Lattice QCD at finite baryon density using analytic continuation

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Outline

- Introduction
- Some results obtained by analytic continuation
- New method to compute canonical partition functions Z_n
- Conclusions

The work presented is completed by joint FEFU(Vladivostok) – ITEP(Moscow) – IHEP(Protvino) lattice group :

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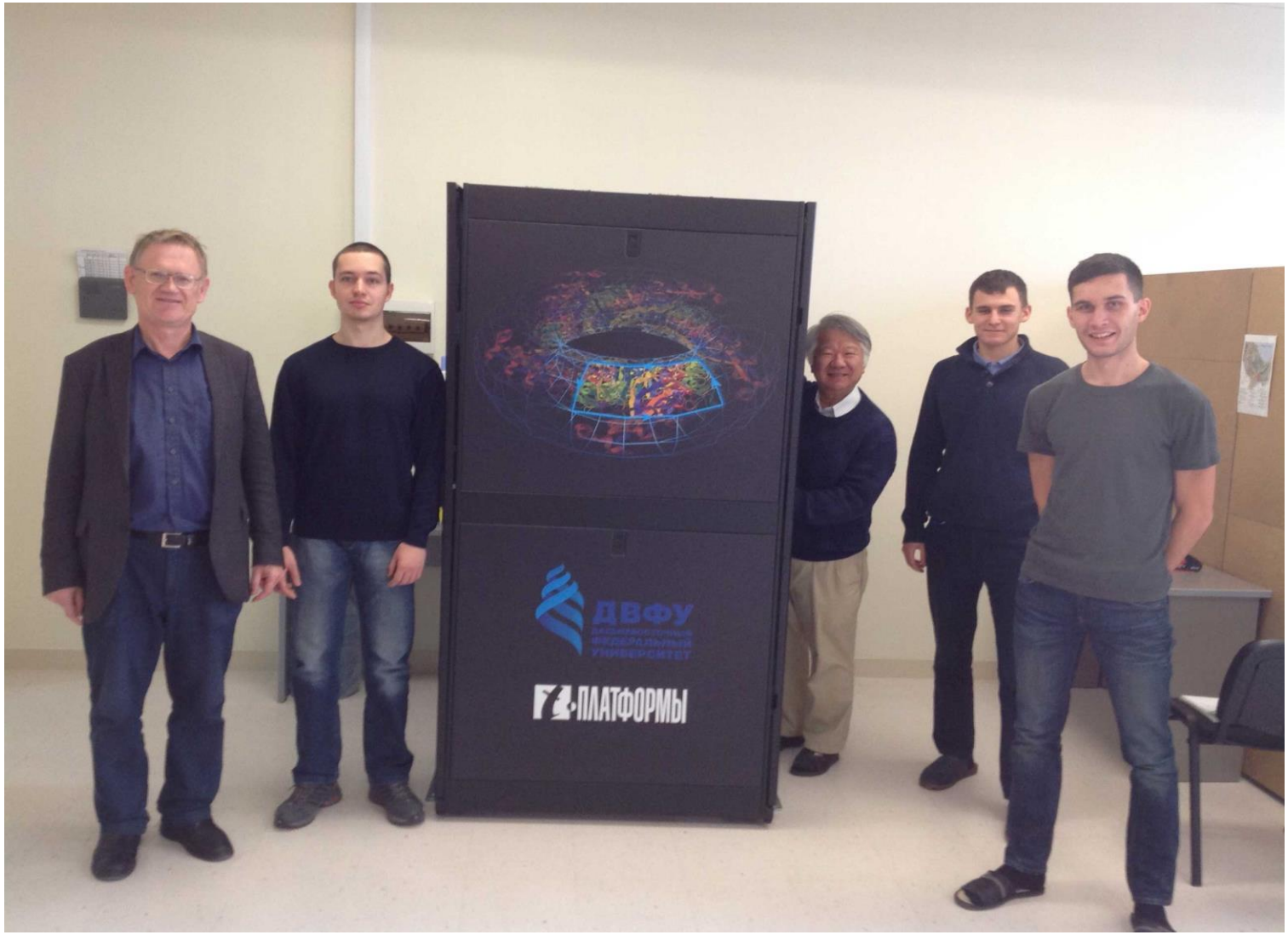
Denis Boyda
Hideaki Iida
Masayuki Wakayama

FEFU lattice group

‘QCD at nonzero baryon density’



The talk is based on publications:

- New approach to canonical partition functions computation in N_f=2 lattice QCD at finite baryon density.

  Phys.Rev. D95 (2017) no.9, 094506

- Study of lattice QCD at finite baryon density using the canonical approach.

  EPJ Web Conf. 137 (2017) 07017

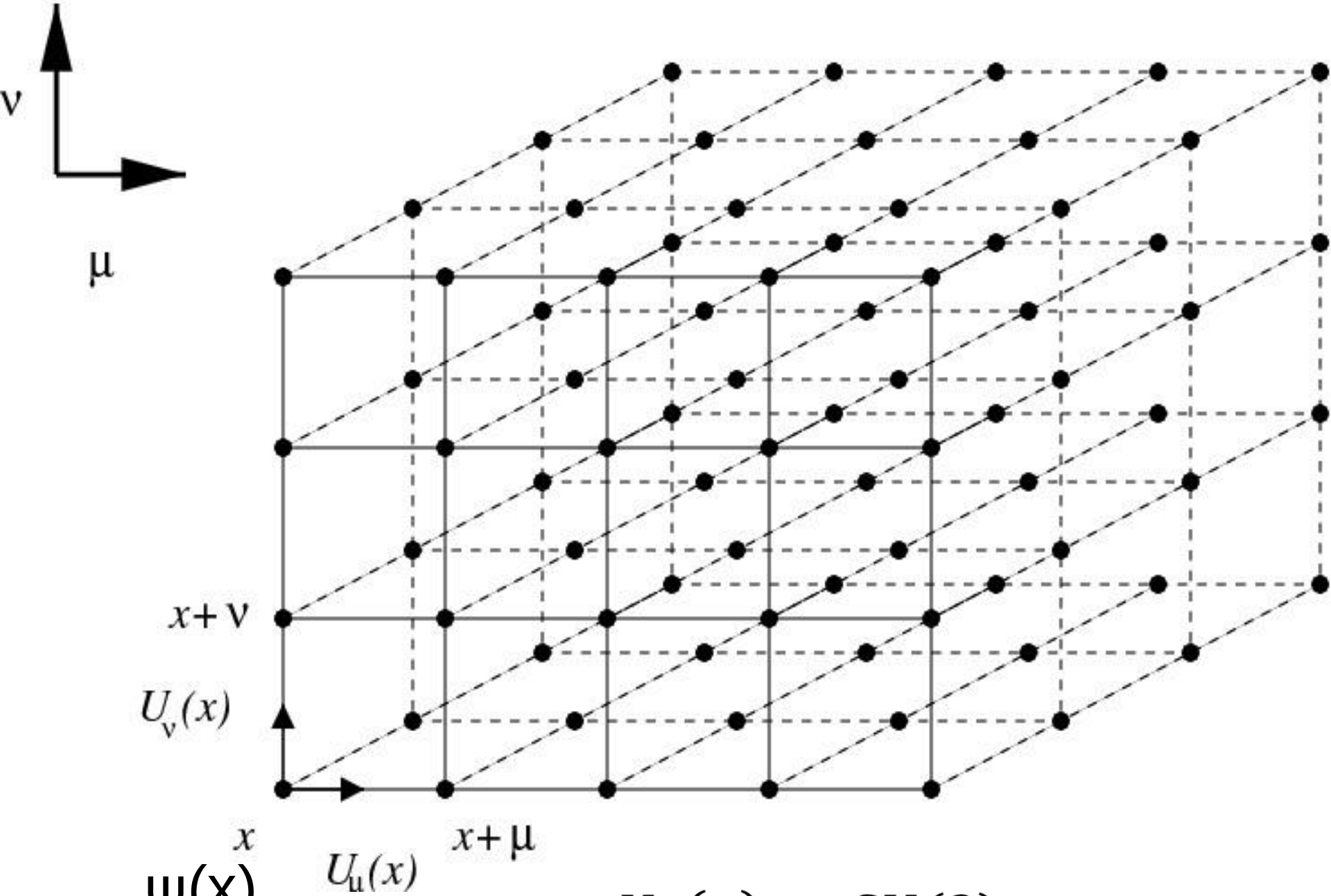
- Sign problem in finite density lattice QCD.

  PTEP 2017 (2017) no.3, 031D01

We study QCD in lattice regularization (aka Lattice QCD)

Results (at $\mu=0$) obtained via numerical computation of the path integral have statistical as well as systematic uncertainties.

Important: These uncertainties are under control, i.e. they can be estimated and decreased.



$$U_\mu(x) \in SU(3)$$

Lattice QCD action

$$S_W^G = \beta \sum_P \left(1 - \frac{1}{3}\mathrm{Re}\ \mathrm{Tr} U_P\right)$$

$$U_{\mu\nu}(s) = U_\mu(s) U_\nu(s + \hat{e}_\mu) U_\mu^\dagger(s + \hat{e}_\nu) U_\nu^\dagger(s)\,.$$

$$S_W^F = \bar{\psi}\, M(U)\, \psi$$

$$S_W^G \xrightarrow{a\to 0} \frac{1}{2\,g^2}\int \mathrm{Tr}\,F_{\mu\nu}^2(x)\,d^4x + O(a^2)\,,$$

$$S_W^F \xrightarrow{a\to 0} \int \bar{\psi}_f(x)(\gamma_\mu D_\mu + m_f)\psi_f(x)\,d^4x + O(a)$$

Fermion field integration

$$\int \mathcal{D}\psi \mathcal{D}\bar{\psi}\, e^{-\bar{\psi} M(U) \psi} = \det M(U)$$

$$\int \mathcal{D}\psi \mathcal{D}\bar{\psi}\ \bar{\psi}^a(s')\psi^b(s)\ e^{-\bar{\psi} M(U) \psi}$$

$$= (M^{-1}_{s,s'}(U))^{ab} \det M(U)$$

$$< \mathcal{O} >= \frac{1}{\mathcal{Z}} \int \mathcal{D}U \, \mathcal{O}(U) \, e^{-S_{\rm eff}(U)}$$

$$\mathcal{Z} = \int \mathcal{D}U \, e^{-S_{\rm eff}(U)}$$

$$S_{\rm eff}(U) = S_W^G(U) - \sum_f \ln \det M_f(U)$$

$$\mathcal{D}U = \prod_{s,\mu} dU_\mu(s)$$

Sign problem

$\det(\not{D} + m + \mu\gamma_0)$ -- In the integral

We use $$\gamma_5 \not{D} \gamma_5 = \not{D}^\dagger$$

$$\gamma_5(\not{D} + m + \mu\gamma_0)\gamma_5 = \not{D}^\dagger + m - \mu\gamma_0$$
$$= (\not{D} + m - \mu^*\gamma_0)^\dagger$$

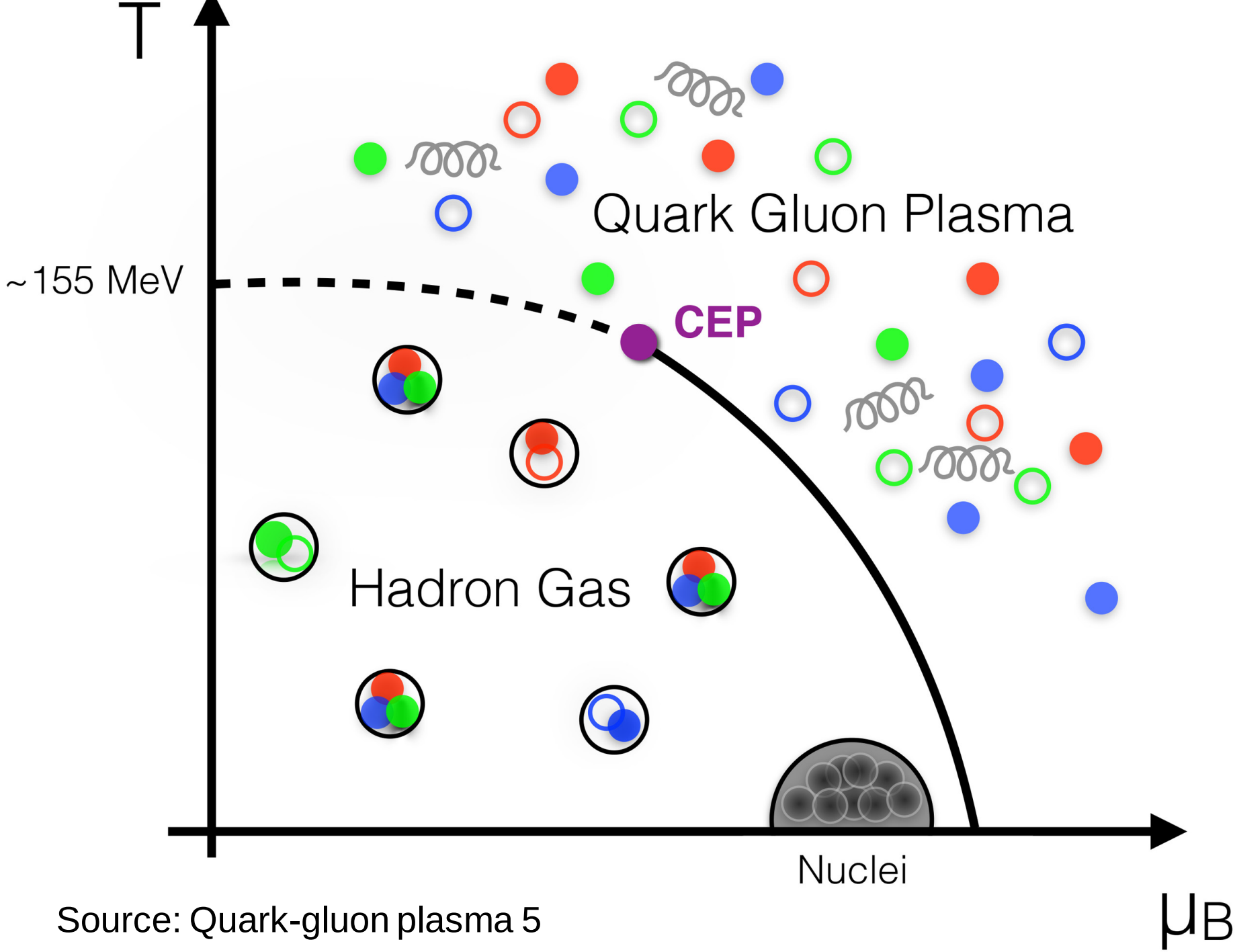
$$\det(\not{D} + m + \mu\gamma_0) = \det{}^*(\not{D} + m - \mu^*\gamma_0)$$

$$\det(\not{D} + m + \mu\gamma_0) = \det{}^*(\not{D} + m - \mu^*\gamma_0)$$

Determinant is real only for μ =0 and $\mu = i\mu_I$

This makes impossible to apply usual MCMC algorithm In case of real μ

Note, that for imaginary μ this problem is absent



Source: Quark-gluon plasma 5

Methods to solve sign problem

- Multi-Parameter Reweighting

Fodor, Katz, 2002

- Taylor expansion

Gottlieb et al. Phys.Rev.Lett. 59, 2247 (1987) (up to μ^2)
Allton et al., Phys.Rev. D71, 054508 (2005) (up to μ^6)

- Imaginary Chemical Potential

D'Elia, Lombardo, 2002

- Canonical ensemble approach

de Forcrand, Philipsen, 2002

- Complex Langevin

- Density of states

- Dual formulation

- Lefschetz thimble

Notations

pressure

$$\frac{p}{T^4} = \frac{1}{VT^3} \log Z(V, T, \mu)$$

Quark number density

$$n_f/T^3 = \frac{\partial p/T^4}{\partial \mu_f/T}$$

Susceptibility

$$\chi_{ff}/T^2 = \frac{\partial n_f/T^3}{\partial \mu_f/T}$$

High and low temperature limits

For free quark-gluon gas (Stefan-Boltzmann limit):

$$\frac{p_{SB}}{T^4} = \frac{8\pi^2}{45} + \sum_{f=u,d,..} \left[\frac{7\pi^2}{60} + \frac{1}{2}\left(\frac{\mu_f}{T}\right)^2 + \frac{1}{4\pi^2}\left(\frac{\mu_f}{T}\right)^4 \right]$$

This is valid for very high T

For low T – Hadron resonance gas (HRG) model

$$\frac{p}{T^4} = G(T) + F(T)\cosh\left(\frac{3\mu_q}{T}\right)$$

Imaginary μ_q

At imaginary chemical potential $\mu_q = i\mu_{qI}$ the sign problem is absent and standard Monte Carlo algorithms can be applied to simulate Lattice QCD. Can we use this?

Study of QCD at nonzero μ_{qI} can provide us with information about physical range of μ_q

- extrapolation to $\mu_q = 0$ or analytical continuation to nonzero real μ_q

The QCD partition function Z is a periodic function of $\theta = \mu_{qI}/T$:

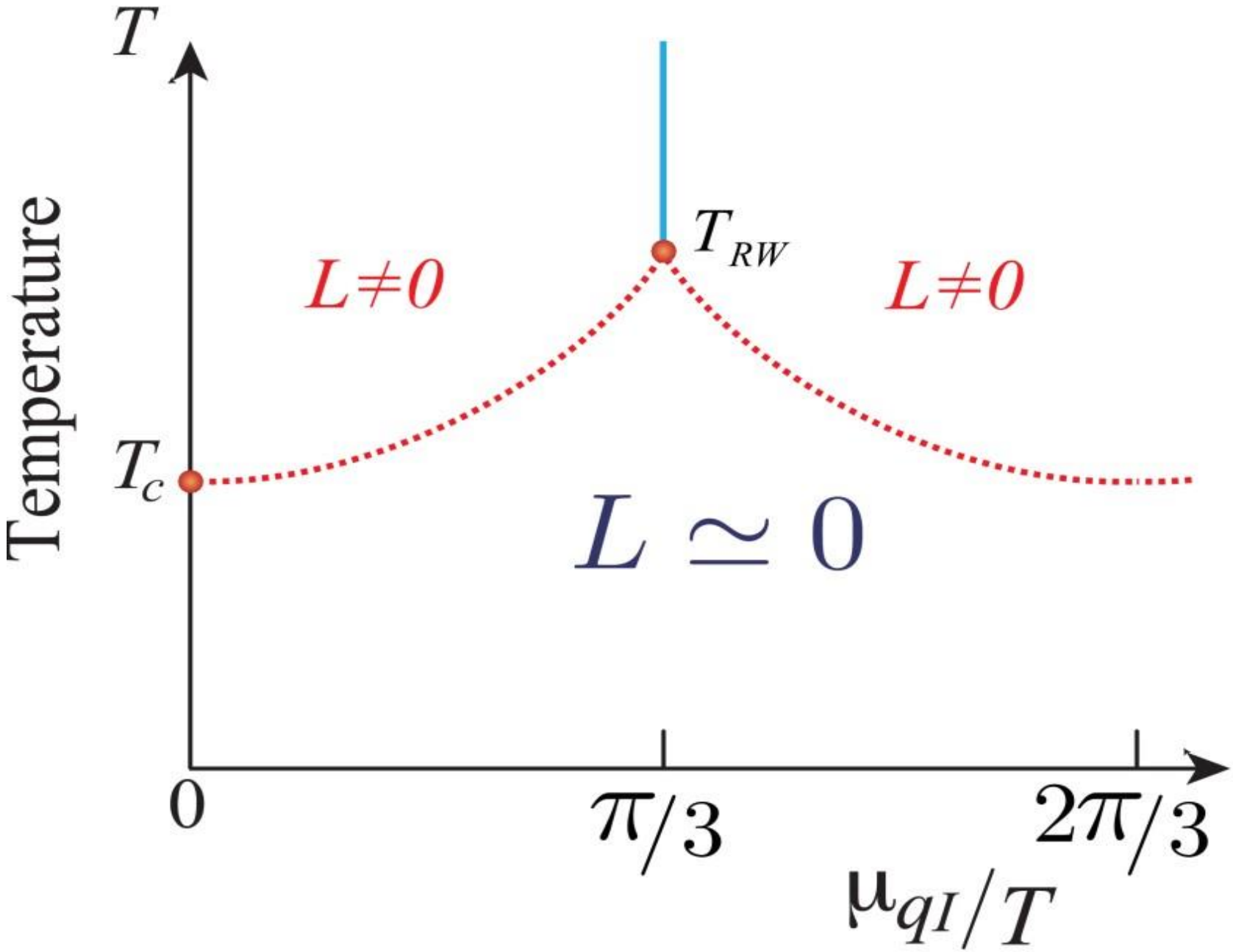
$$Z(\theta) = Z(\theta + 2\pi k/3)$$

There are 1st order phase transitions at $\theta = (2k+1)\frac{\pi}{3}$

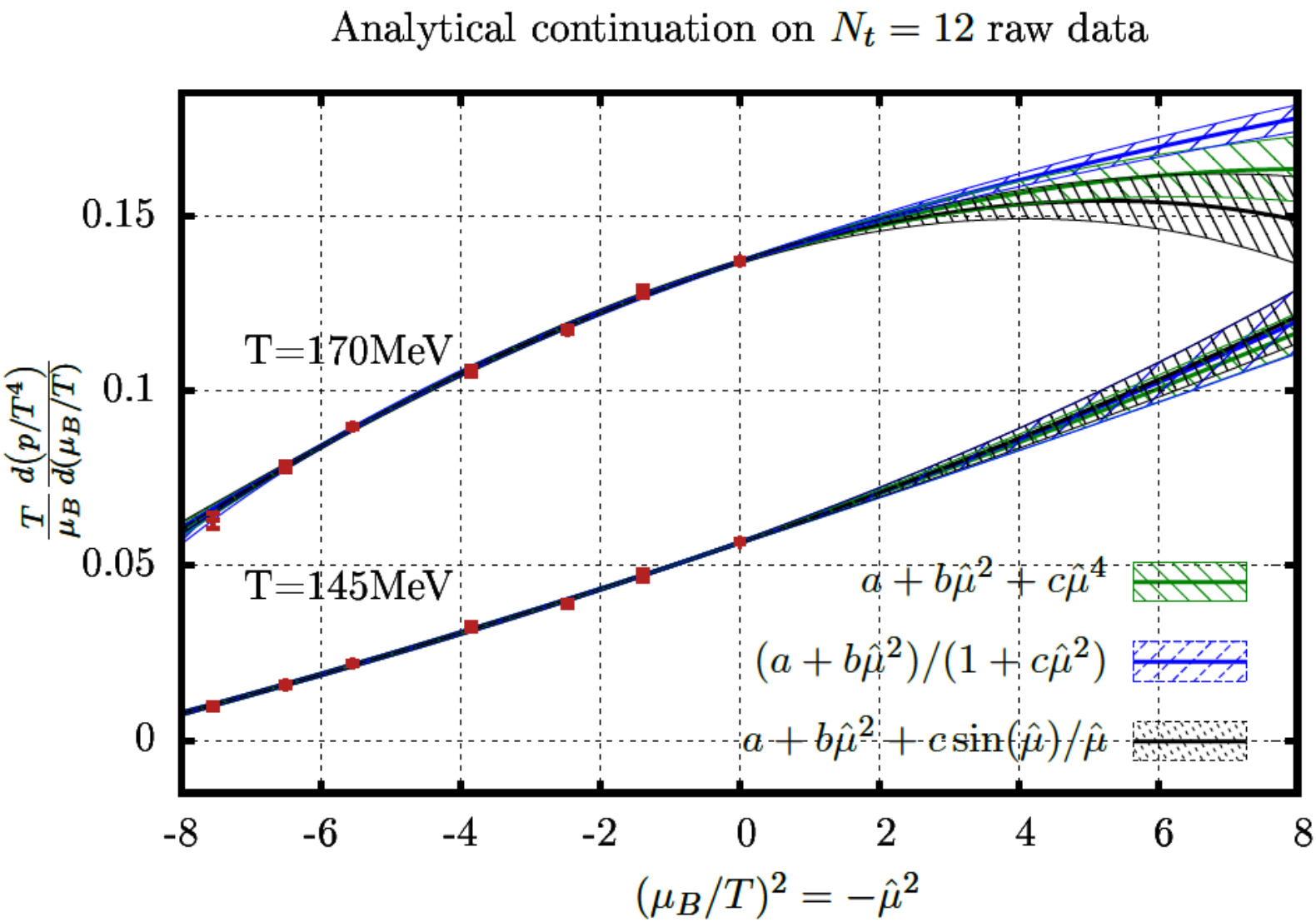
This symmetry is called Roberge-Weiss symmetry

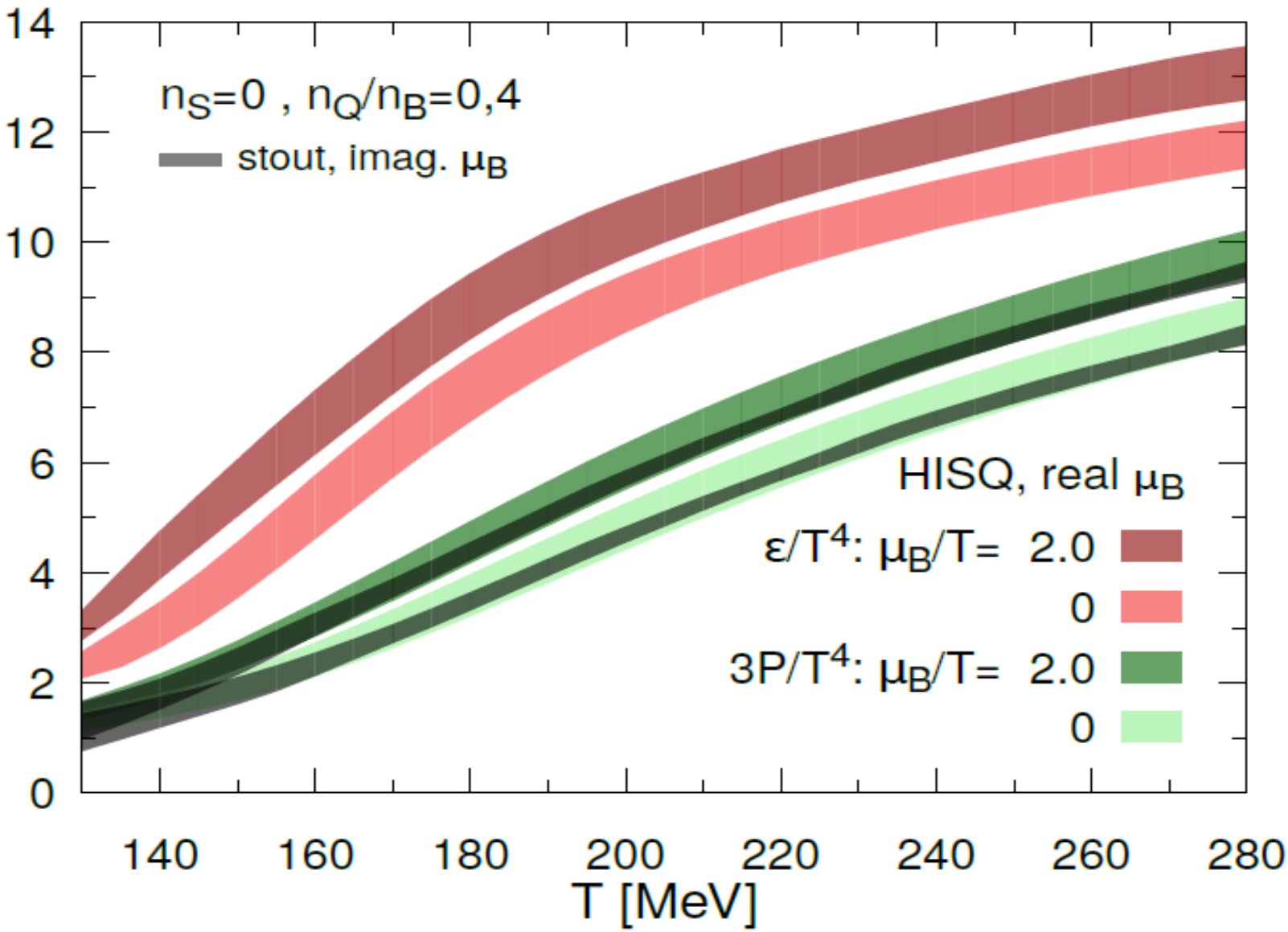
Roberge,Weiss, 1986

QCD phase diagram at imaginary μ



N_f=2+1, N_t=10,12,16, N_s=40,48,64
Fodor et al., 2016





Pressure obtained by two different methods

from Phys.Rev. D95 (2017) by F.Karsch et al.

Simulation settings

We simulate $N_f = 2$ lattice QCD with clover improved Wilson fermions and Iwasaki improved gauge field action.

Lattice size: 16^3 x 4
lattice spacing: 0.2 fm
lattice spatial size: 3.2 fm
pion mass 700 MeV

We make simulations at imaginary chemical potential
- $T > T_{RW}$ $(T / T_c = 1.20, 1.35)$
- $T_c < T < T_{RW}$ $(T / T_c = 1.08)$
- $T > T_c$ $(T / T_c = 0.84, 0.93, 0.99)$

Canonical approach

The canonical approach is based on the following relations.
- Relation between grand canonical partition function Z_{GC}(μ, T, V) and canonical one Z_C(n, T, V) :

$$Z_{GC}(\mu_q, T, V) = \sum_{n=-\infty}^{\infty} Z_C(n, T, V)\xi^n, \qquad \xi = e^{\mu/T}$$

- The inverse of this equation : (Hasenfratz, Toussaint, 1992)

$$Z_C(n, T, V) = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-in\theta} Z_{GC}(i\theta, T, V).$$

$\theta = \mu_I/T$

Standard Monte Carlo simulations are possible

Quark number density n_q defined by equation

$$\begin{aligned}\frac{n_q}{T^3} &= \frac{1}{VT^2}\frac{\partial}{\partial\mu_q}\ln Z_{GC} \\ &= \frac{N_f N_t^3}{N_s^3}\frac{1}{Z_{GC}}\int \mathcal{D}U e^{-S_G}(\det\Delta(\mu_q))^{N_f}\mathrm{tr}\left[\Delta^{-1}\frac{\partial\Delta}{\partial\mu_q/T}\right],\end{aligned}$$

can be computed numerically for this partition function.

It is imaginary for imaginary chemical potential: $n_q = i n_{qI}$.
n_{qI} in terms of $Z_n = \frac{Z_C(n,T,V)}{Z_C(0,T,V)}$

$$\frac{n_{qI}}{T^3} = \frac{N_t^3}{N_s^3}\frac{\sum_n nZ_n\sin(n\theta)}{\sum_n Z_n\cos(n\theta)}$$

In the deconfining phase we fit the data for n_{ql} to a polynomial

$$n_{ql}(\theta) = \sum_{n=1}^{n_{max}} a_n \theta^{2n-1}$$

in the confining phase (below Tc) we fit it to a Fourier expansion

$$n_{ql}(\theta) = \sum_{n=1}^{n_{max}} f_{3n} sin(3n\theta)$$

These or similar fits were used before

- Thermodynamics of two flavor QCD from imaginary chemical potentials

M. D'Elia, F. Sanfilippo, Phys.Rev. D80 (2009) 014502

- Quark number densities at imaginary chemical potential in N_f=2 lattice QCD with Wilson fermions and its model analyses

J. Takahashi, H. Kouno, M. Yahiro Phys.Rev. D91 (2015) no.1, 014501

- The QCD equation of state at finite density from analytical continuation

J. Gunther, R. Bellwied, S. Borsanyi , Z. Fodor, S.D. Katz, A. Pasztor, C. Ratti. EPJ Web Conf. 137 (2017) 07008

- Higher order quark number fluctuations via imaginary chemical potentials in Nf=2+1 QCD

M. D'Elia, G. Gagliardi, F. Sanfilippo Phys.Rev. D95 (2017) no.9, 094503

Using numerical data or fitted form of n_{ql} one can compute the grand canonical partition function by integration over imaginary chemical potential

$$LZ(\theta) \equiv \log \frac{Z_G(\theta)}{Z_G(0)} = \int_0^\theta d\tilde{\theta} n_{ql}(\tilde{\theta}) \tag{10}$$

Then

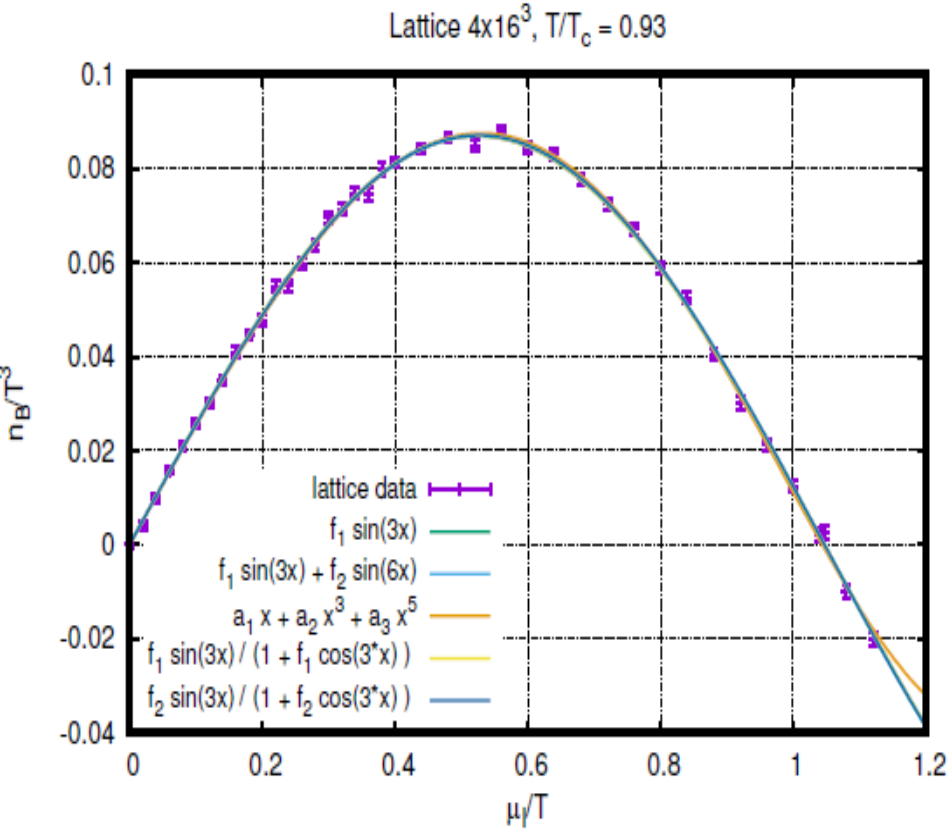
$$\frac{Z_G(\theta)}{Z_G(0)} = e^{LZ(\theta)} \tag{11}$$

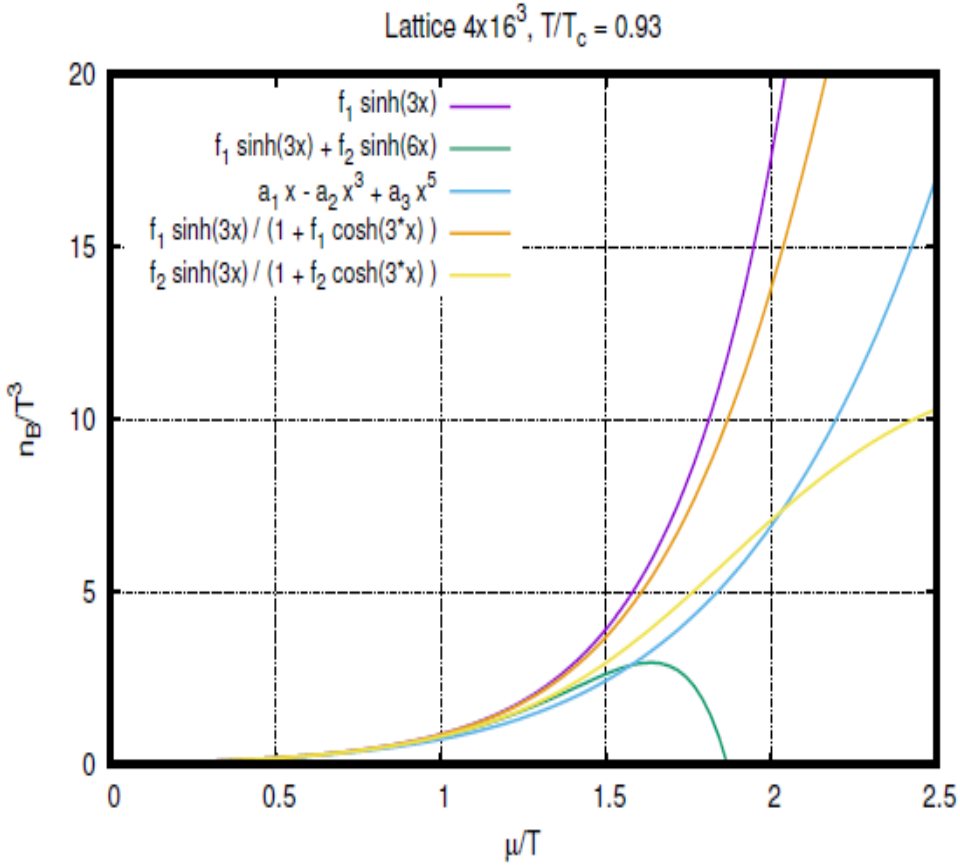
Z_n can be also computed

$$\frac{Z_n}{Z_G(0)} = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-in\theta} e^{LZ(\theta)} \tag{12}$$

We obtained very promising results for canonical partition functions Z_n.

Problem: many functions provide good fits of data.
Analytical continuation is ambiguous





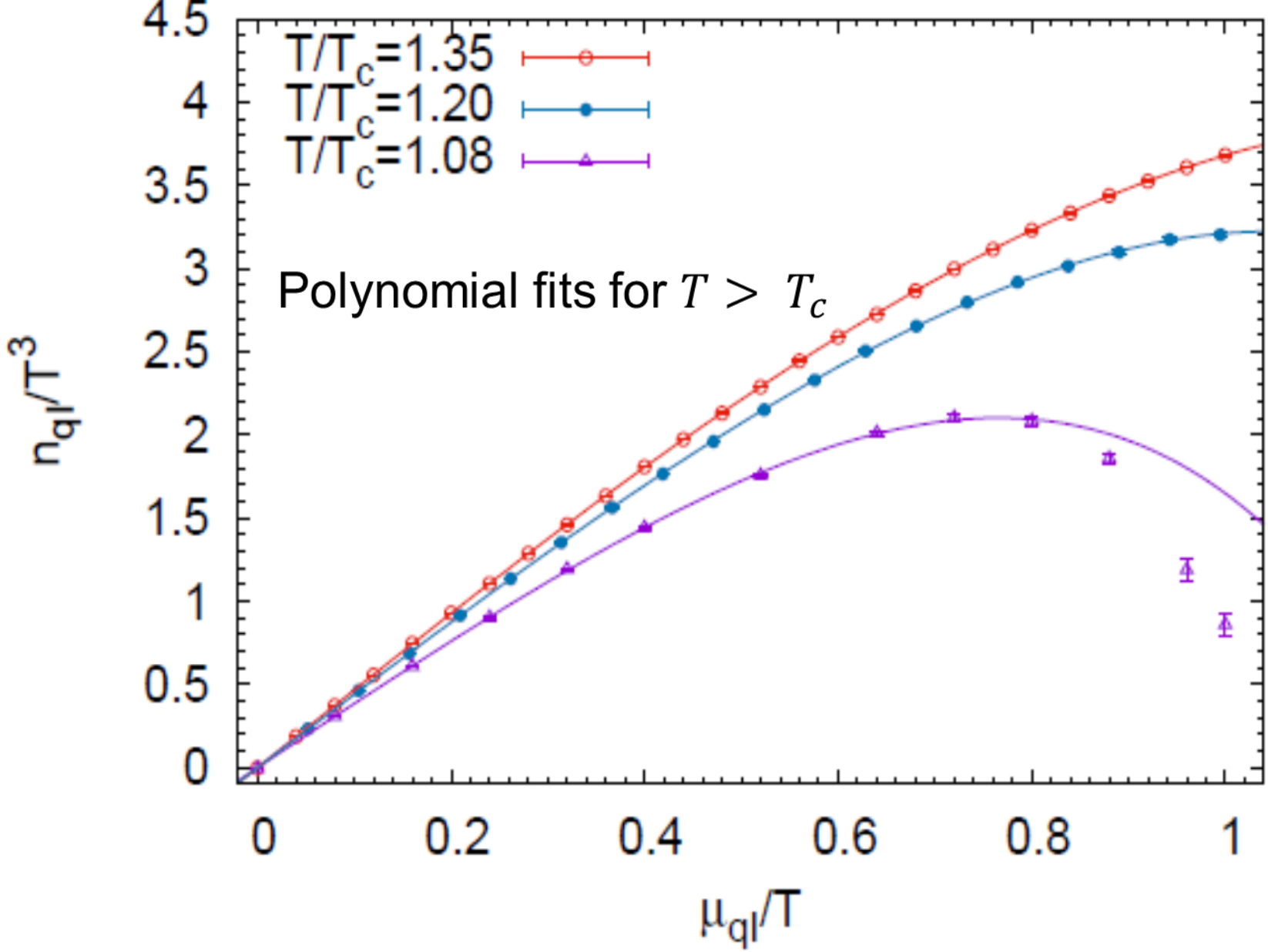
Restrictions on fitting functions

- At $T > T_{RW}$ n_{qI} has a gap at $\mu_{qI}/T = \frac{\pi}{3}$, Fourier series is unacceptable

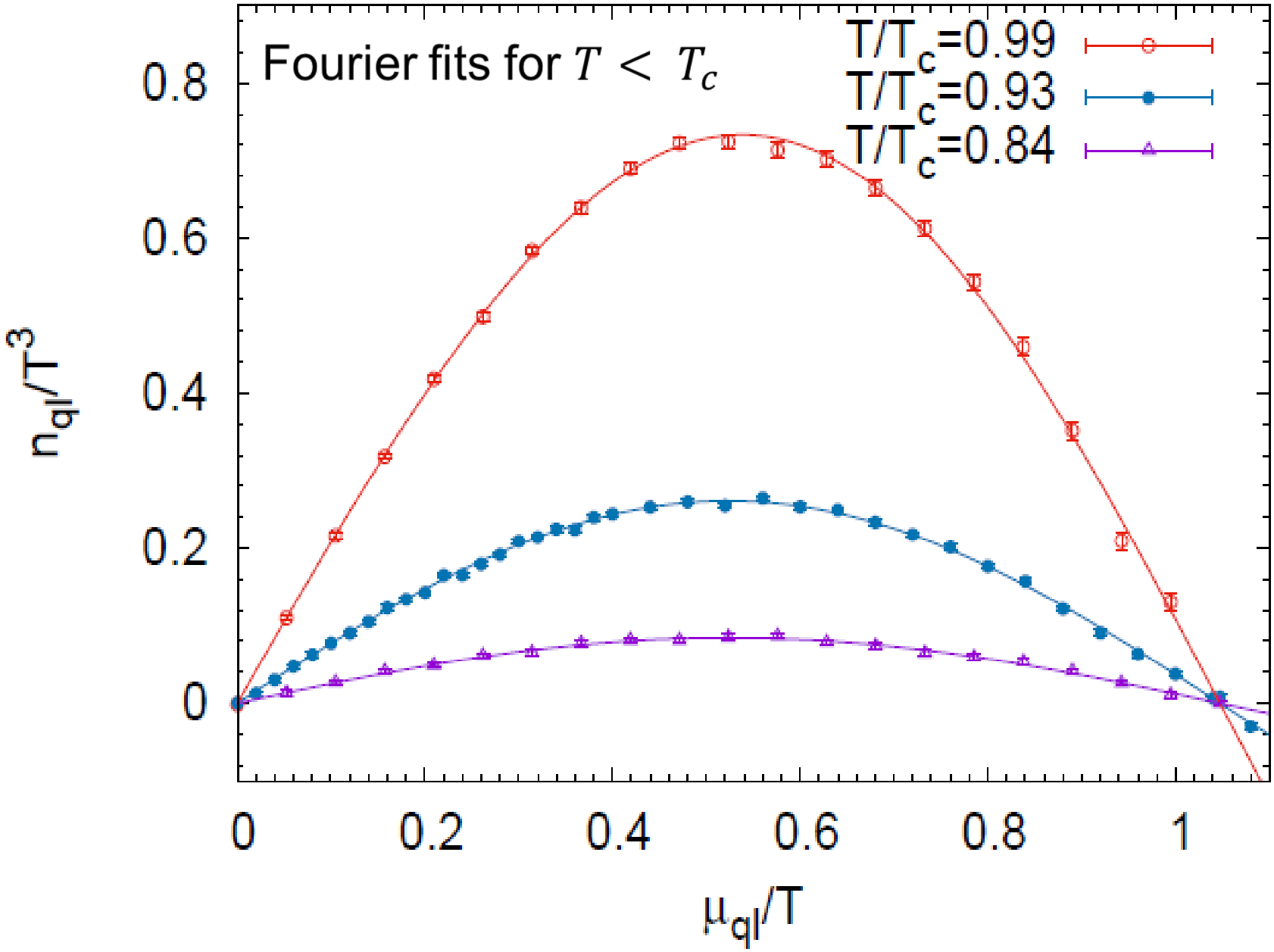
- At $T_c < T < T_{RW}$ and $T < T_c$ analytical behavior at $\mu_{qI}/T = \frac{\pi}{3}$ and periodicity exclude polynomials

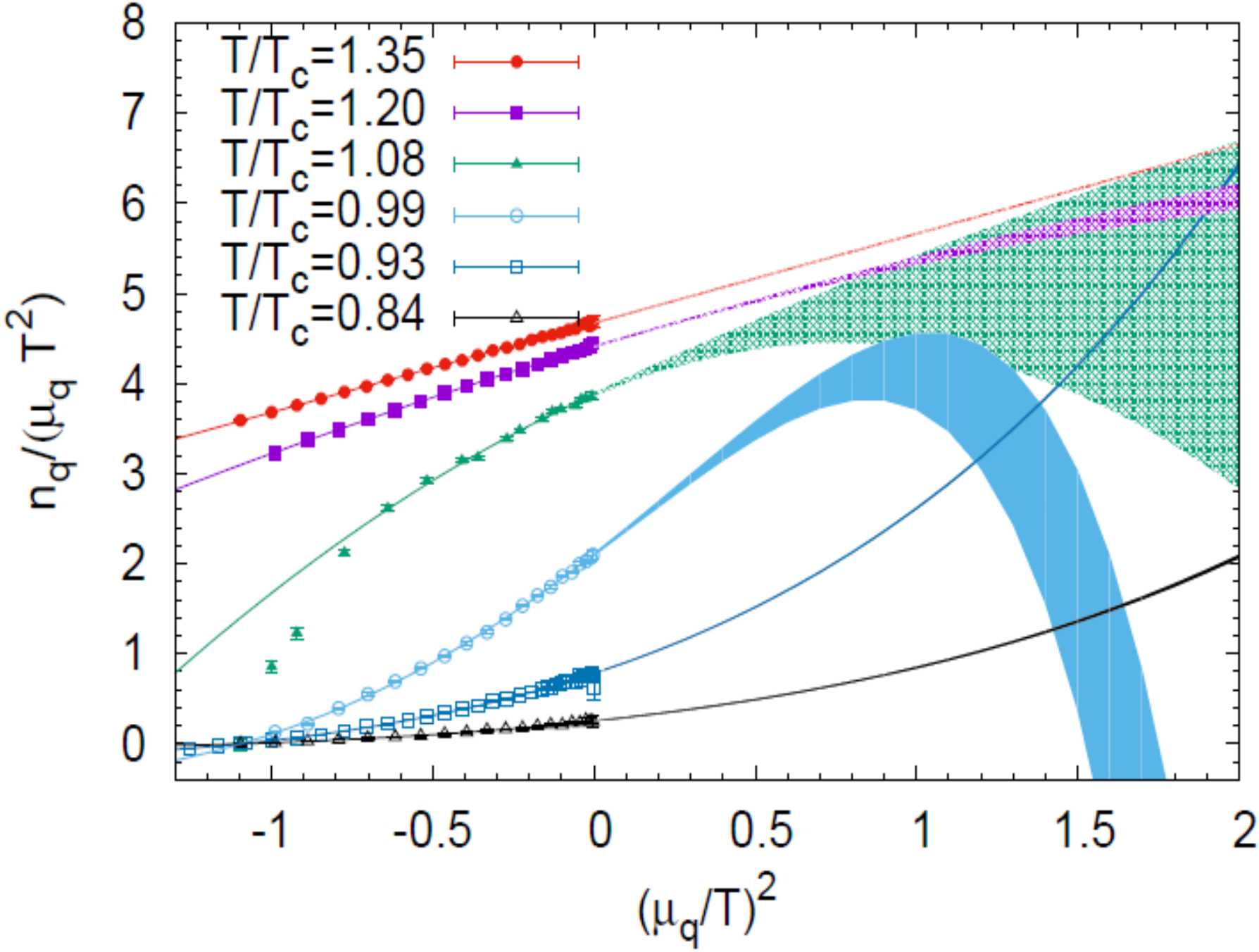
- New restriction on the fitting functions:

$$Z_n > 0$$

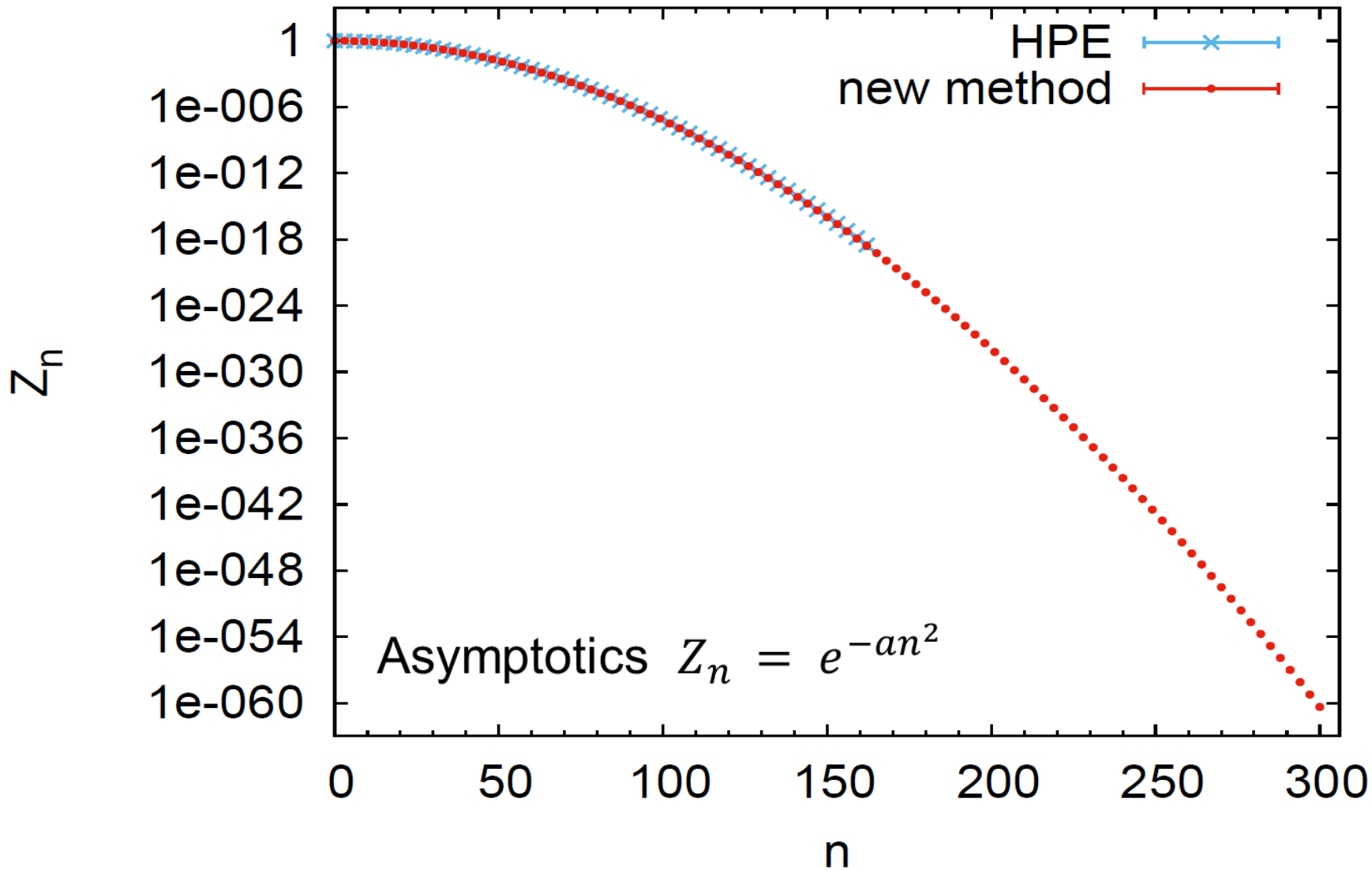


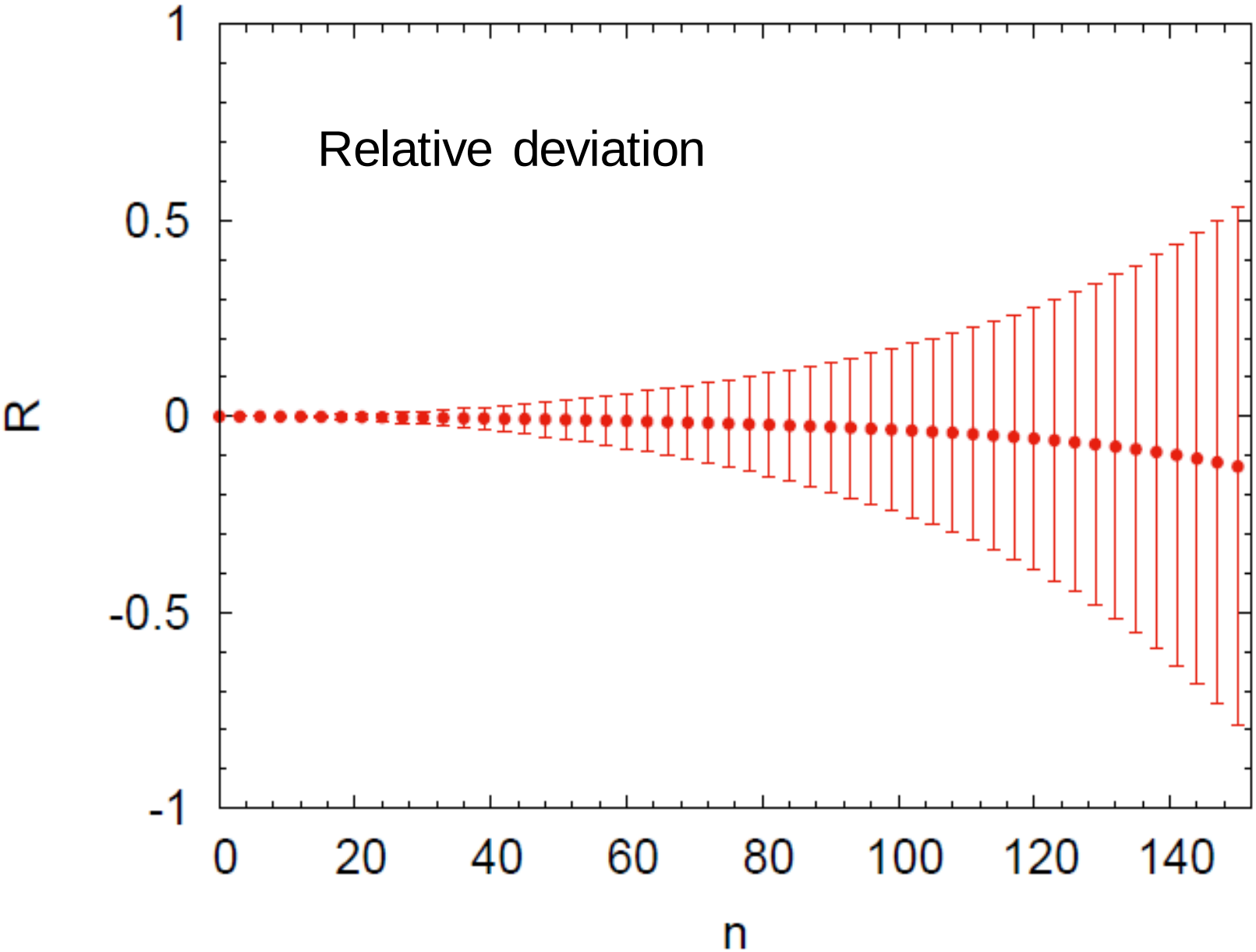
Imaginary number density at $T > T_{RW}$ and $T_c < T < T_{RW}$


Fourier fits for $T < T_c$
T/T$_c$=0.99
T/T$_c$=0.93
T/T$_c$=0.84
0.8
0.6
0.4
0.2
0
n_{ql}/T^3
0
0.2
0.4
0.6
0.8
1
μ_{ql}/T

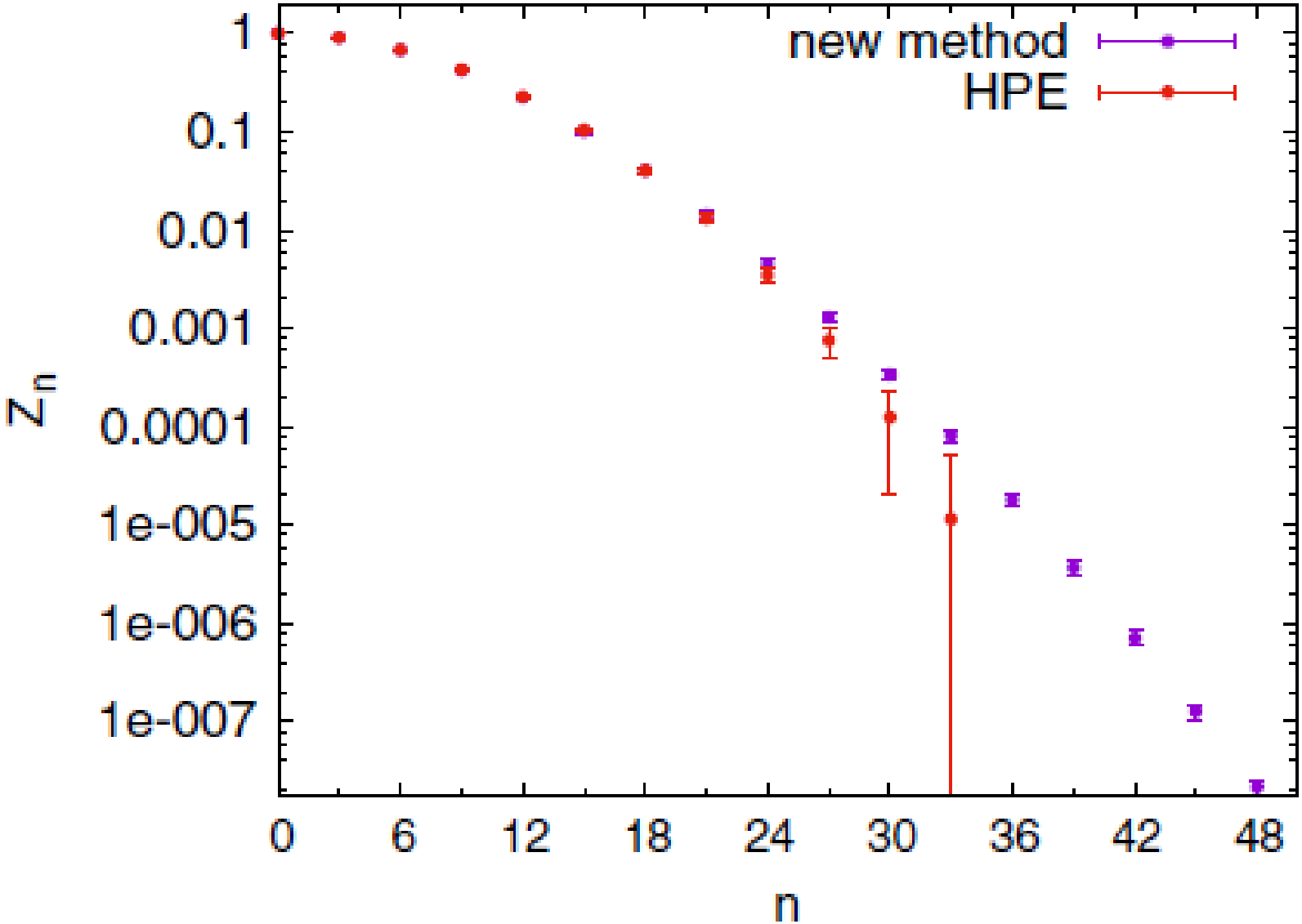

T/T_c=1.35
T/T_c=1.20
T/T_c=1.08
T/T_c=0.99
T/T_c=0.93
T/T_c=0.84
n_q/(μ_q T^2)
(μ_q/T)^2
8
7
6
5
4
3
2
1
0
-1
-0.5
0
0.5
1
1.5
2

Deconfining phase:




Relative deviation
1
0.5
0
-0.5
-1
R
0
20
40
60
80
100
120
140
n

Confinement phase



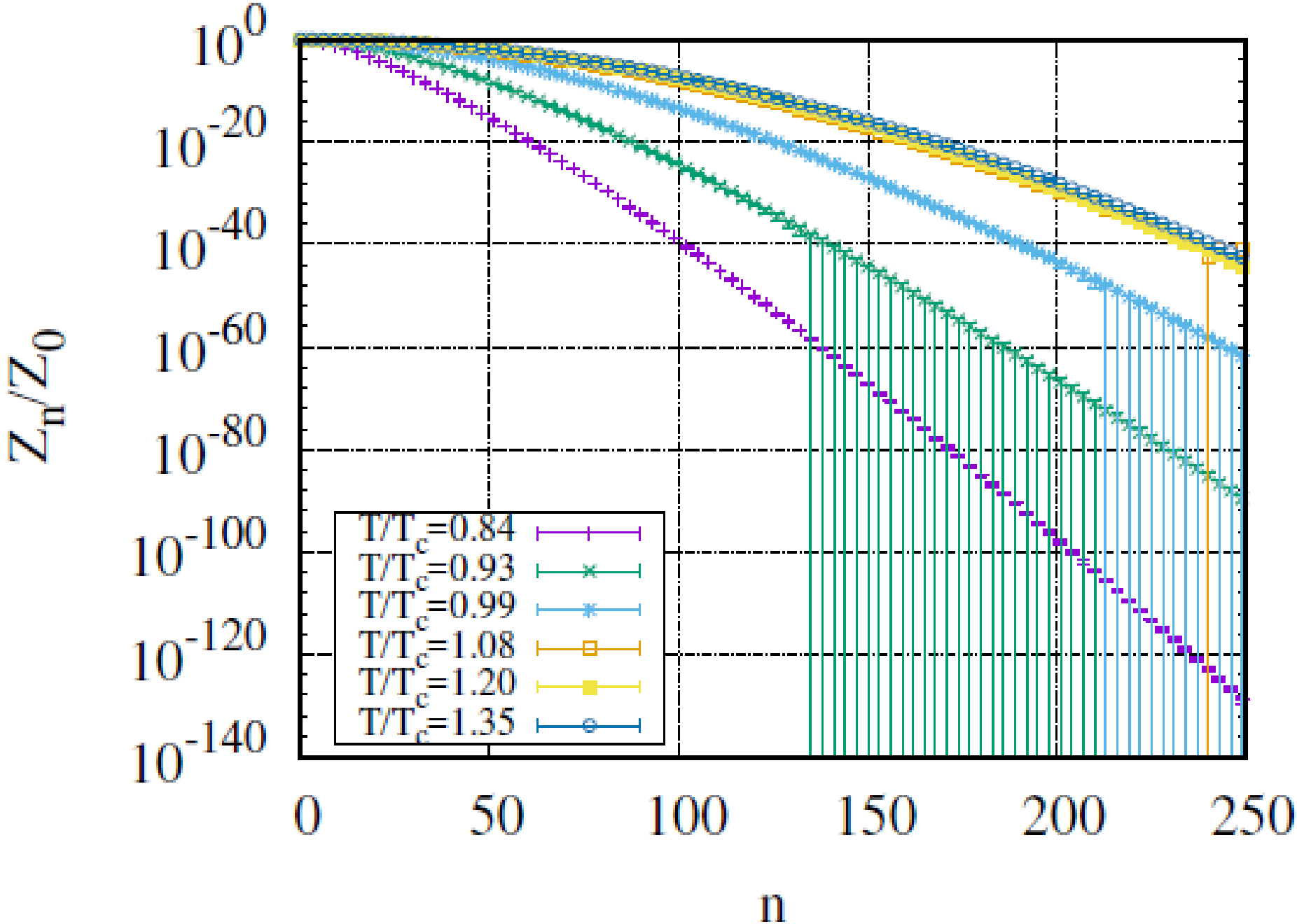
At T/T_c=1.35 and 0.93 we compared new method results for Z_n with Z_n computed by HPE

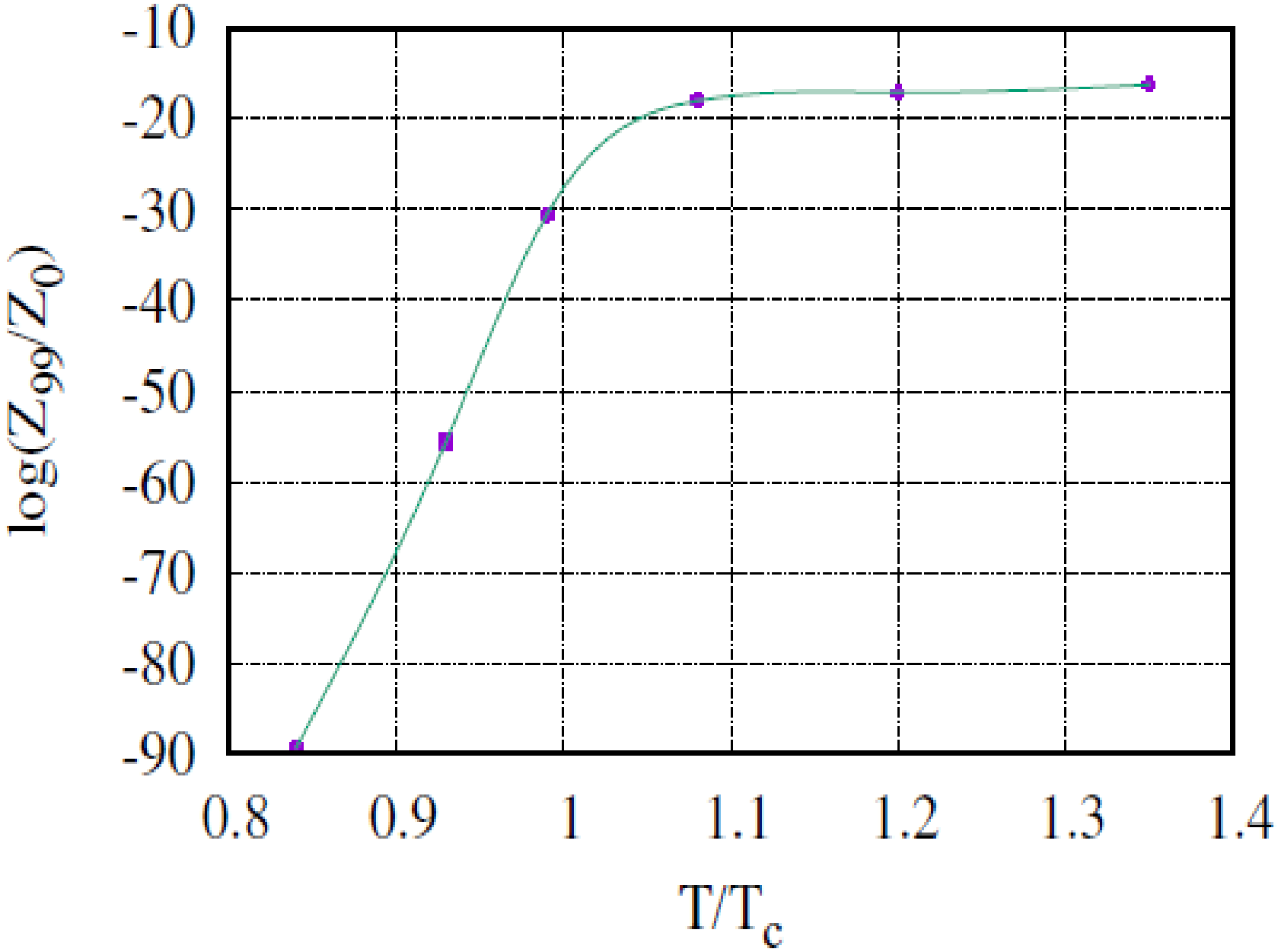
We found that two sets of Z_n computed by completely independent methods agree well, especially at T/T_c=1.35

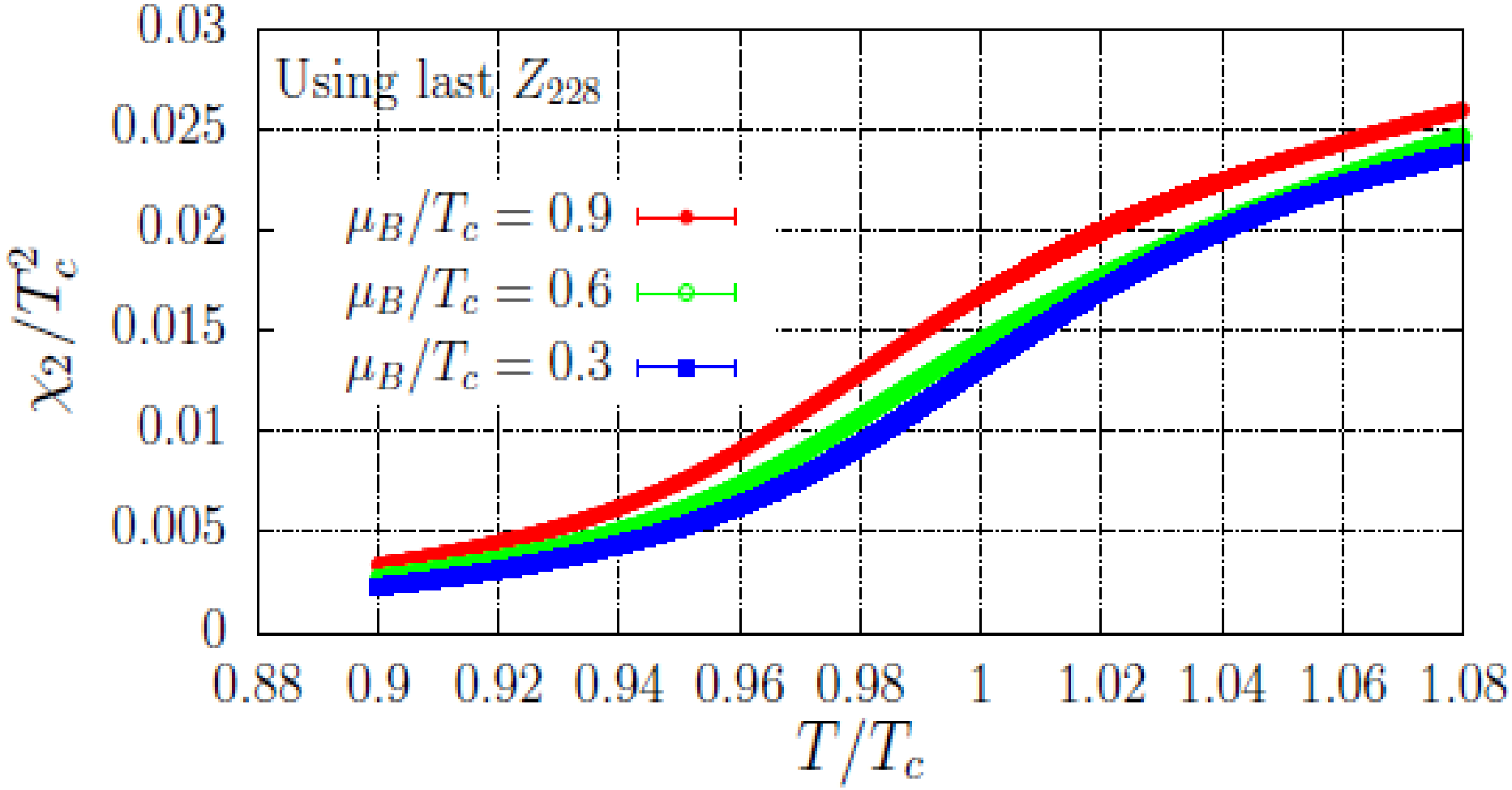
(For T/T_c=0.93 HPE results should be improved)

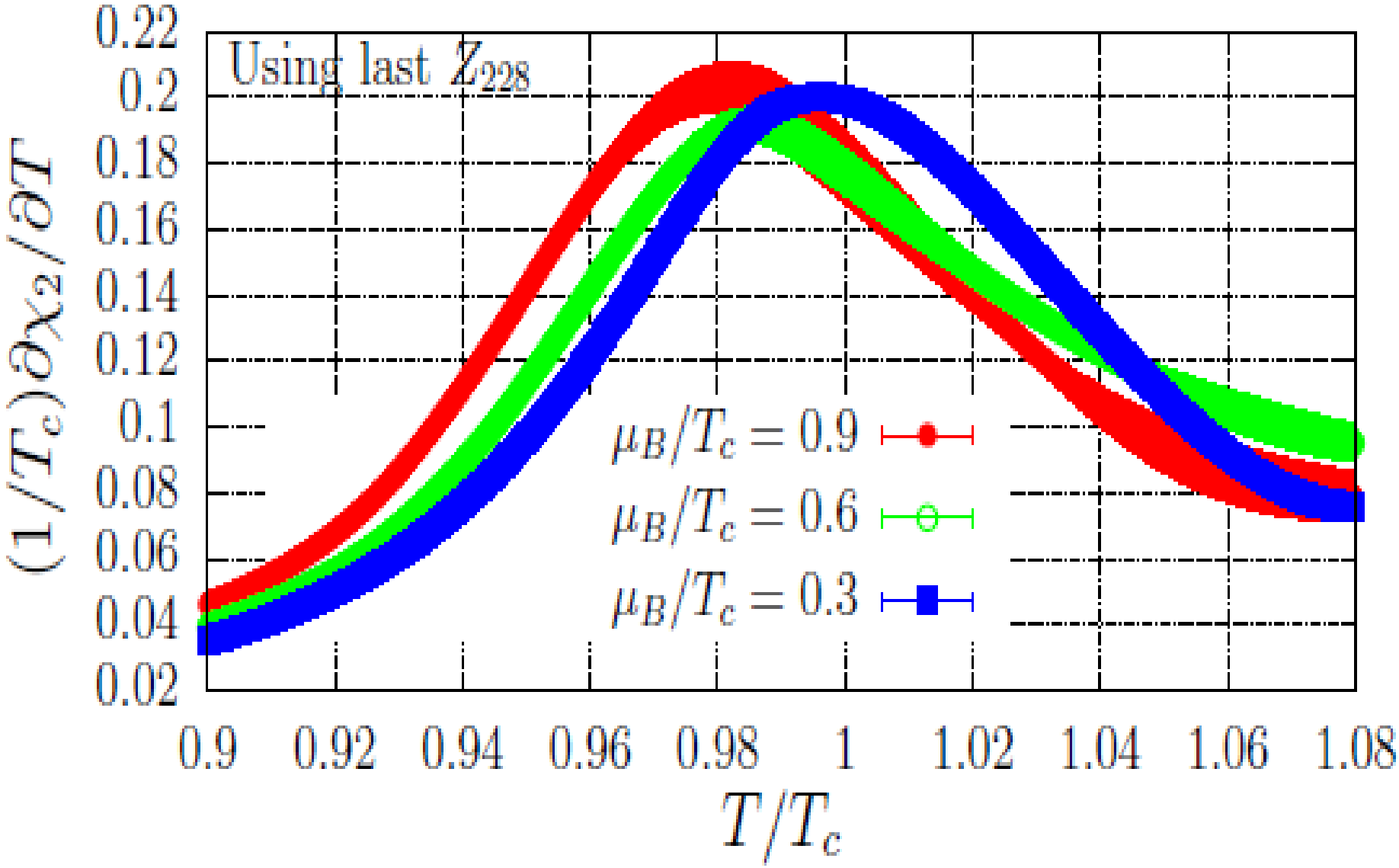
This means that

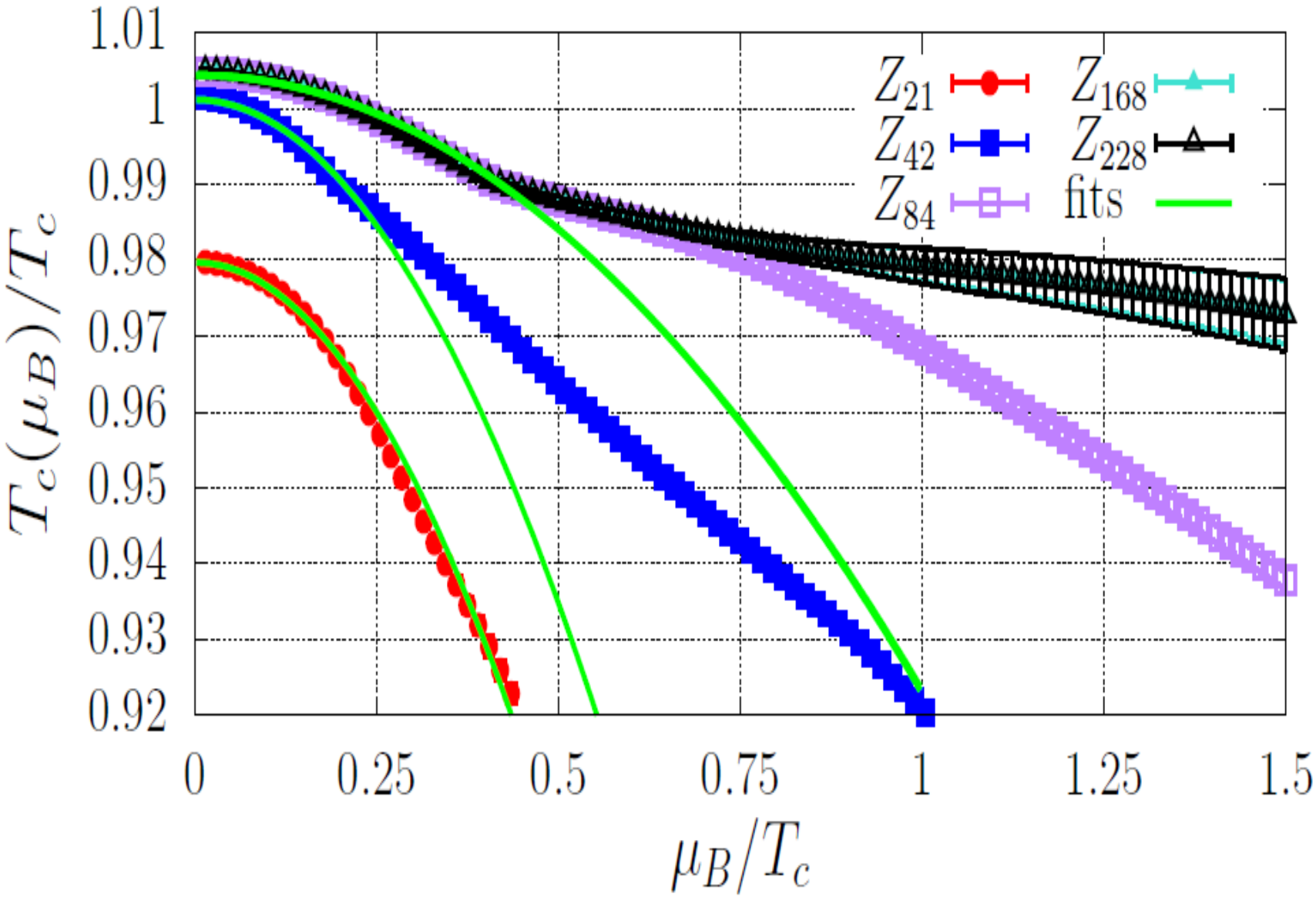
- we use correct fitting functions
- analytical continuation goes beyond Taylor expansion since this analytical continuation coincides with n_q computed independently via correctly determined Z_n
- also provides the way to determine the range of validity of the analytical continuation


10^{0}
10^{-20}
10^{-40}
10^{-60}
10^{-80}
10^{-100}
10^{-120}
10^{-140}
Z_n/Z_0
0
50
100
150
200
250
n
T/T$_c$=0.84
T/T$_c$=0.93
T/T$_c$=0.99
T/T$_c$=1.08
T/T$_c$=1.20
T/T$_c$=1.35


-10
-20
-30
-40
-50
-60
-70
-80
-90
log(Z99/Z0)
0.8
0.9
1
1.1
1.2
1.3
1.4
T/Tc


Using last Z_{228}
$\mu_B/T_c = 0.9$
$\mu_B/T_c = 0.6$
$\mu_B/T_c = 0.3$
χ_2/T_c^2
T/T_c
0.03
0.025
0.02
0.015
0.01
0.005
0
0.88
0.9
0.92
0.94
0.96
0.98
1
1.02
1.04
1.06
1.08


Using last Z_{228}
$\mu_B/T_c = 0.9$
$\mu_B/T_c = 0.6$
$\mu_B/T_c = 0.3$
$(1/T_c)\partial\chi_2/\partial T$
T/T_c
0.22
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0.9
0.92
0.94
0.96
0.98
1
1.02
1.04
1.06
1.08


1.01
1
0.99
0.98
0.97
0.96
0.95
0.94
0.93
0.92
$T_c(\mu_B)/T_c$
0
0.25
0.5
0.75
1
1.25
1.5
μ_B/T_c
Z_{21}
Z_{42}
Z_{84}
Z_{168}
Z_{228}
fits

C=0.033(10)

Conclusions

- Our group is developing a combination of the canonical ensemble and analytical continuation approaches. Results are encouraging.
- Agreement of two methods (HPE and Integration) found for large quark mass allows to separate proper fitting functions. Hopefully same fitting functions work at small quark masses.
- Positivity $Z_n > 0$ imposes additional restrictions on the fitting functions
- This condition also restricts range of reliability of the analytical continuation for $n_q(\mu)$.

Backup slides

Main project: Study of the quark-gluon plasma using lattice QCD Supported by the Russian Science Foundation

Leader: A. Nakamura

Main goal: phase diagram of QCD in μ-T plane

Machine :
10 nodes (2x Intel E5-2680-v2, 64Gb; 2 x NVidia Tesla K40X Kepler)
33 Tflops (peak); 23.5 Tflops (Linpack)

Code: Hybrid Monte Carlo code for GPU was created from scratch. Its performance is comparable to QUDA code (library for lattice QCD on GPUs (http://lattice.github.com/quda)

- coefficients of Taylor expansion agree with direct computation, smaller errors
- in the deconfining phase our results are in nice agreement with hopping parameter expansion
- in the confining phase agreement is not so good but there is hope for improvement
- contrary to hopping parameter expansion - no limitations on quark mass
- observed agreement with the hopping parameter expansion means method works beyond Taylor expansion validity range.
- Pressure, number density and higher cumulants can be computed beyond Taylor expansion

We use hopping parameter expansion (HPE) to evaluate the determinant ($\xi = e^{\mu_B a N_f} = e^{\mu_B/T}$):

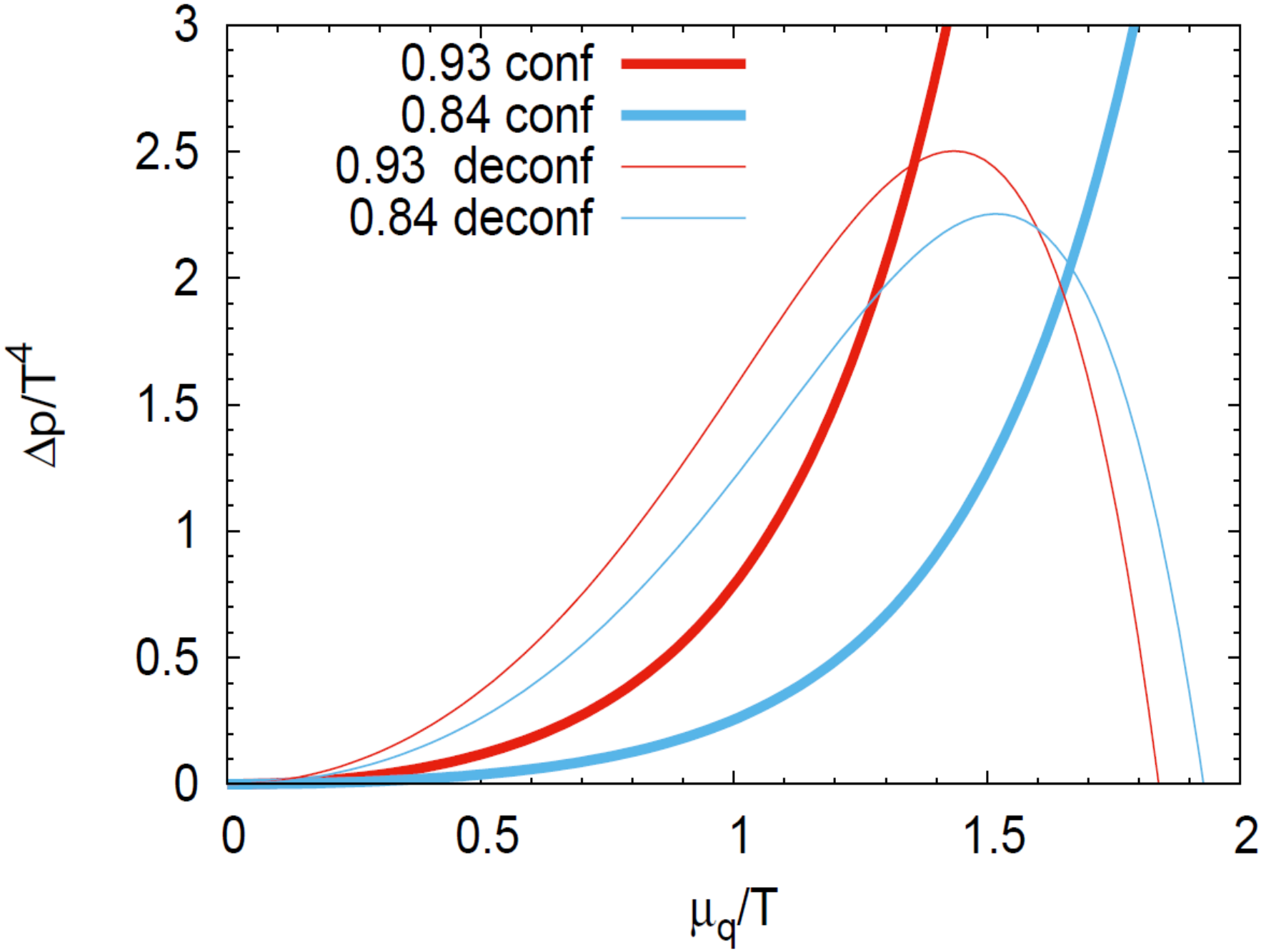
$$Tr\left[ln\,\Delta\right] = Tr\left[ln\left(I - \kappa Q\right)\right] = -\sum_{n=1}^{\infty} \frac{\kappa^n}{n} Tr\left[Q^n\right] = \sum_{n=-\infty}^{\infty} W_n \left(e^{\mu_B a N_\tau}\right)^n$$

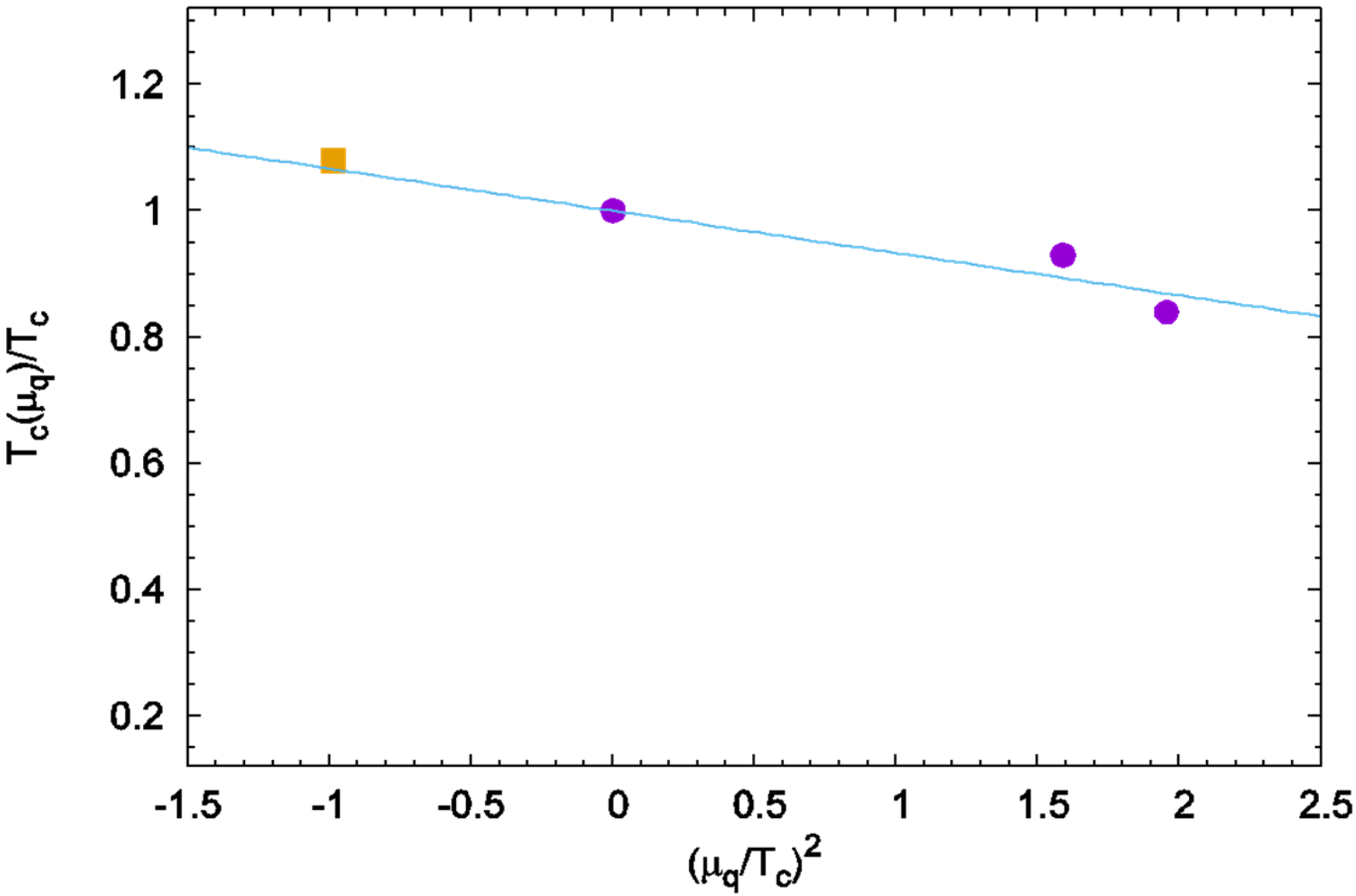
$$\det \Delta(U) = e^{Tr[ln\Delta]} = exp\left[\sum_{n=-N_{cut}}^{N_{cut}} W_n[U]\xi^n\right]$$

$W_n[U]$ may be calculated using stochastic estimators for $Tr\left[Q^n\right]$.

$$\det \Delta(U) = \sum_{n=-2N_xN_yN_zN_c}^{2N_xN_yN_zN_c} z_n[U]\xi^n$$

To determine the transition line in the $\mu - T$ plane we extrapolate pressure from $T > T_c$ to $T < T_c$


0.93 conf
0.84 conf
0.93 deconf
0.84 deconf
3
2.5
2
1.5
1
0.5
0
0
0.5
1
1.5
2
Δp/T^4
μq/T


1.2
1
0.8
0.6
0.4
0.2
$T_c(\mu_q)/T_c$
-1.5
-1
-0.5
0
0.5
1
1.5
2
2.5
$(\mu_q/T_c)^2$

$$T_c(\mu_q)/T_c = 1 - C\left(\mu_q/T_c\right)^2$$

Our result: C=0.07 is in nice agreement with other results for N_f=2 lattice QCD:

C=0.051(3) De Forcrand, Philipsen, 2002

C=0.065(7) Wu, Luo, Chen, 2007