Why can we trust canonical approach to finite density QCD ?

Ryutaro Fukuda

SCHOOL OF SCIENCE
THE UNIVERSITY OF TOKYO

Zn collaboration

A. Nakamura (Hiroshima), S. Oka (Rikkyo),
Y. Taniguchi (Tsukuba), A. Suzuki (Tsukuba)

YITP, HHIQCD 2015, March 12, 2015

Our motivation

http://www.bnl.gov/physics/news/news.asp?a=1870&t=today
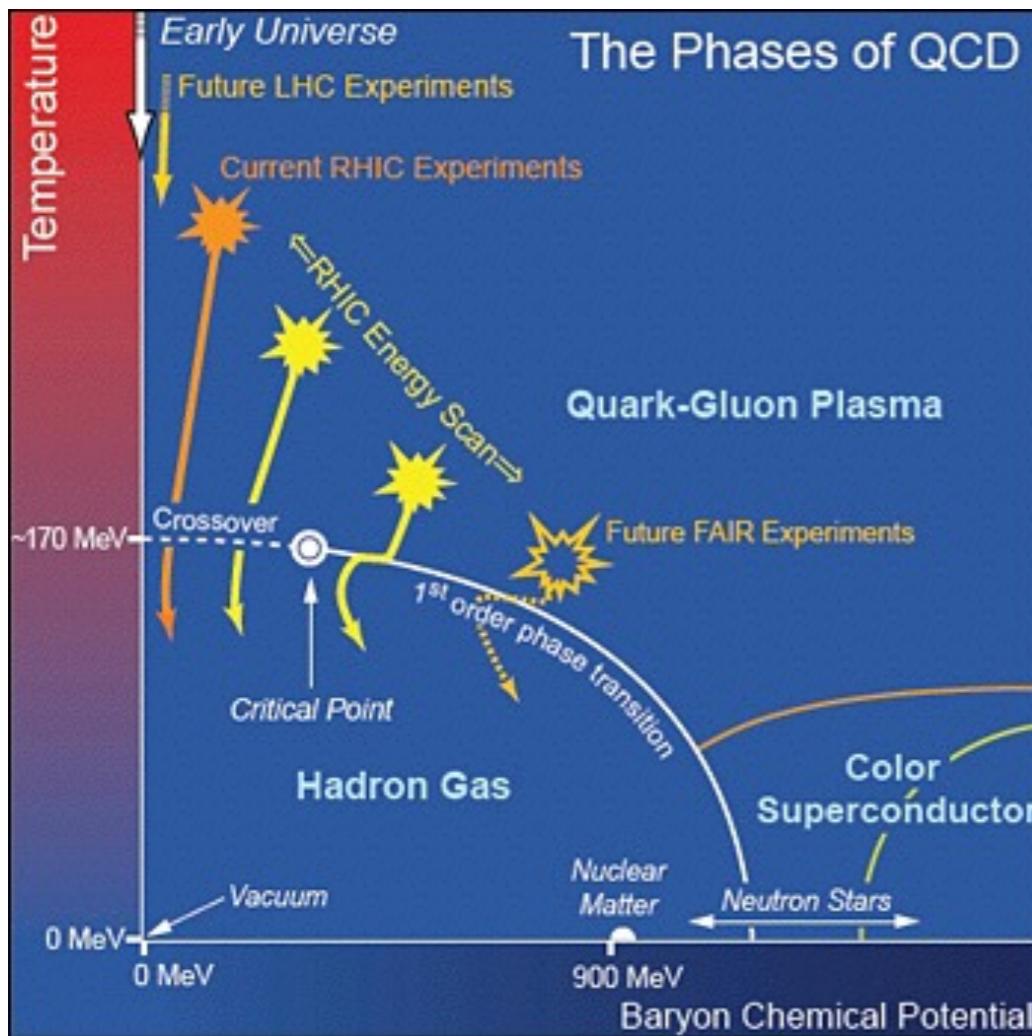
Many types of QCD phase diagram at finite density have been proposed by lots of calculations.

However...

The most part is **still unknown** !!
All phase diagram is just an outlook chart.

Our purpose is to break this present situation with **First-principle calculation**!!

We adopt the **canonical approach** !!

What is canonical approach ?

To get the grand canonical partition function in the following form.

$$Z_{GC}(\mu, T) = \sum_{n=-\infty}^{\infty} Z_n(T) \left(\underbrace{e^{\mu/T}}_{\text{fugacity}} \right)^n$$

Question : Above relation is reasonable ?

Absolutely, yes !!

$$Z_{GC}(\mu, T) = \text{Tr } e^{-(\hat{H} - \mu \hat{N})/T} = \sum_n \langle n | e^{-(\hat{H} - \mu \hat{N})/T} | n \rangle$$

If $\left[\hat{H}, \hat{N} \right] = 0$ $= \sum_n \langle n | e^{-\hat{H}/T} | n \rangle e^{n\mu/T} \equiv \sum_n Z_n(T) e^{n\mu/T}$

Is canonical approach useful ?

Absolutely, yes !!

(A. Hasenfratz and D. Toussaint (1992))

① No sign problem at pure imaginary chemical potential

$$Z_n(T) = \frac{1}{2\pi} \int_0^{2\pi} d\left(\frac{\mu_I}{T}\right) \underline{Z_{GC}(i\mu_I)} e^{-in\mu_I/T}$$

$$\mu_I \in \mathbb{R}$$

However, Fourier transformation (F.T.) is numerically unstable because of the oscillatory integral.
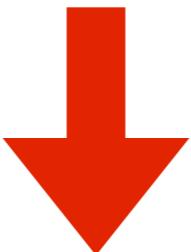
Our solution : **Multiple-precision calculation**

Is canonical approach useful ?

Absolutely, yes !!

② Available at any chemical potential

$$Z_{GC}(\mu, T) = \sum_{n=-\infty}^{\infty} Z_n(T) \left(e^{\mu/T} \right)^n$$

Chemical potential dependence is **only in fugacity**.

Desired density can be got by **tuning the fugacity**.

Is canonical approach useful ?

Absolutely, yes !!

③ We can get thermodynamic observables directly.

$$\frac{p(\mu, T)}{T^4} = \frac{1}{V_s T^3} \log Z_{GC}(\mu, T) = \frac{1}{V_s T^3} \log \left(\sum_n Z_n(T) e^{n\mu/T} \right)$$

$$\frac{n(\mu, T)}{T^3} = \frac{\partial}{\partial(\mu/T)} \frac{p(\mu, T)}{T^4} \quad , \quad \frac{\chi(\mu, T)}{T^2} = \frac{\partial^2}{\partial(\mu/T)^2} \frac{p(\mu, T)}{T^4}$$

How to evaluate $Z_{GC}(i\mu_I)$?

$$Z_n(T) = \frac{1}{2\pi} \int_0^{2\pi} d\left(\frac{\mu_I}{T}\right) \boxed{Z_{GC}(i\mu_I)} e^{-in\mu_I/T}$$

$\boxed{\text{Our proposal}}$

To regard the calculation of grand canonical partition function as the calculation of expectation value of fermion determinant.

$$\left\langle \frac{\det \Delta(i\mu_I)}{\det \Delta(\mu_0)} \right\rangle_{\mu_0} \quad \Longrightarrow \quad Z_{GC}(i\mu_I)$$

Our strategy to calculate $Z_{GC}(i\mu_I)$

$$Z_{GC}(i\mu_I) = \int [dU] \left(\frac{\det \Delta(i\mu_I)}{\det \Delta(\mu_0)} \right) \det \Delta(\mu_0) \, e^{-S_g} = Z_{GC}(\mu_0) \left\langle \frac{\det \Delta(i\mu_I)}{\det \Delta(\mu_0)} \right\rangle_{\mu_0}$$
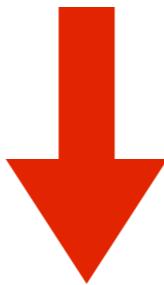
$$Z_n(T) = \underbrace{Z_{GC}(\mu_0)}_{\text{constant}} \times \frac{1}{2\pi} \int_0^{2\pi} d\left(\frac{\mu_I}{T} \right) \left\langle \frac{\det \Delta(i\mu_I)}{\det \Delta(\mu_0)} \right\rangle_{\mu_0} e^{-in\mu_I/T}$$
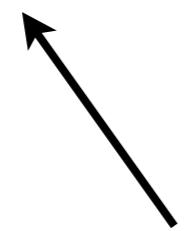
To avoid this constant, we consider $\dfrac{Z_n(T)}{Z_0(T)}$.

We have only to evaluate $\left\langle \dfrac{\det \Delta(i\mu_I)}{\det \Delta(\mu_0)} \right\rangle_{\mu_0}$.

How to evaluate the fermion determinant ?

We adopt **Wilson fermions** formulation.

$\left\langle \dfrac{\det \Delta(i\mu_I)}{\det \Delta(\mu_0)} \right\rangle_{\mu_0}$ is needed at various pure imaginary chemical potentials.
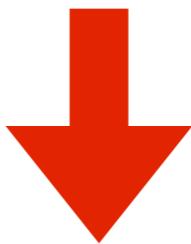
Calculation cost is too high if we compute it directly
at all pure imaginary chemical potential point.

Thus, in our work, we use so-called **winding number expansion**
based on hopping parameter expansion to reduce calculation cost.

Hopping parameter expansion

Wilson fermion matrix : $\Delta(\mu) = 1 - \kappa Q(\mu)$

Key identity : $\det \Delta = e^{\mathrm{Tr}\log \Delta} = e^{\mathrm{Tr}\log(1-\kappa Q)}$

$$\mathrm{Tr}\log(1 - \kappa Q(\mu)) = \sum_{n=1}^{\infty} \frac{\kappa^n}{n} \boxed{\mathrm{Tr}\, Q^n(\mu)}$$

$$\sum_{x,\alpha,a} \langle x, \alpha, a | \, Q^n(\mu) \, | x, \alpha, a \rangle$$

x : space-time α : spinor a : color
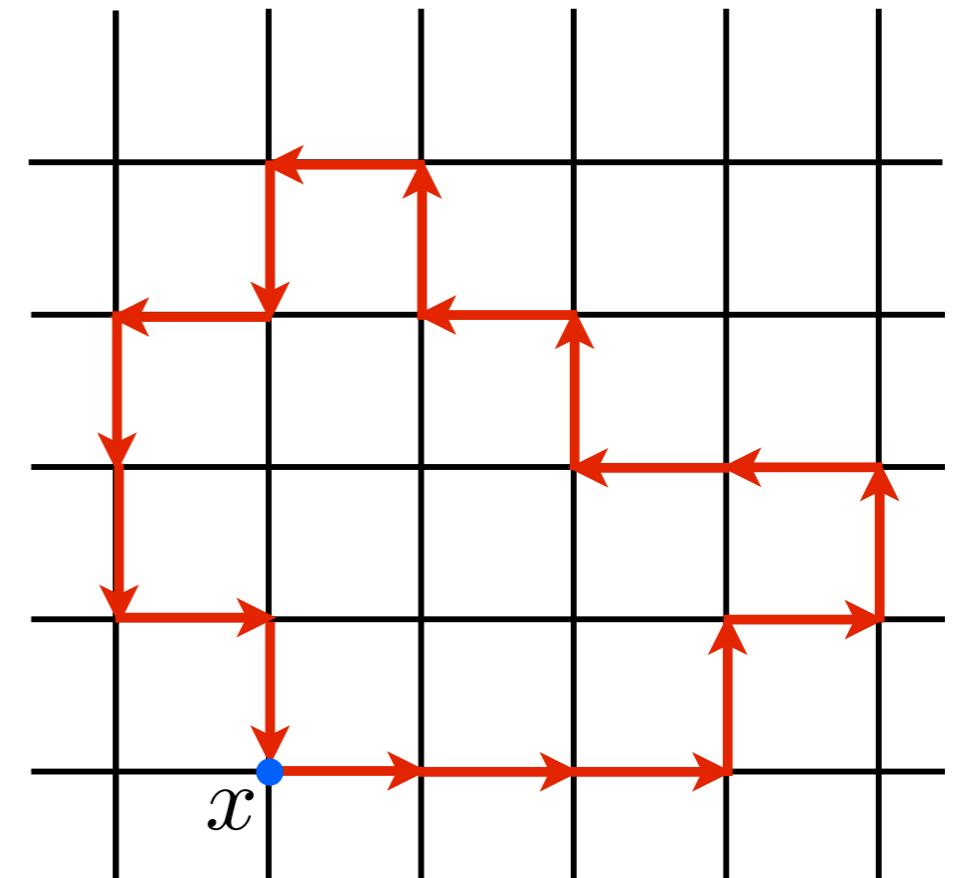
Non-zero contribution comes from **closed loops**.

Winding number expansion (WNE)

$$\det D = \exp(\mathrm{Tr}\log D)$$

$$= \exp\left(e^{+\mu/T}Q^+ + e^{-\mu/T}Q^- + \cdots\right)$$
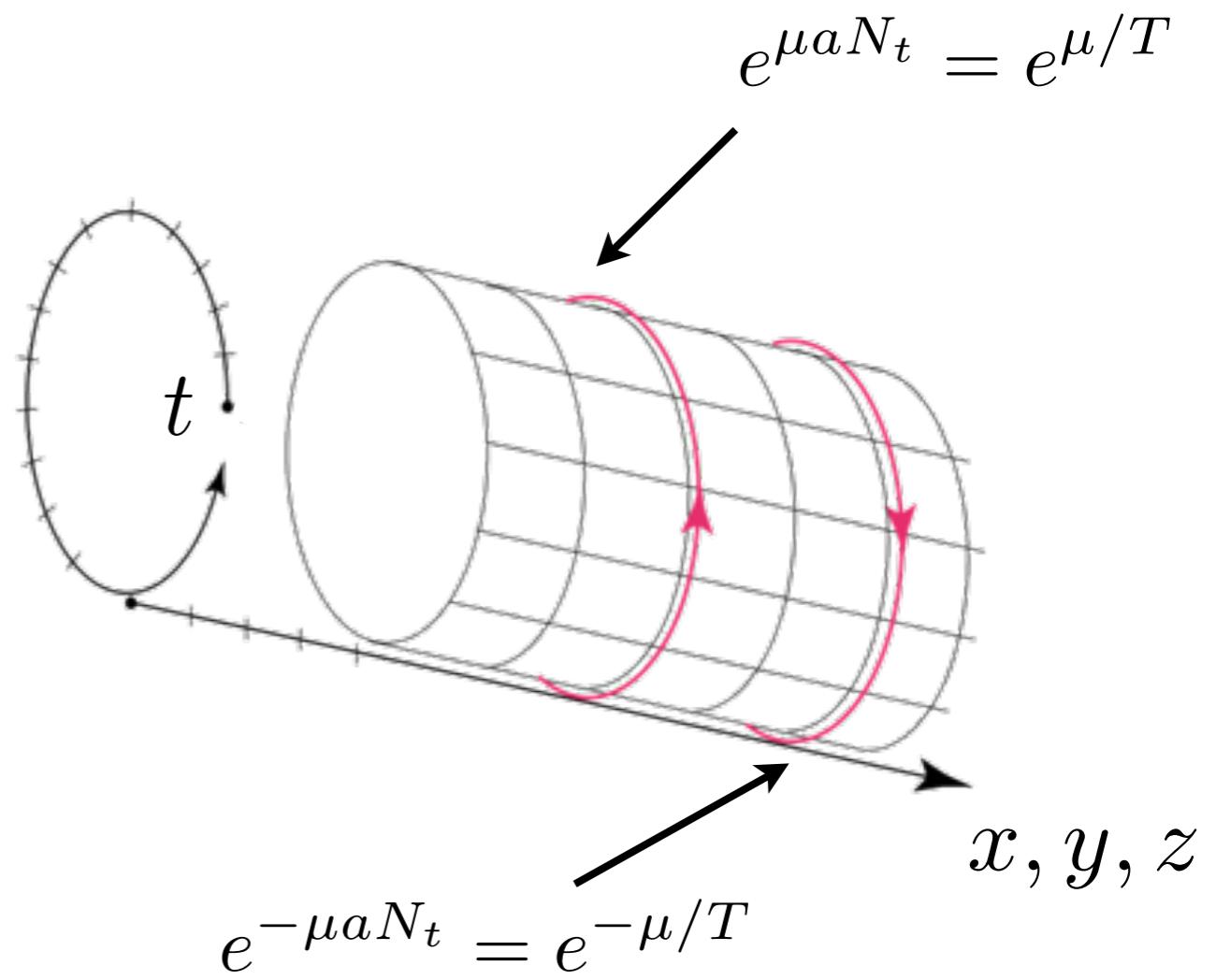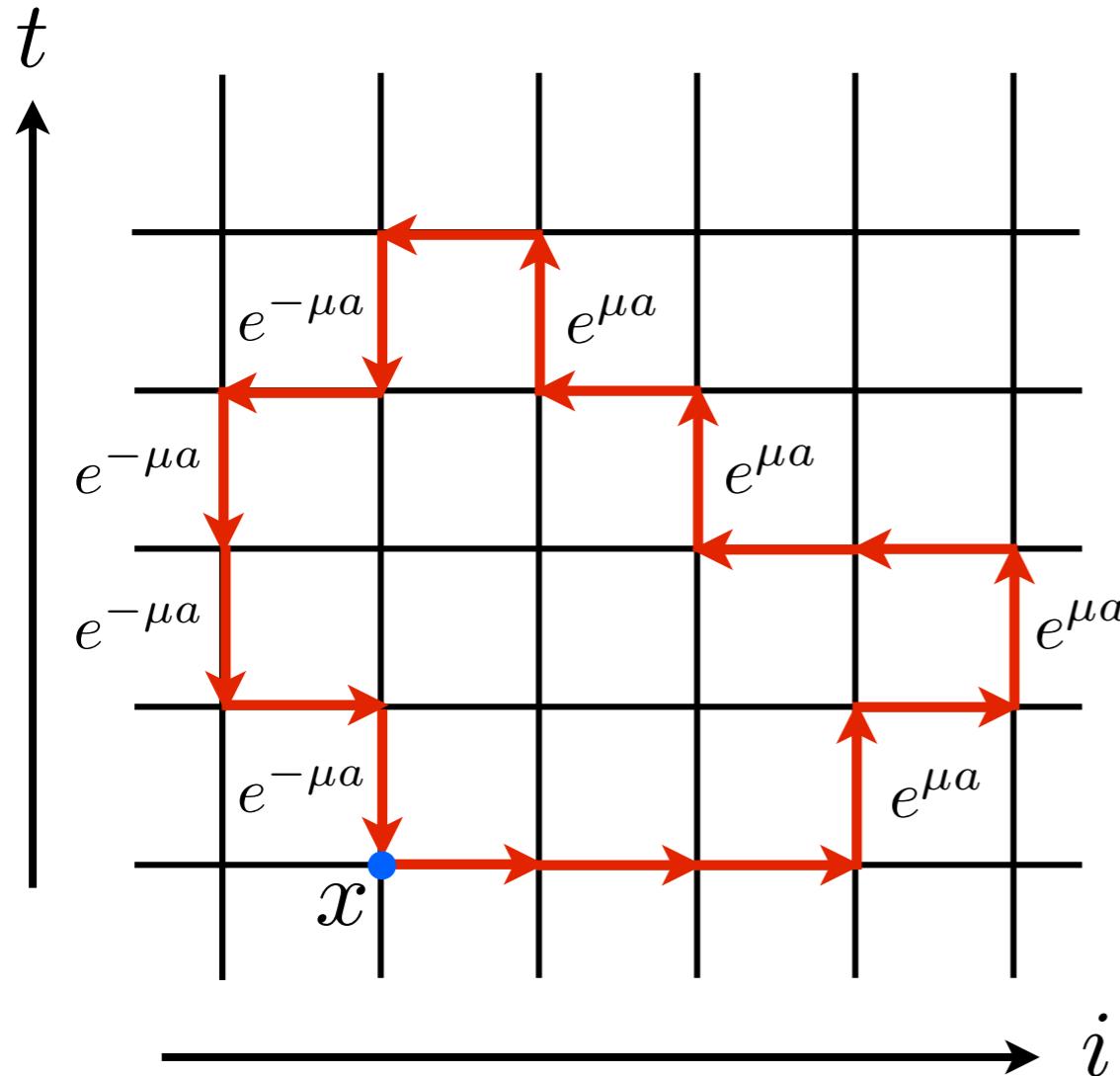
Loops winding $\pm n$ times along time direction have chemical potential dependence $e^{\pm n\mu/T}$.

$$\det \Delta(\mu) = e^{\mathrm{Tr}\log(1-\kappa Q(\mu))} \equiv \exp\left[\sum_{n=-\infty}^{\infty} W_n e^{n\mu/T}\right]$$

Summary of our strategy

$$\left\langle \frac{\det \Delta(i\mu_I)}{\det \Delta(\mu_0)} \right\rangle_{\mu_0} \quad \Longrightarrow \quad Z_{GC}(i\mu_I) \quad \Longrightarrow \quad Z_n$$

$$\det \Delta(\mu) = e^{\mathrm{Tr} \log(1-\kappa Q(\mu))} \equiv \exp\left[\sum_{n=-\infty}^{\infty} W_n e^{n\mu/T} \right]$$

Step ① : Make gauge configurations at $\mu_0 = 0$.

Step ② : Calculate the sets of coefficients W_n .

Step ③ : Calculate $Z_{GC}(i\mu_I)$ from the expectation
value of fermion determinant with WNE.

Step ④ : Calculate Z_n through F.T. .

Step ⑤ : Calculate thermodynamic observables.

Numerical set up

$\boxed{\text{Action}}$

Fermion part : 2-flavor clover improved Wilson fermion action

Gauge part : RG-improved gauge action

$\boxed{\text{Parameters}}$ (S. Ejiri et al, Phys. Rev. D82:014508, 2010)

$$N_s^3 \times N_t = 8^3 \times 4 \,, \quad m_{\rm ps}/m_{\rm v} = 0.8$$

$$T/T_c = 1.35(7), 1.20(6), 1.08(5), 0.93(5)$$

$\boxed{\text{Observables}}$

$$\frac{\delta p(\mu_B/T)}{T^4} \equiv \frac{p(\mu_B/T) - p(0)}{T^4} \,, \qquad \frac{n_B(\mu_B/T)}{T^3} \,, \qquad \frac{\chi(\mu_B/T)}{T^2}$$

Truncation error estimation

$$Z_{GC}(\mu) = \sum_{n=-\infty}^{\infty} Z_n \, e^{n\mu/T} \sim \boxed{\sum_{n=-N_{\max}}^{N_{\max}} Z_n \, e^{n\mu/T}}$$

In numerical calculation, fugacity expansion is finite series.
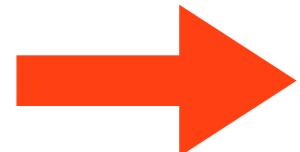
→ Truncation error cannot be negligible.

Two types of analyses

Choose suitable baryon number $N_{\max}$ and calculate observables with

$$① \sum_{n=-N_{\max}}^{N_{\max}} Z_n \, e^{n\mu/T} \qquad ② \sum_{n=-N_{\max}+1}^{N_{\max}-1} Z_n \, e^{n\mu/T} \, .$$

Chemical potential region where no deviation between both two results of above analysis is reliable.

Pressure at $T/T_c = 1.08(5)$

Red : $N_{\max} = 23$

Green : $N_{\max} - 1$

Blue : Multi-parameter reweighting (MPR)

(K.Nagata, A,Nakamura
10.1007/JHEP04(2012)092)
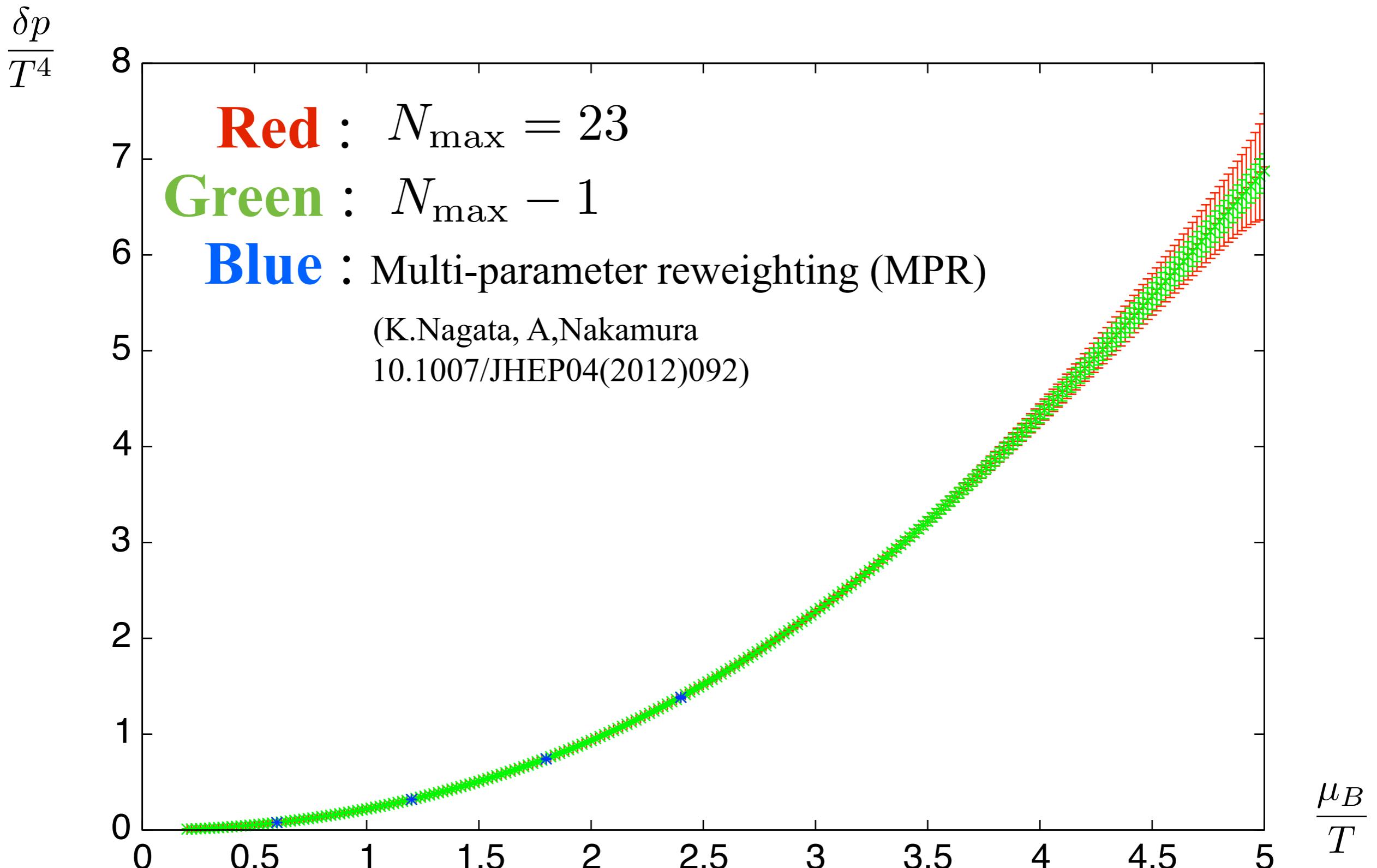
reliable up to around $\frac{\mu_B}{T} = 4.5$

Pressure at $T/T_c = 0.93(5)$

Red : $N_{\max} = 11$
**Green** : $N_{\max} - 1$
Blue : MPR (K.Nagata, A,Nakamura 10.1007/JHEP04(2012)092)
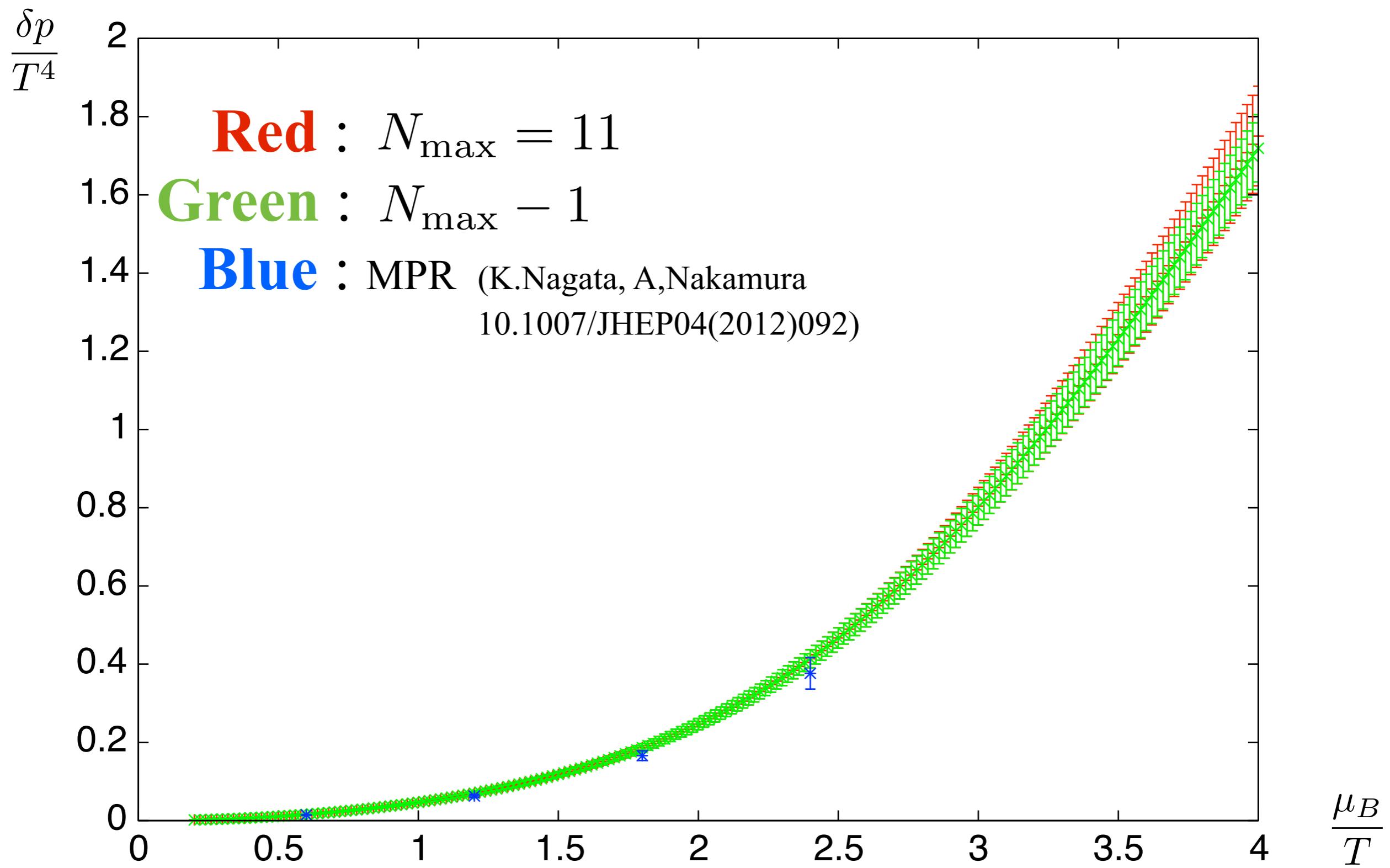
reliable up to around $\frac{\mu_B}{T} = 3.5$

Temperature dependence of pressure
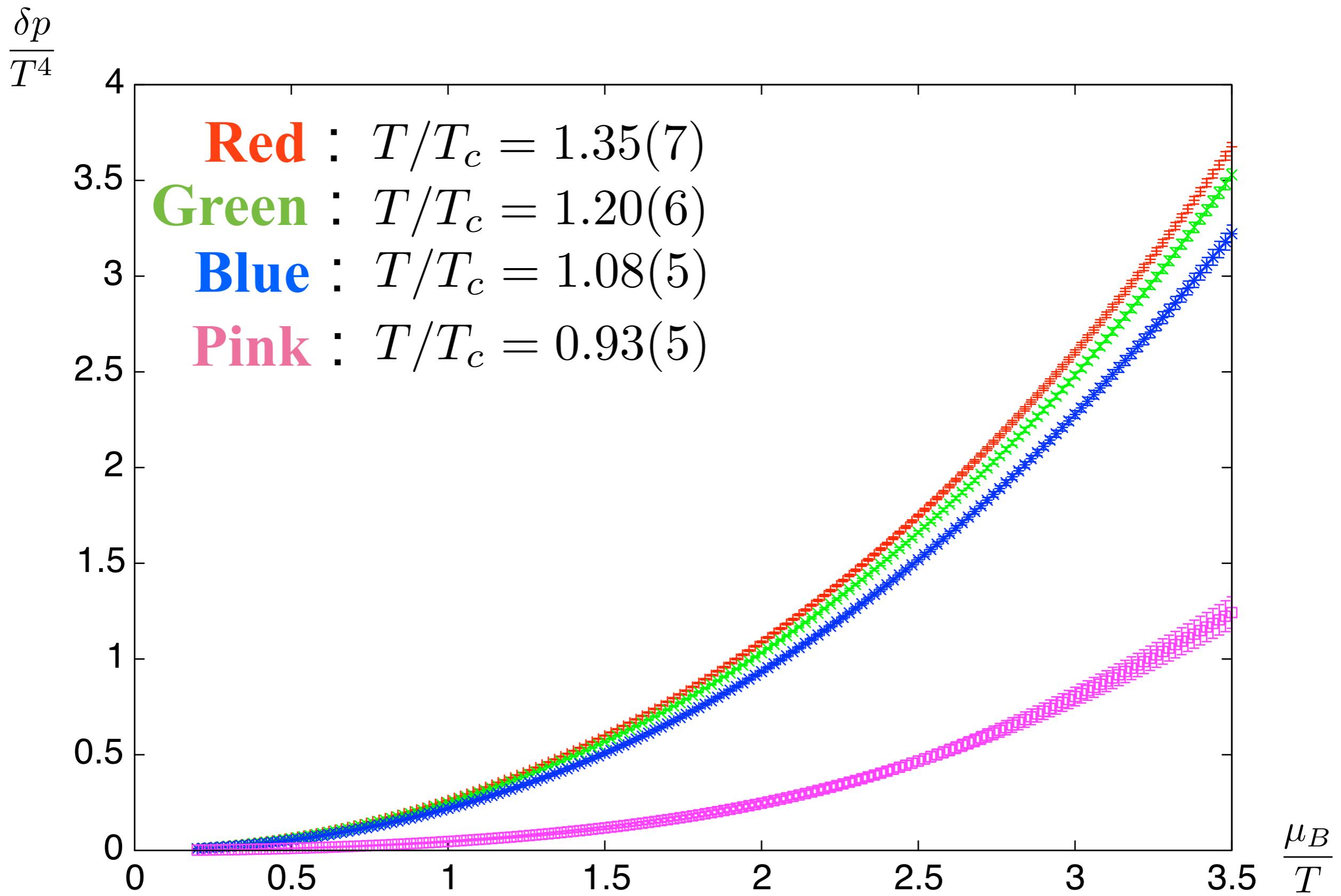
Baryon number density at $T/T_c = 1.08(5)$

Red : $N_{\max} = 23$
Green : $N_{\max} = 22$
Blue : MPR (K.Nagata, A,Nakamura
10.1007/JHEP04(2012)092)

reliable up to around $\frac{\mu_B}{T} = 4$

Baryon number density at $T/T_c = 0.93(5)$

Red : $N_{\max} = 11$
Green : $N_{\max} - 1$
Blue : MPR (K.Nagata, A,Nakamura
10.1007/JHEP04(2012)092)

reliable up to around $\frac{\mu_B}{T} = 3$
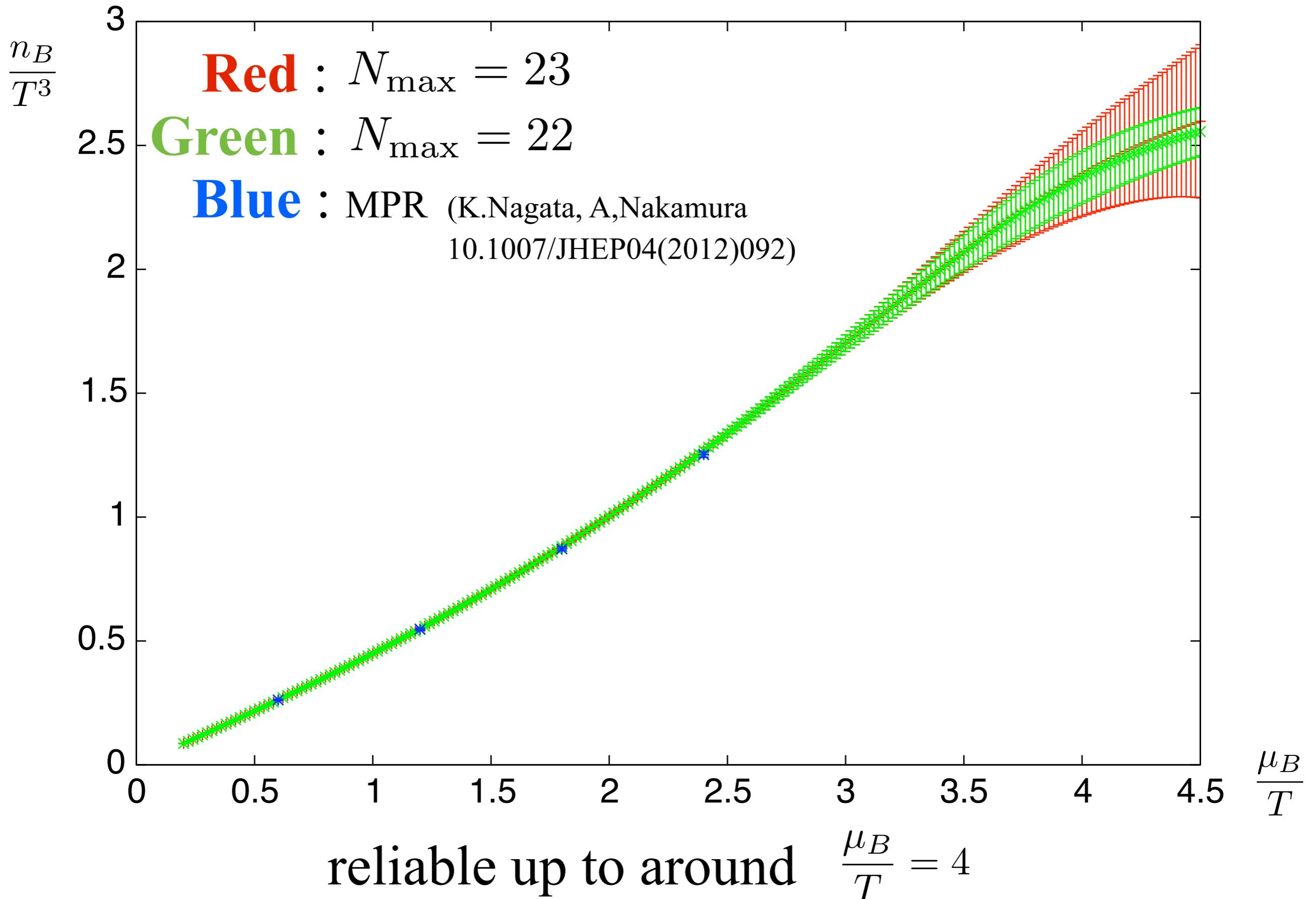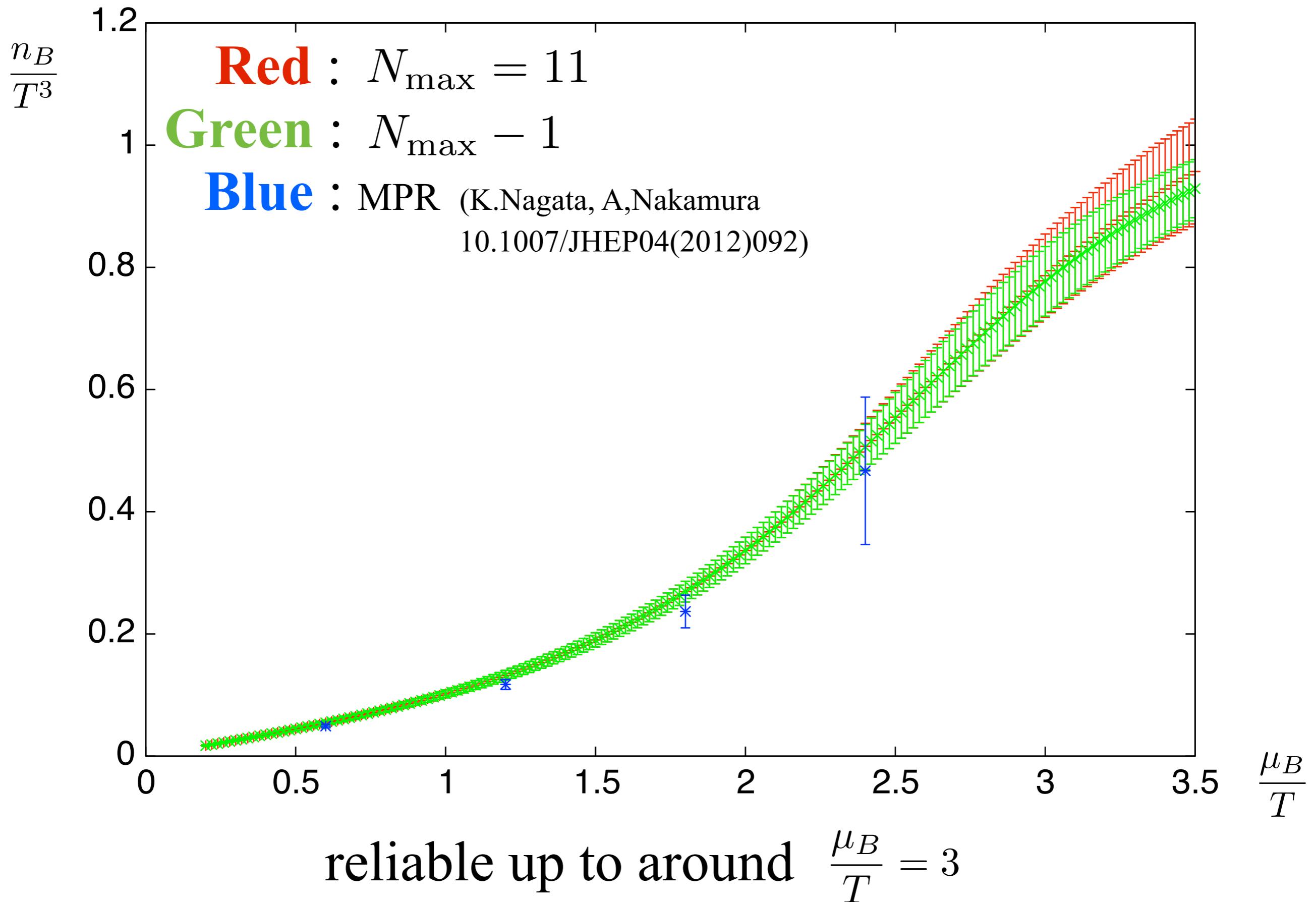
Temperature dependence of baryon number density

Red : $T/T_c = 1.35(7)$
Green : $T/T_c = 1.20(6)$
Blue : $T/T_c = 1.08(5)$
Pink : $T/T_c = 0.93(5)$

Susceptibility at $T/T_c = 1.08(5)$

Red : $N_{\max} = 23$
Green : $N_{\max} - 1$
Blue : MPR (K.Nagata, A,Nakamura 10.1007/JHEP04(2012)092)

This peak is caused by the truncation error.

reliable up to around $\frac{\mu_B}{T} = 3$

Susceptibility at $T/T_c = 0.93(5)$

Red : $N_{\max} = 11$
Green : $N_{\max} - 1$
Blue : MPR (K.Nagata, A,Nakamura 10.1007/JHEP04(2012)092)

This peak is caused by the truncation error.

reliable up to around $\frac{\mu_B}{T} = 2.3$
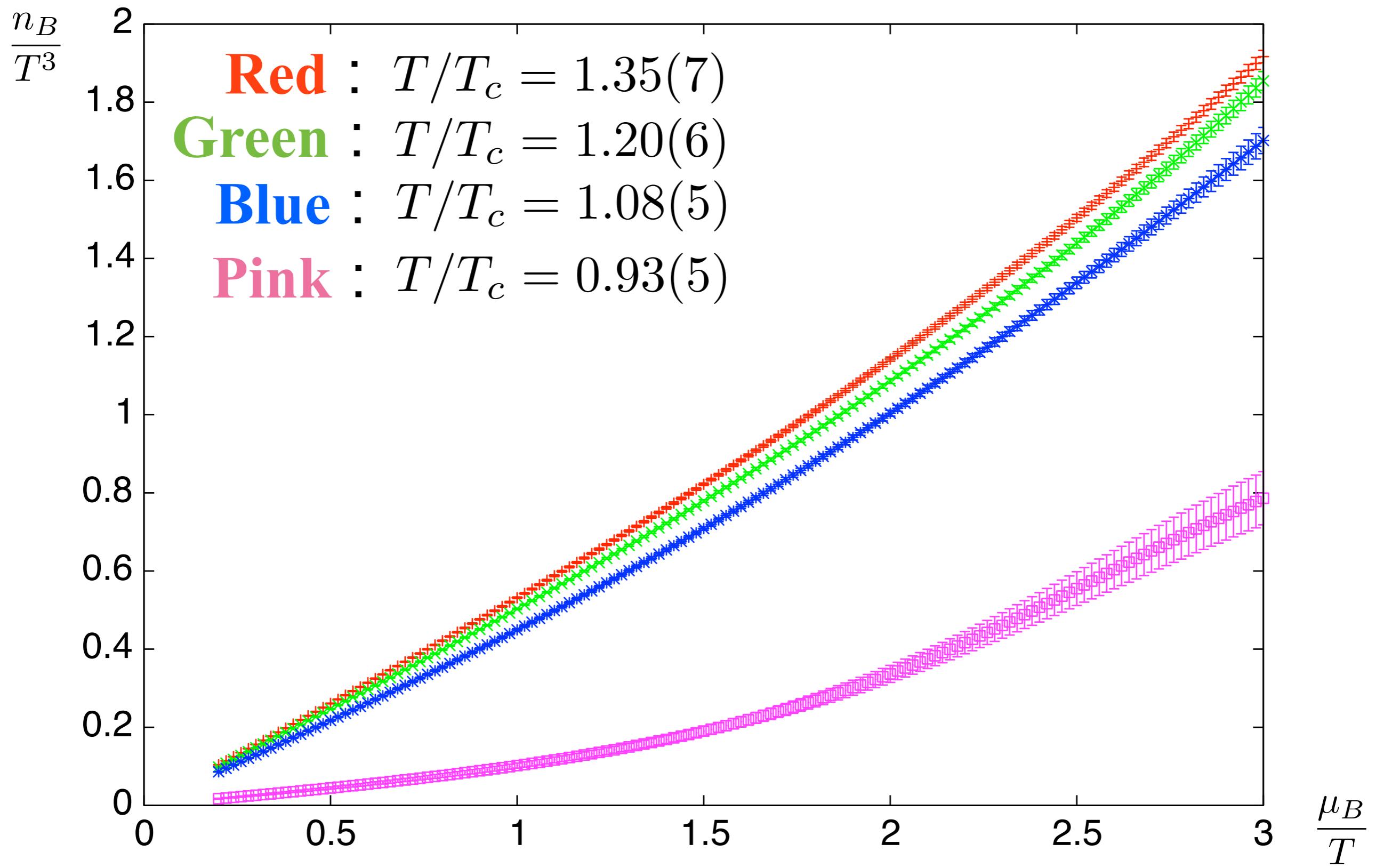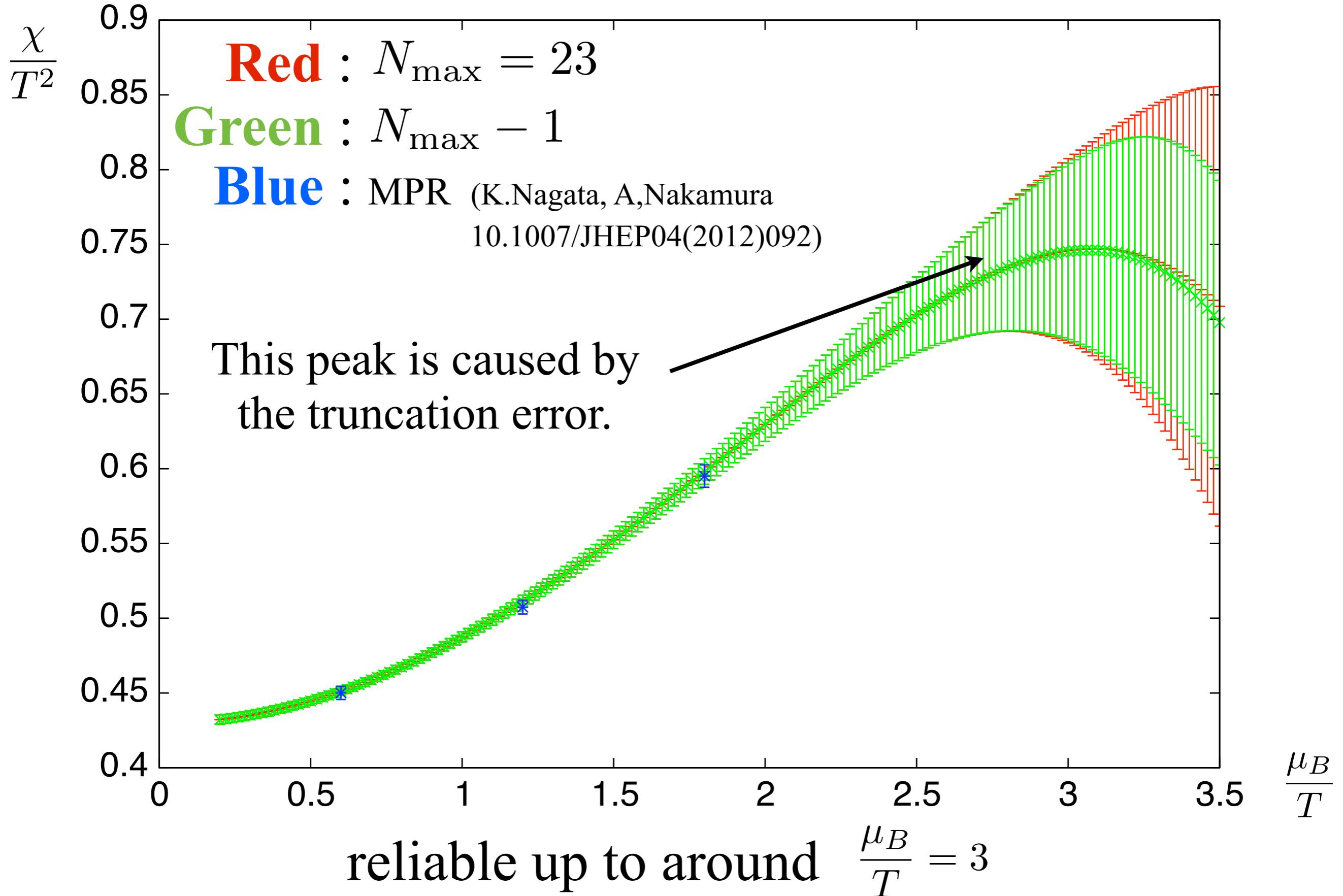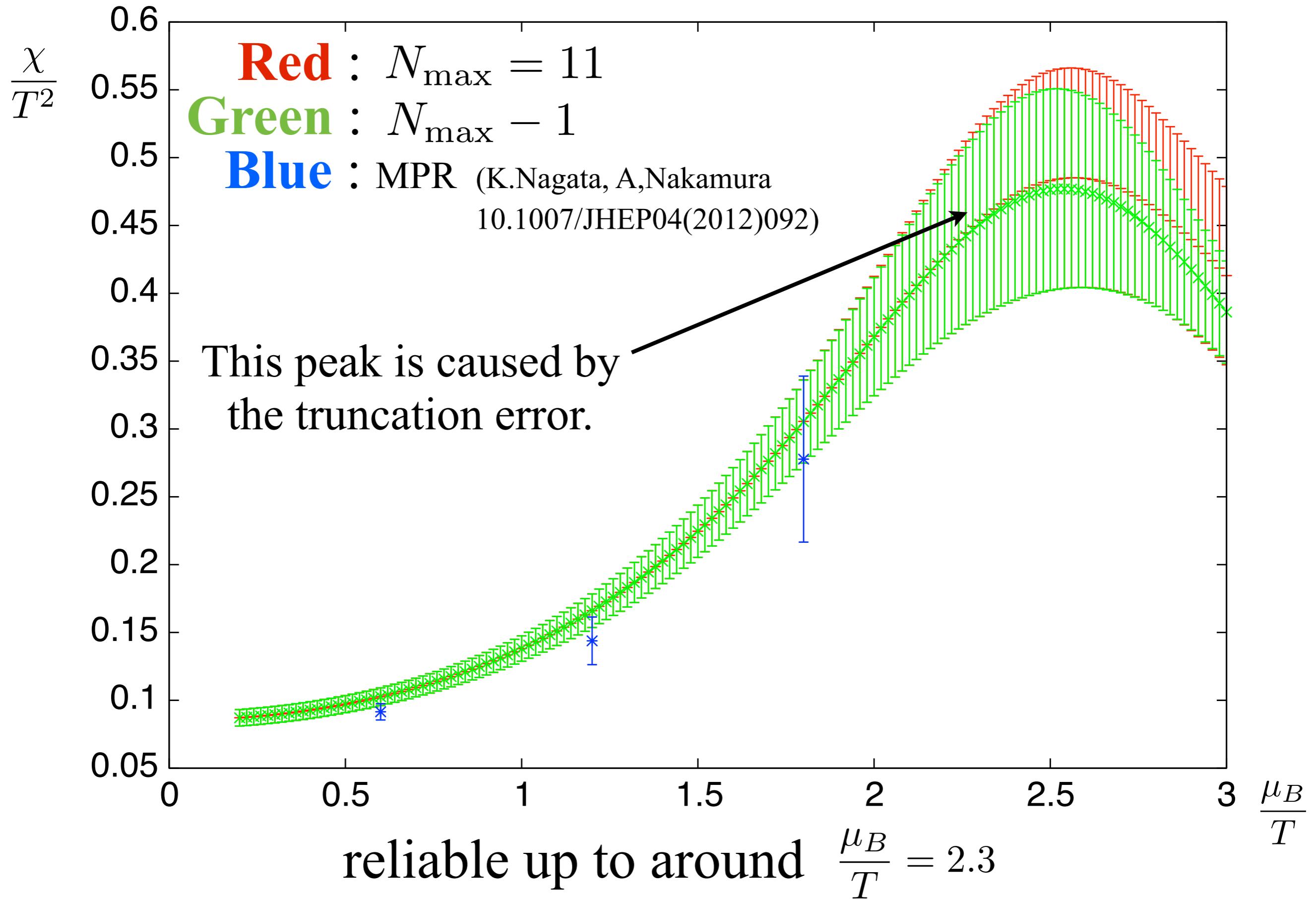
Summary

We checked
**canonical approach is consistent
with multi-parameter reweighting**.

Moreover, in many cases,
canonical approach is available **over** $\mu_B/T = 3$.

Conclusion ： **Canonical approach is reliable !!**

Outlook

Our purpose is to catch the phase transition at below T_c.

⬇
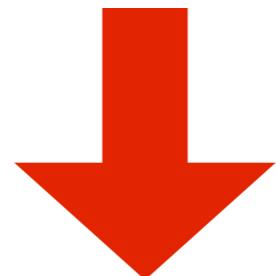
It is needed to calculate Z_n at more larger n.

Is it possible ?   *Yes !!*

We have to fight against calculation cost.

Thank you for your attention.

Cancelled significant digits in F.T.

Legend:
- $+$ $\beta = 1.80$ ($T/T_c = 0.93(5)$)
- $\times$ $\beta = 1.90$ ($T/T_c = 1.08(5)$)

y-axis: Cancelled significant digits [digits]

x-axis: n_B