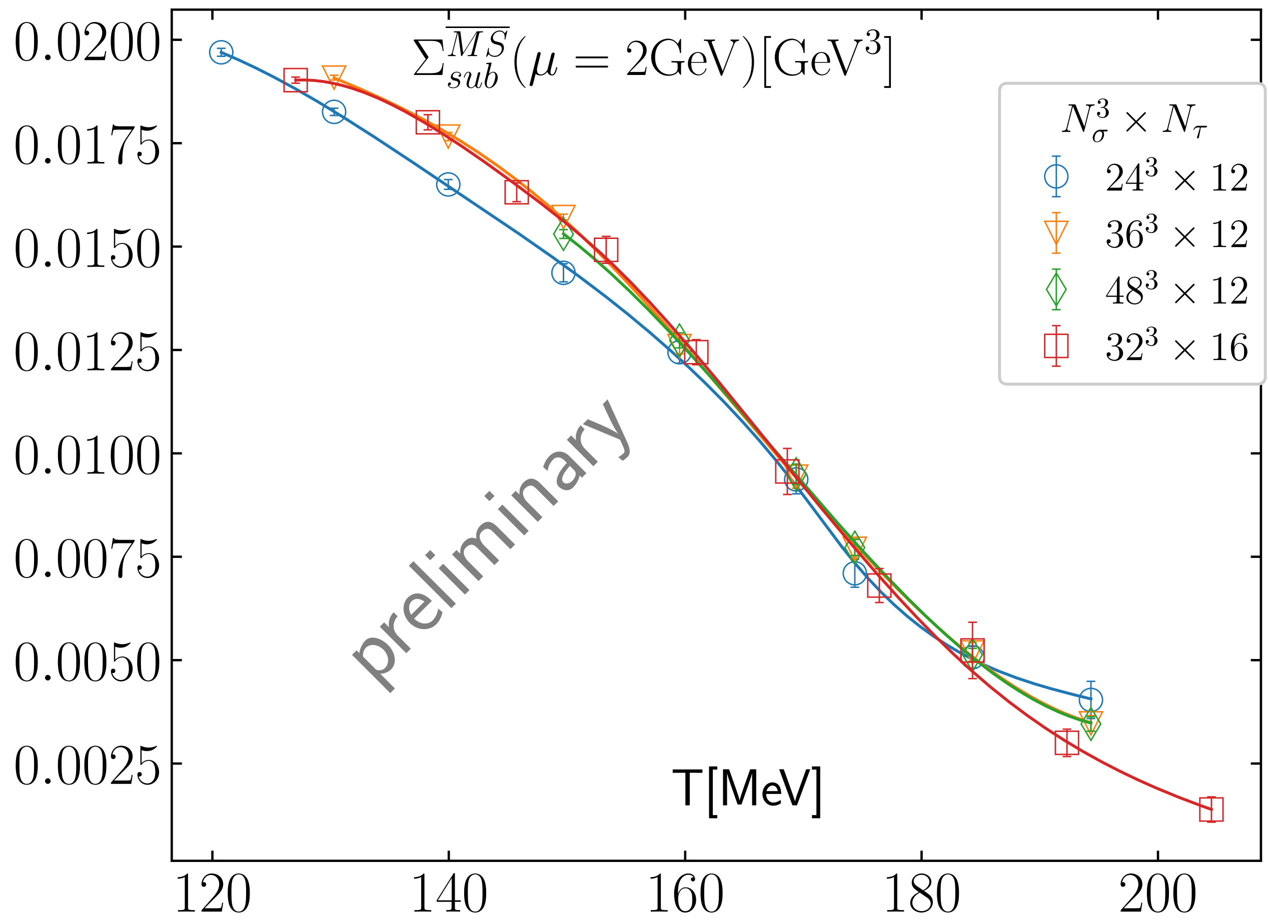
- Additionally, we present preliminary results of conserved charge fluctuations. To understand the effects of m_{res} on the ground state hadron masses, we use HRG (Hadron Resonance Gas) model.

- Calculations at $m_l = m_s/27$ are currently ongoing.

Thank you for your attention !!

- Back up slides

Chiral observables

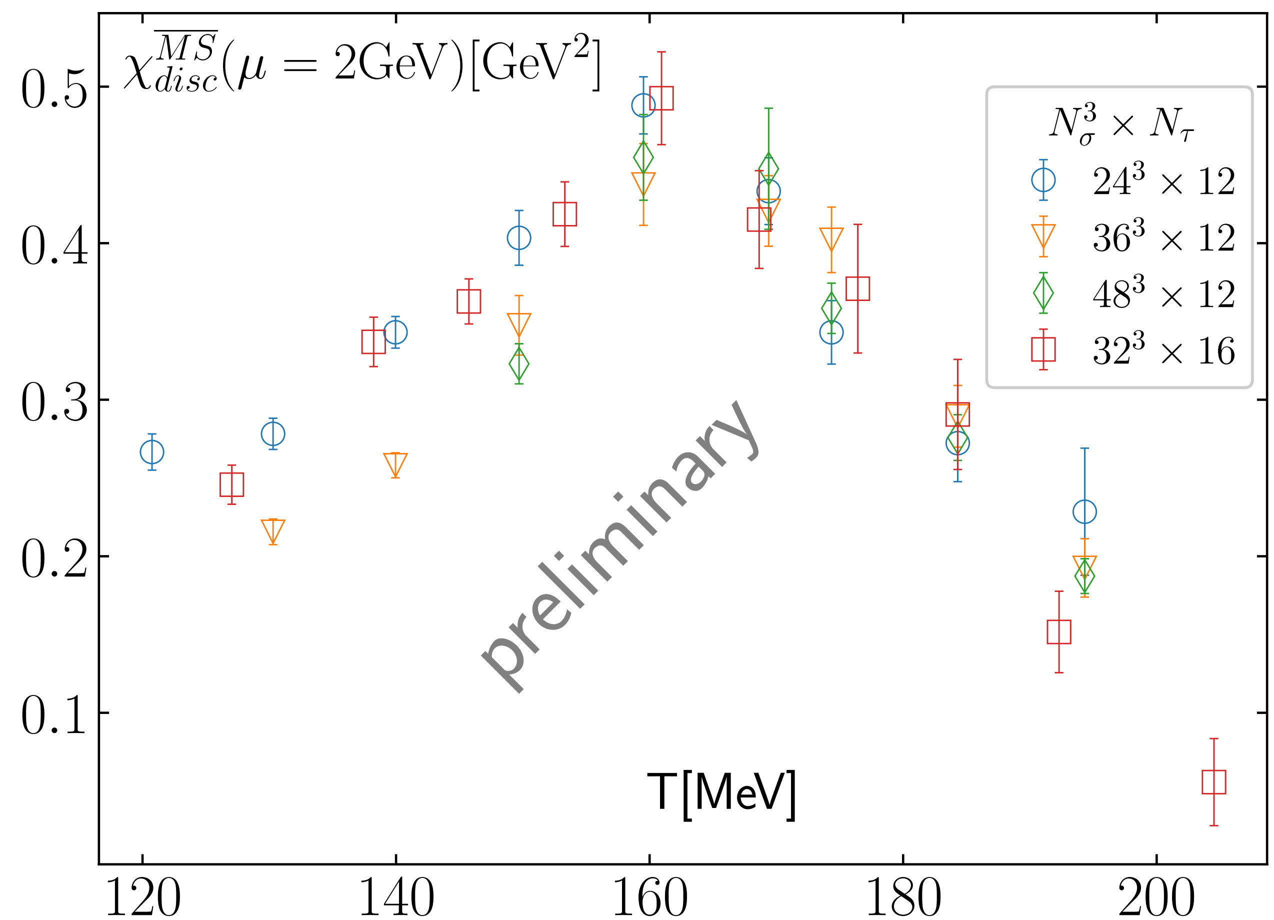


$\langle\bar{\psi}\psi\rangle_l$ is the order parameter for chiral phase transition at, $m_l \to 0$. The renormalised chiral condensate ,

$$\Sigma_{sub} = \langle\bar{\psi}\psi\rangle_l - \frac{m_l}{m_s}\langle\bar{\psi}\psi\rangle_s$$

The disconnected part of the chiral susceptibility,

$$\chi^{disc} = \left(\langle(\mathrm{TrM_l^{-1}})^2\rangle - \langle\mathrm{TrM_l^{-1}}\rangle^2\right)$$



Michael I. Buchoff et al, Phys. Rev. D 89, 054514 (2014)

Ongoing work and computer resources

Ongoing research on QCD thermodynamics with Möbius Domain Wall fermions: (JLQCD collaboration)

(1) talks by Y. Aoki & I. Kanamori (*PoS* LATTICE2022 (2023) 176) at Lattice 2022
(2) Yu Zhang et al., *PoS* LATTICE2022 (2023) 197
(3) Y. Nakamura et al., *PoS* LATTICE2021 (2022) 080
4) S. Aoki et al., *PoS* LATTICE2021 (2022) 609

Etc …..

Code base and resources:

(I) Grid, Hadrons and Bridge++2.0

(III) Current : Fugaku (hp200130, hp210165, hp220174, ra000001)
(IV) Past : Oakforest-PACS (hp200130), Polaire and Grand Chariot (hp200130)

Configuration generation: Grid(https://github.com/paboyle/Grid)
Measurements : Hadrons (https://github.com/aportelli/Hadrons)
Bridge++ version 2.0.1(https://bridge.kek.jp/Lattice-code/)
Data Analysis : https://github.com/LatticeQCD/LatticeToolbox

Quark number susceptibility

$$Z = \int DU \prod_{f=u,d,s} detM(m_f)\exp[-S_g], \qquad \det M(m_f, \mu_f) = \left[\frac{\det D(m_f, \mu_f)^{DWF}}{\det D(m_{PV}, \mu_f)^{DWF}} \right]$$

$$U_4(x) \to \exp(\mu_f) U_4(x),\ U_4^\dagger(x) \to \exp(-\mu_f) U_4^\dagger(x),$$

J. Bloch and T. Wettig, Phys. Rev. Lett. 97, 012003 (2006)

The diagonal and off-diagonal quark number susceptibilities can be written as,

$$\chi_2^f = \frac{N_\tau}{N_\sigma^3} \langle D_2^f \rangle + \langle (D_1^f)^2 \rangle,\ f = \{u, d, s\}$$

$$\chi_{11}^{fg} = \frac{N_\tau}{N_\sigma^3} \frac{\partial^2 \ln Z}{\partial \hat{\mu}_f \partial \hat{\mu}_g} = \langle D_1^f D_1^g \rangle,\ f \neq g,\ f, g = \{u, d, s\}$$

M. Cheng et al, Phys.Rev.D81:054510,2010 ;
P. Hegde et al, PoS LATTICE2008:187,2008

$\hat{\mu}_f = \mu_f / T$, **where ,** μ_f **is the quark chemical potential.**

$(D_1^f)^2$ and $D_1^f D_1^g$ are the most noisy part in our calculation

Matrix size : $12V_5 \times 12V_5$

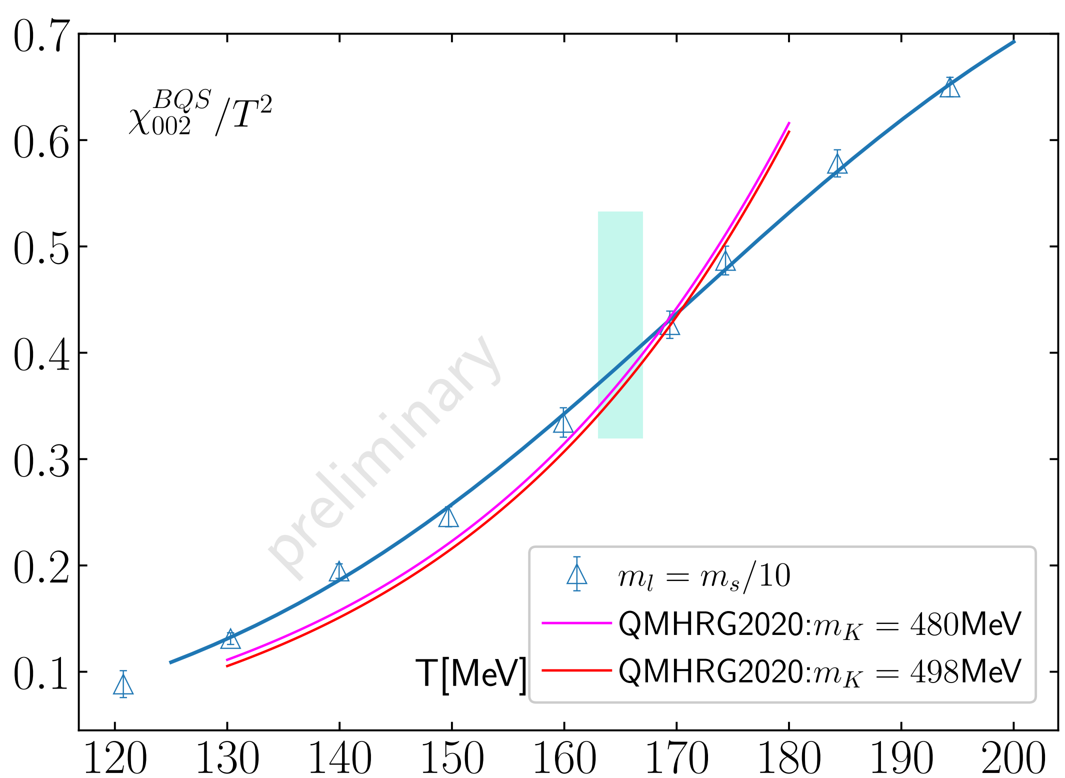
$V_5 = N_\sigma^3 \times N_\tau \times L_s$

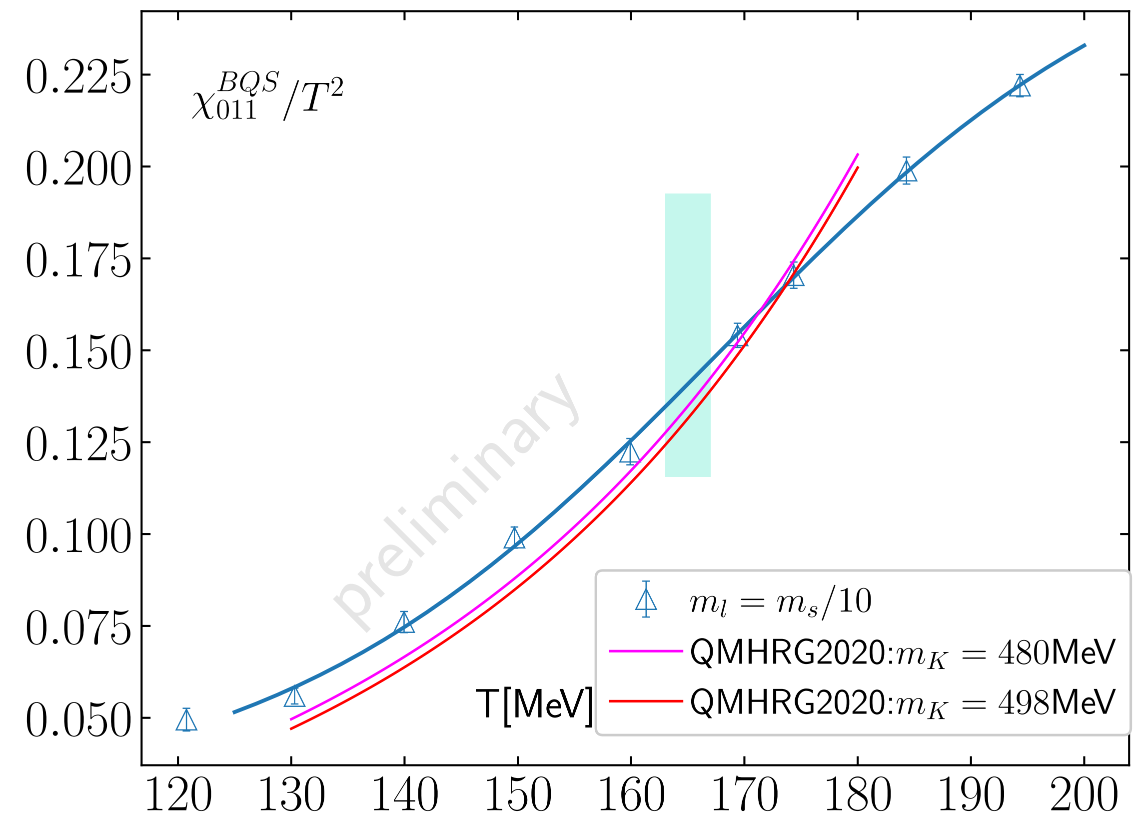
→ **Error reduction in stochastic trace estimators ??**

Conserved charge fluctuations : Strangeness cumulants

The central lines are from $A\tanh(B(T-T_{pc})/t_0)+C$ ansätz, where A, B, C, T_{pc} are the fitting para[meters] and $t_0 = 160$ is an arbitrary scale.

The blue bands are the, T_{pc} obtained from the peak of the χ_{disc}

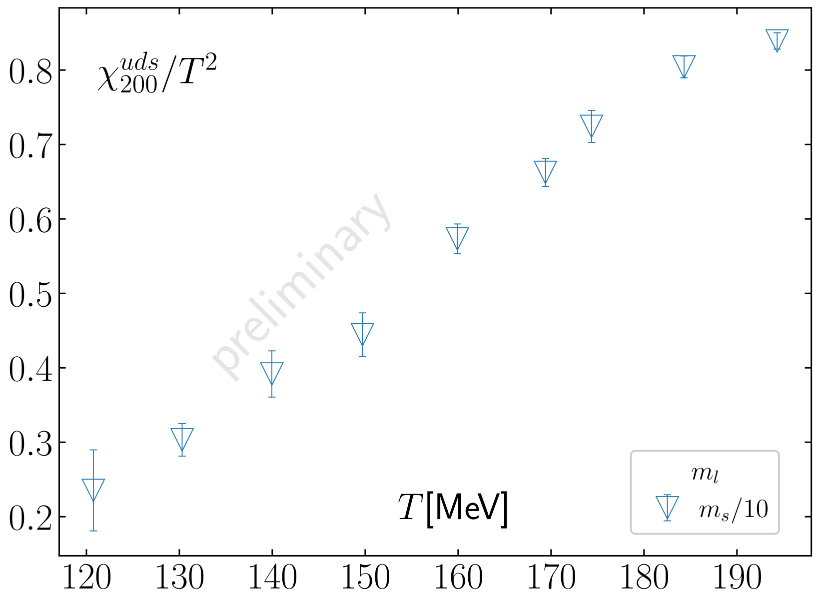


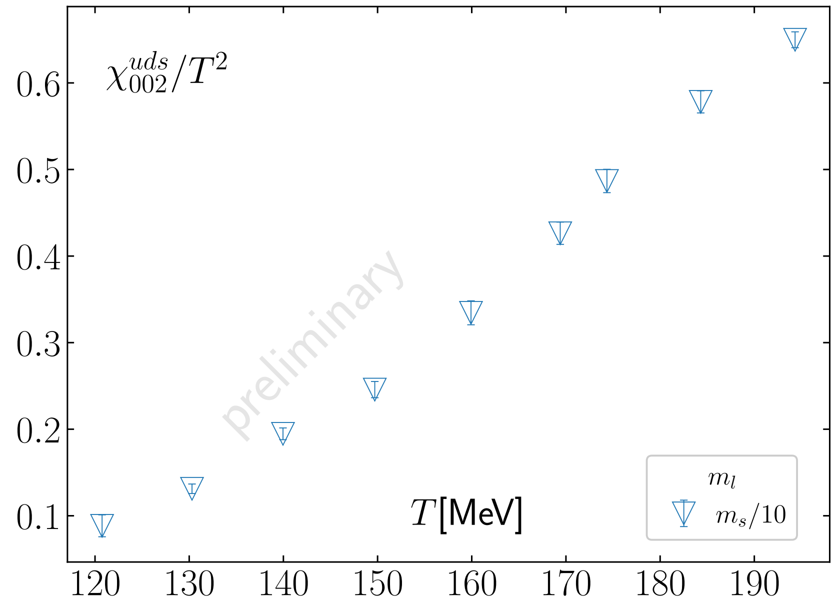


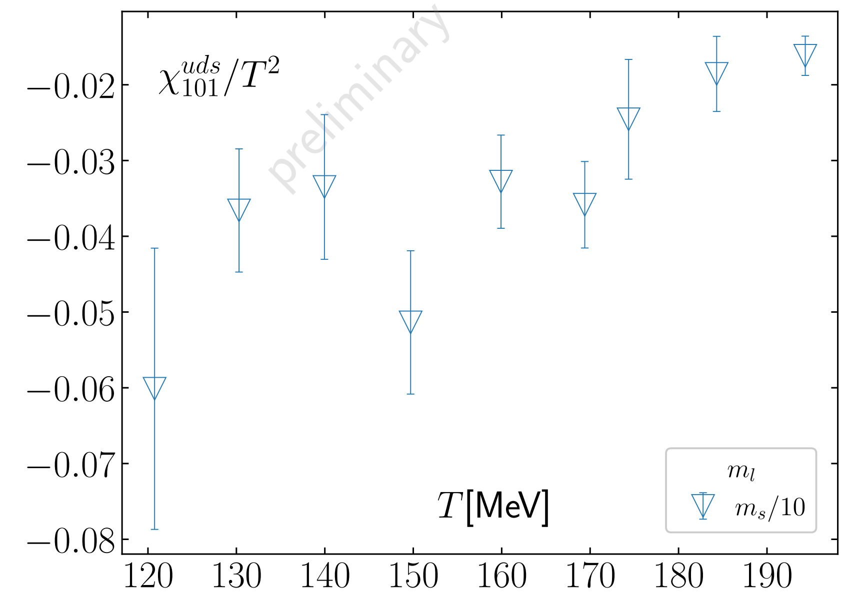
These observables are sensitive to the lowest ground state mass in the spectrum. HRG can provide a good guide to understand the different systematics.

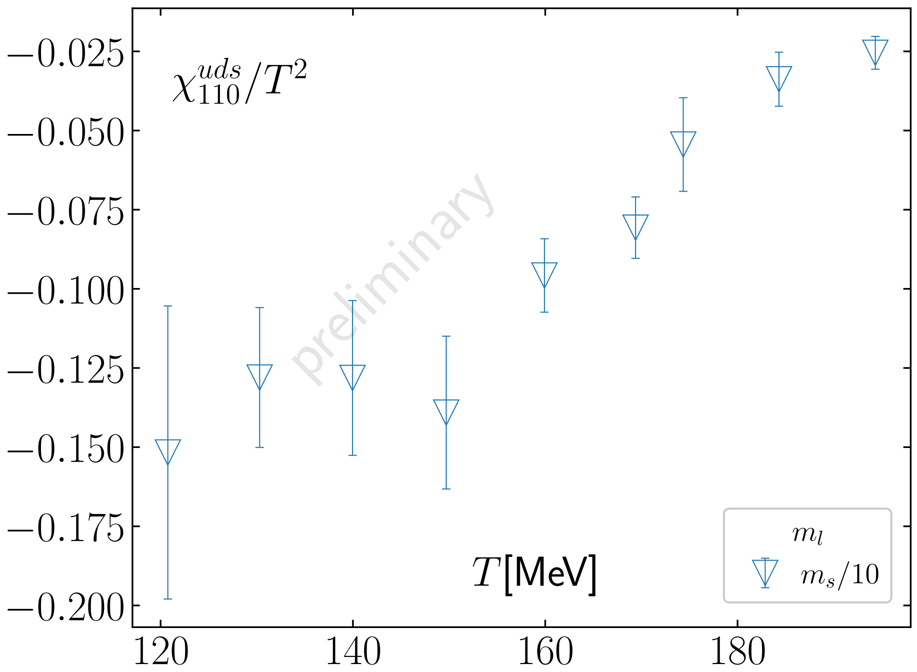
We plan to use $N_\tau = 16$ to understand the m_{res} and cut-off dependence on this observables.

Quark number susceptibility

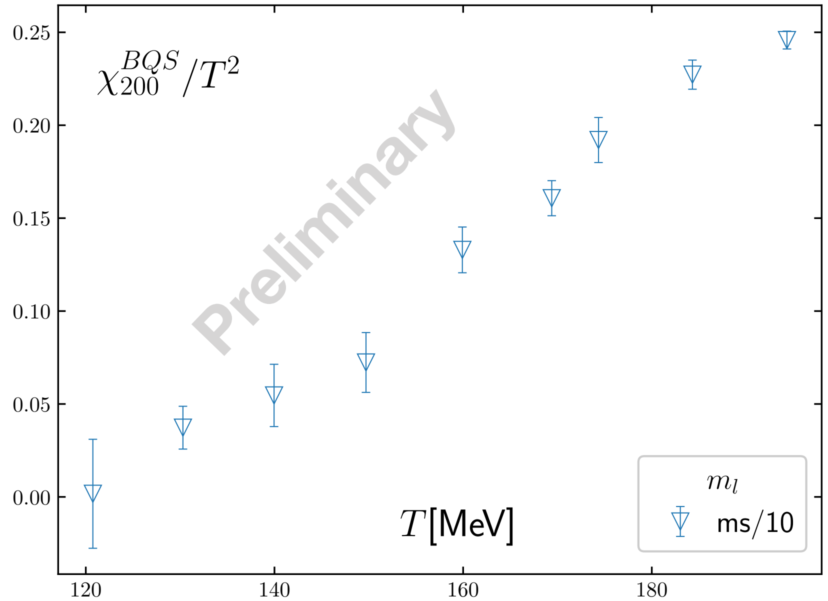


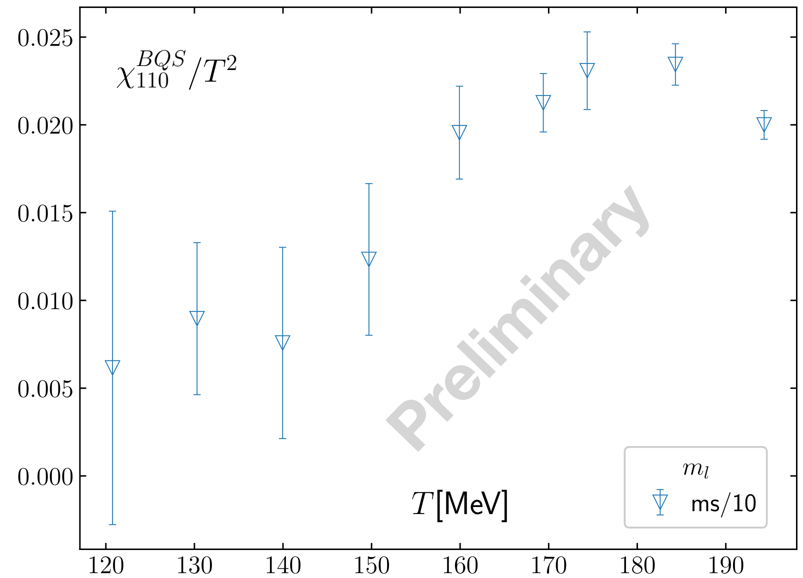


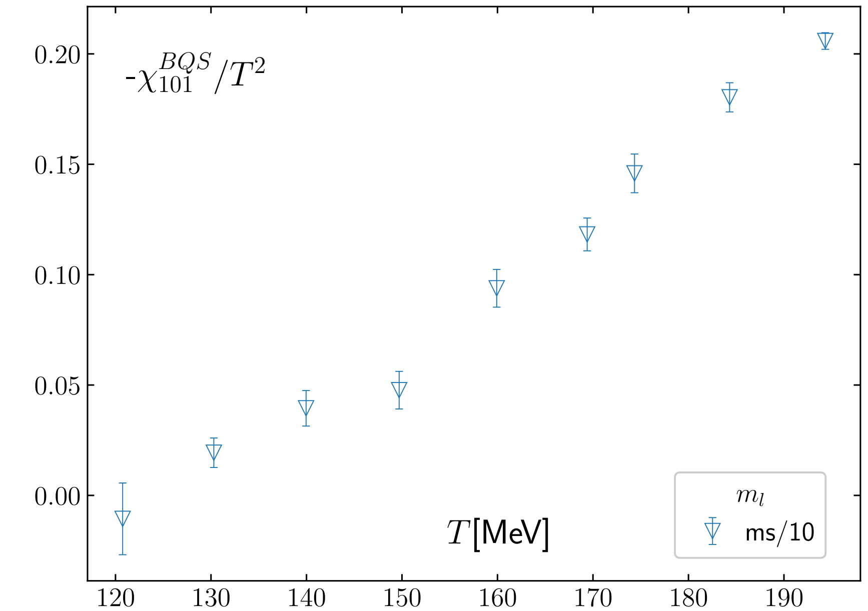


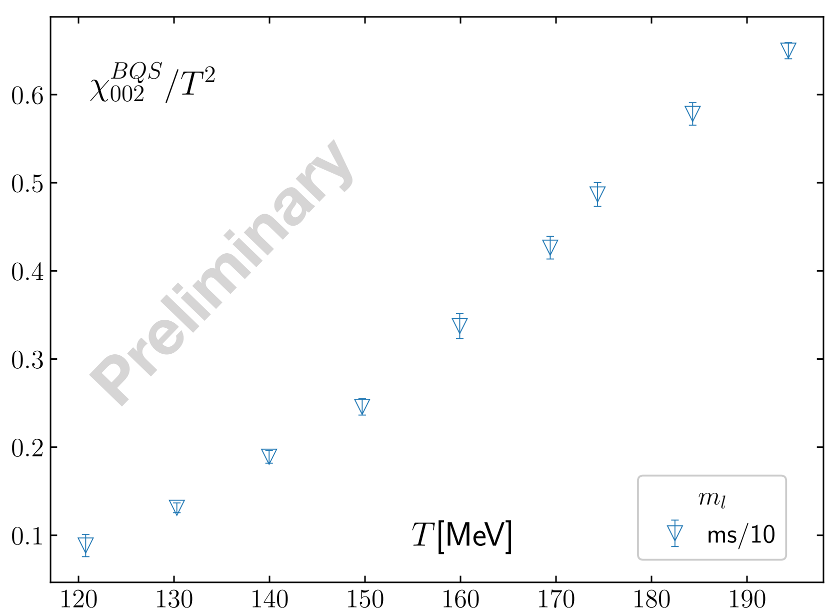


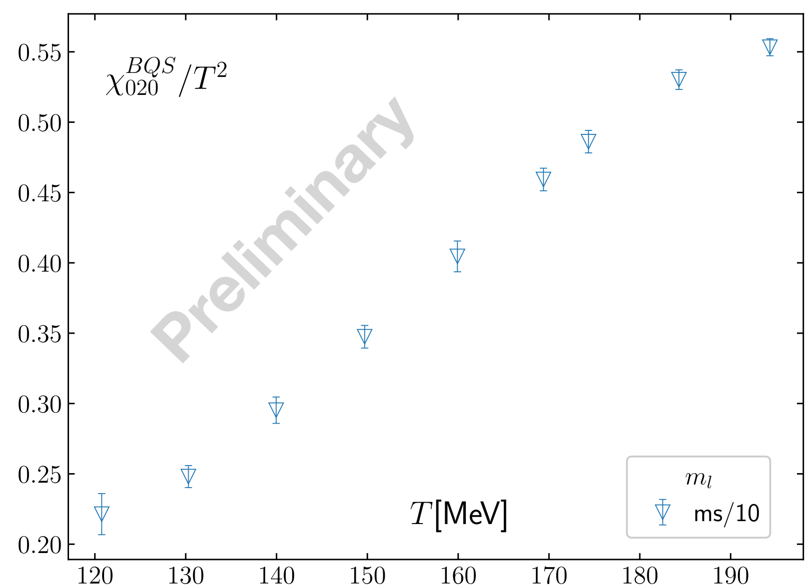
Conserved charge fluctuations

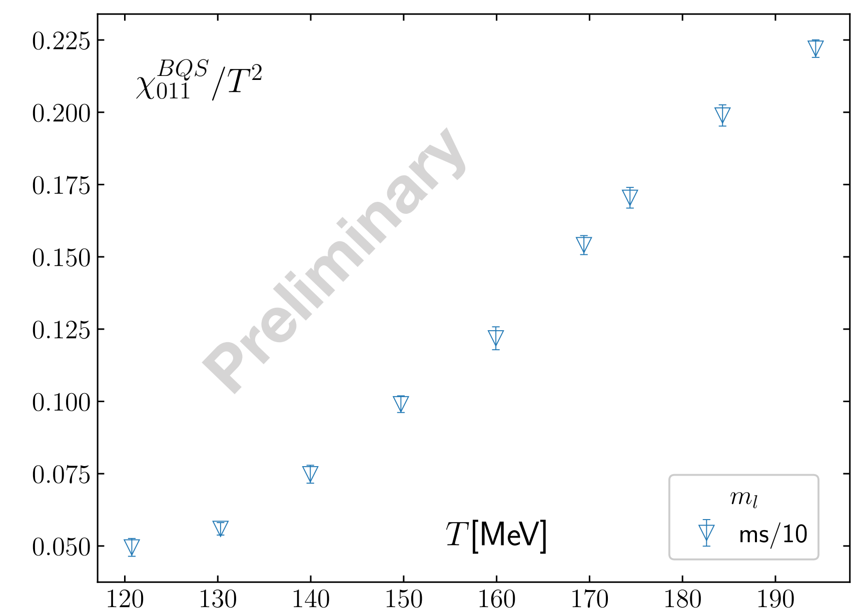




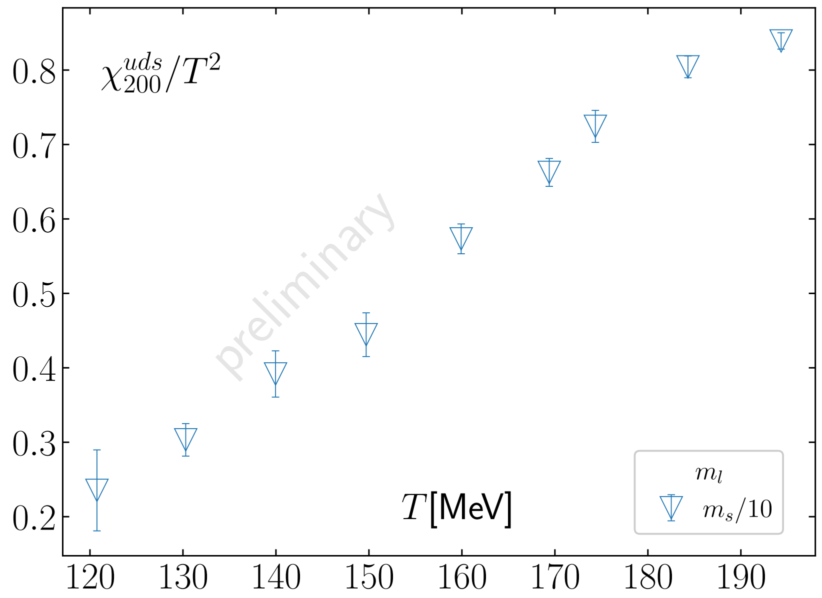


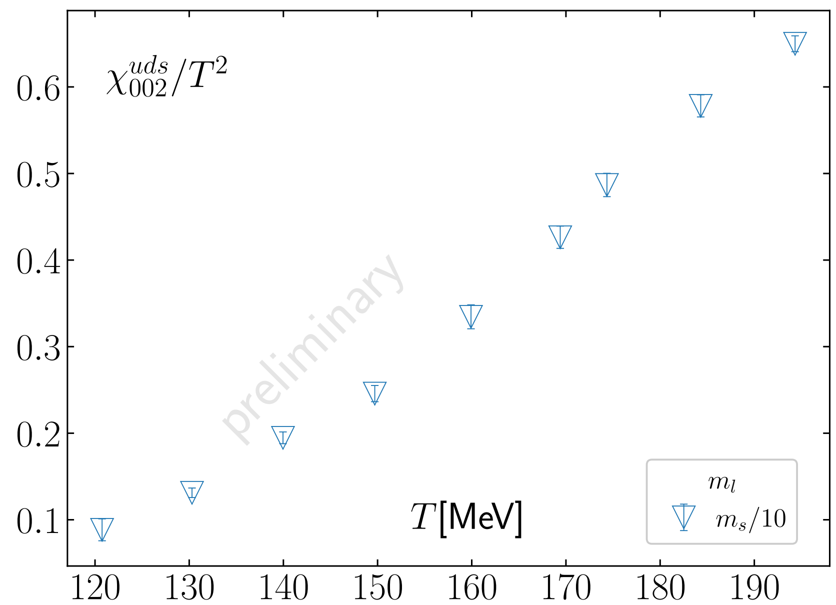


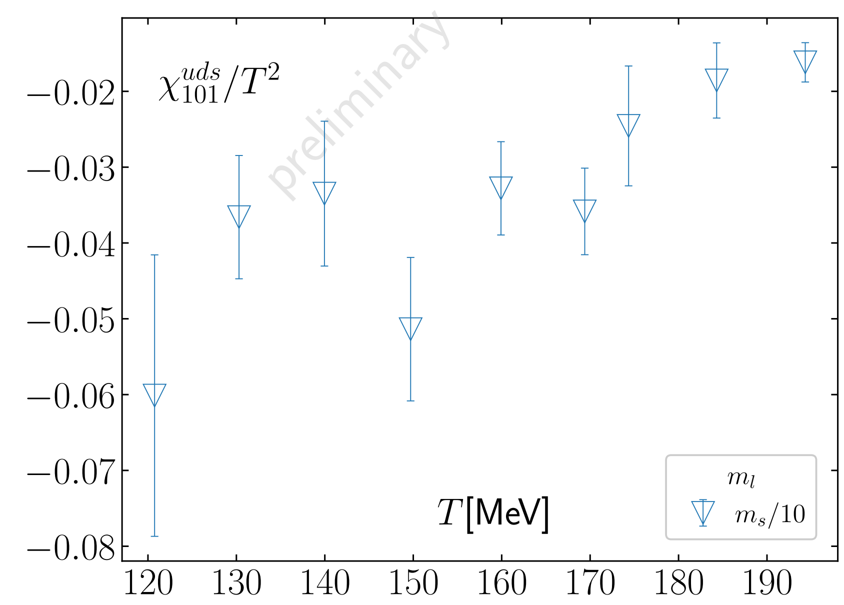


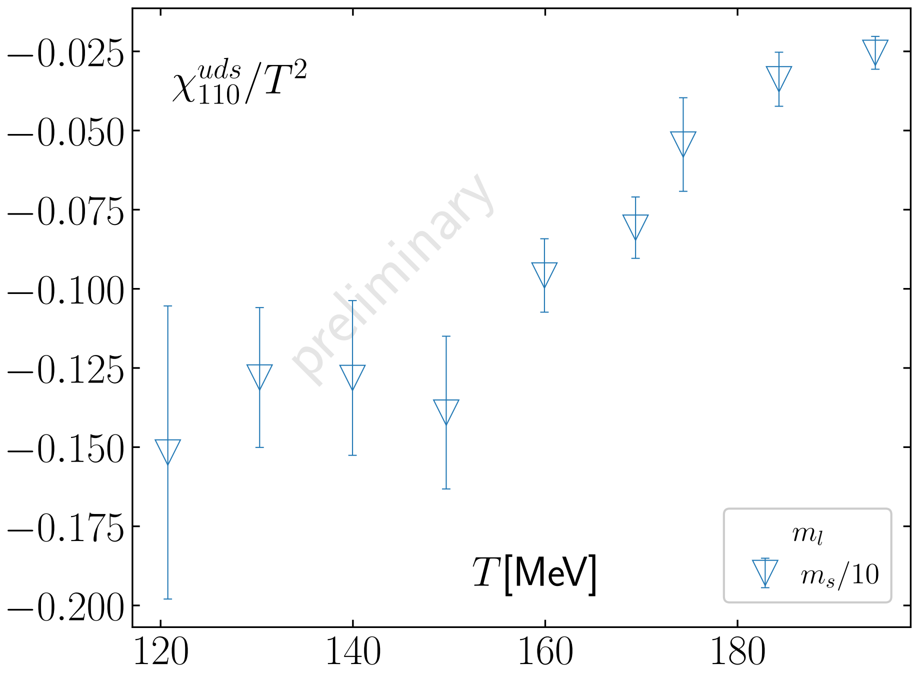


Quark number susceptibility









β	T[MeV]	#conf	sep
4.00	120.75	108	100
4.02	130.29	351	50
4.04	139.95	178	100
4.06	149.70	396	50
4.08	159.91	212	100
4.10	169.39	206	100
4.11	174.35	205	100
4.13	184.30	207	100
4.15	194.32	403	50

Quark number susceptibility

$$Z = \int DU \prod_{f=u,d,s} detM(m_f)\exp[-S_g],$$

$$\det M(m_f, \mu_f) = \left[\frac{\det D(m_f, \mu_f)^{DWF}}{\det D(m_{PV}, \mu_f)^{DWF}}\right]$$

$$\chi_2^f = \frac{N_\tau}{N_\sigma^3}\frac{\partial^2 \ln Z}{\partial \hat{\mu}_f^2} = \langle D_2^f \rangle + \langle (D_1^f)^2 \rangle$$

Matrix size : $N \times N$, **N =** $V \times 4 \times 3$
V = $24^3 \times 12 \times 12$

Noise reduction in stochastic trace estimators ??

Noise induced error reduction from unphysical degrees of freedom :

$$D_1^f = \frac{1}{N_n}\sum_j^{N_n}\left[\eta_j^\dagger D(m_f)^{-1}\frac{dD(m_f)}{d\mu_f}\eta_j - \eta_j^\dagger D(m_{pv})^{-1}\frac{dD(m_{pv})}{d\mu_f}\eta_j\right]$$

Each trace needs proper subtraction from the unphysical degrees of freedom

Noise induced error reduction using dilution vectors :

$$D_1^f = \frac{1}{N_n}\sum_j^{N_n}\left[\sum_{a=1}^{N}\eta_{aj}^\dagger D(m_f)^{-1}\frac{dD(m_f)}{d\mu_f}\eta_{aj} - \sum_{a=1}^{N} D(m_{pv})^{-1}\frac{dD(m_{pv})}{d\mu_f}\eta_{aj}\right]$$