Lattice QCD at imaginary chemical potential

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Outline

- New results in $N_f = 2$ QCD at nonzero chemical potential

- 1d QCD

- Models for the virial expansion coefficients

The work presented is completed by joint
FEFU - ITEP - IHEP lattice group
initiated by late Misha Polikarpov

Atsushi Nakamura, Valentin Zakharov, VB, Alexander Molochkov, Vladimir Goy, Alexander Nikolaev, Denis Boyda, Hideaki Iida, Masayuki Wakayama, Maria-Paola Lombardo

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

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

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

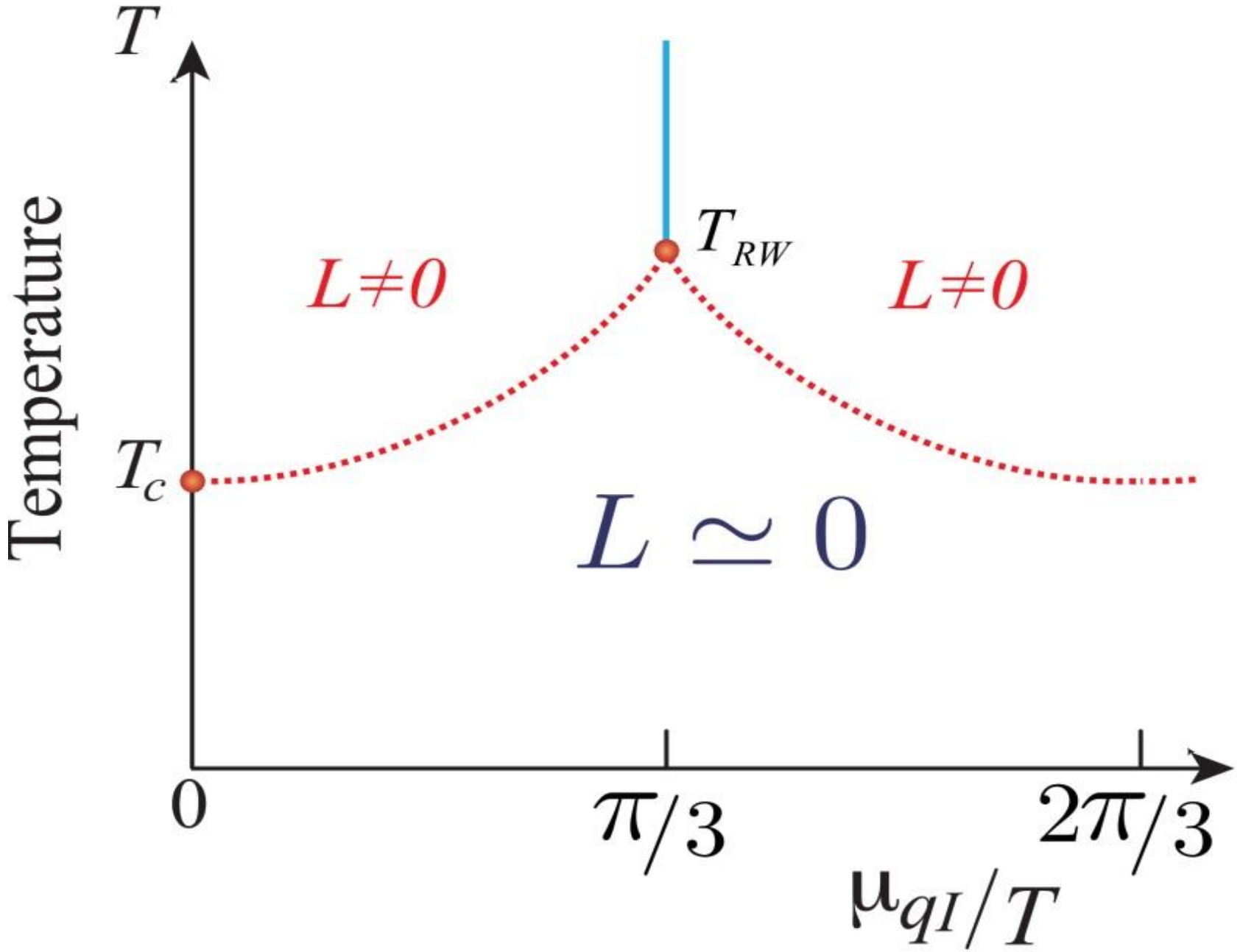
The QCD partition function Z is a periodic function of $\theta = \mu_{qI}/T$:

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

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

This symmetry is called Roberge-Weiss symmetry

QCD phase diagram at imaginary μ



Simulation settings

We simulate lattice QCD with two flavors of clover improved Wilson fermions and Iwasaki improved gauge field action at imaginary baryon chemical potential.

Two values of the quark mass: m_π/m_ρ = 0.8, 0.65

Lattice size: $16^3 \mathrm{x}\, 4$

Lattice spacing: $a \sim 0.2\ fm$

Lattice size: $L \sim 3.2\ fm$

Temperature values

	m_π/m_ρ = 0.8	m_π/m_ρ = 0.65
$T > T_c$	(1.035, 1.08, 1.20, 1.35);	(1.07, 1.18, 1.32)
$T < T_c$	(0.84, 0.93, 0.99);	(0.86, 0.94, 1.00)

Canonical approach

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

$$Z_G(\mu, T, V) = \sum_{n=-\infty}^{\infty} Z_C(n, T, V)\xi^n, \tag{3}$$

where $\xi = e^{\mu/T}$ is called fugacity and this equation - fugacity expansion.
The inverse of this equation : Hasenfratz, Toussaint, 1992

$$Z_C(n, T, V) = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-in\theta} Z_{GC}(i\theta, T, V). \tag{4}$$

$Z_{GC}(i\theta, T, V)$ - the grand canonical partition function for imaginary chemical potential $\mu/T = i\mu_I/T = i\theta$.
Standard Monte Carlo simulations are possible

$$n_{qI}(\theta)/T^3 = \sum_{n=1}^{n_{max}} a_{2n-1}\theta^{2n-1}$$

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

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

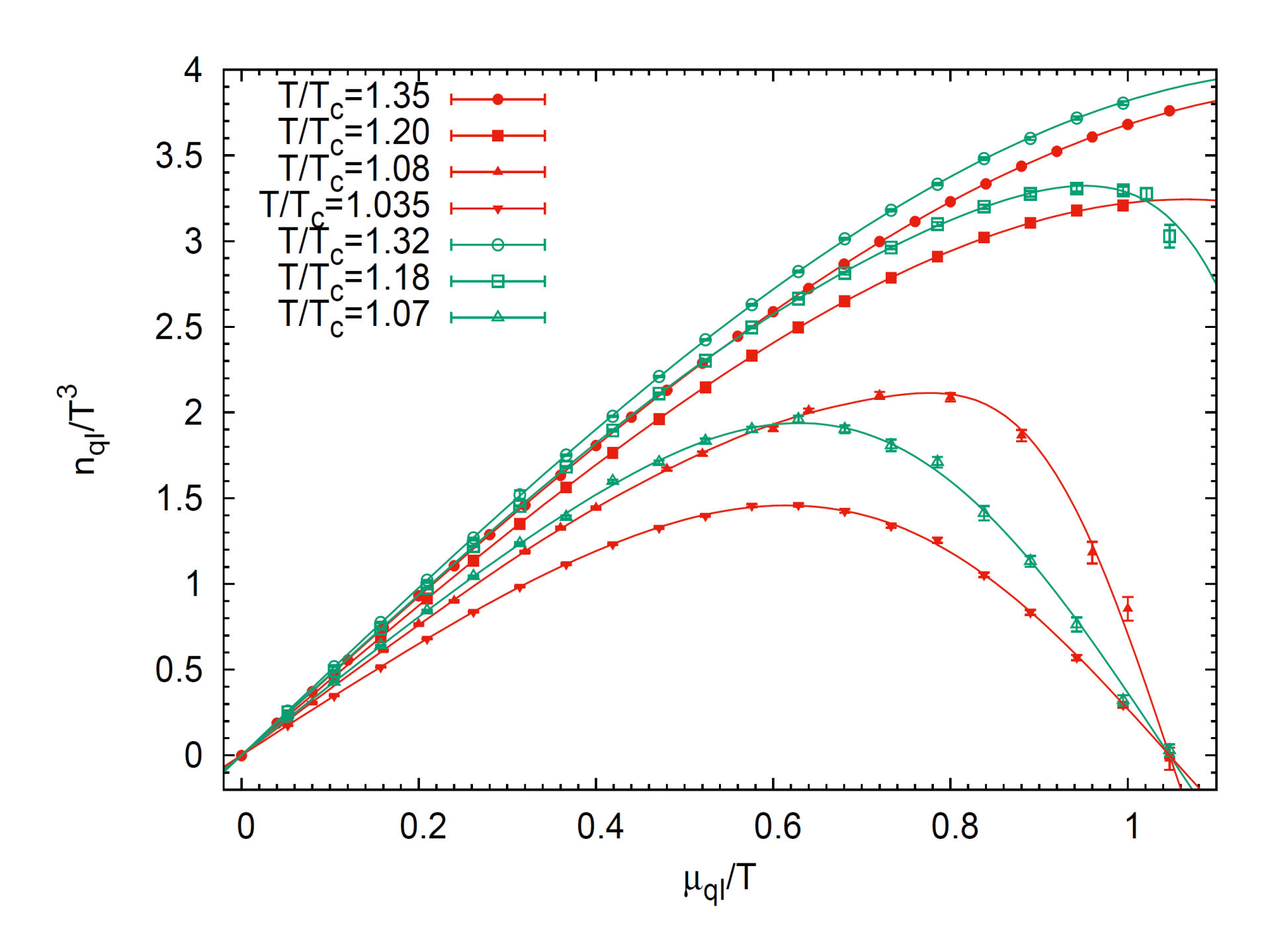
J. Takahashi, H. Kouno, M. Yahiro Phys.Rev. D91 (2015) no.1, 014501

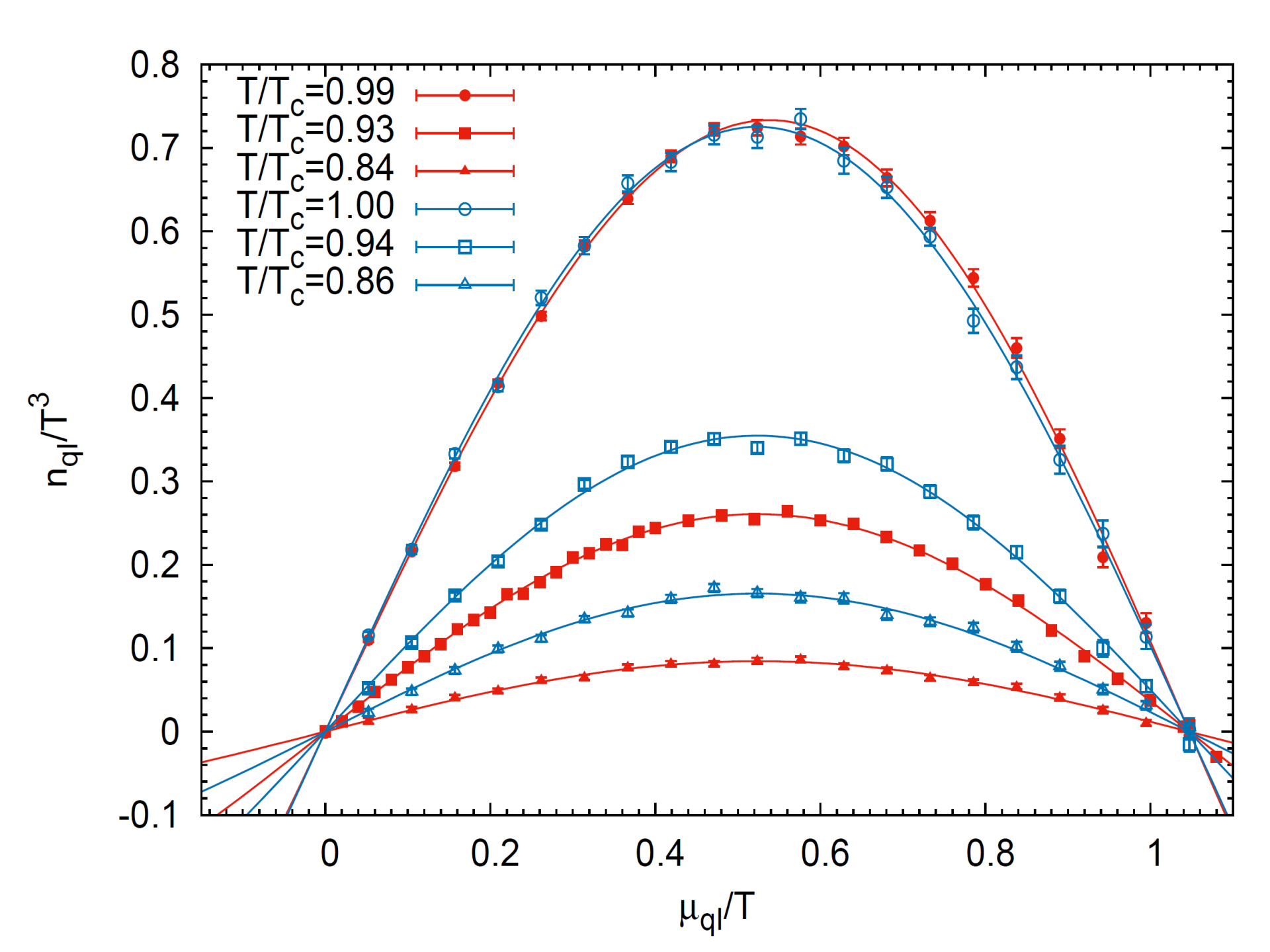
- The QCD equation of state at finite density from analytical continuation

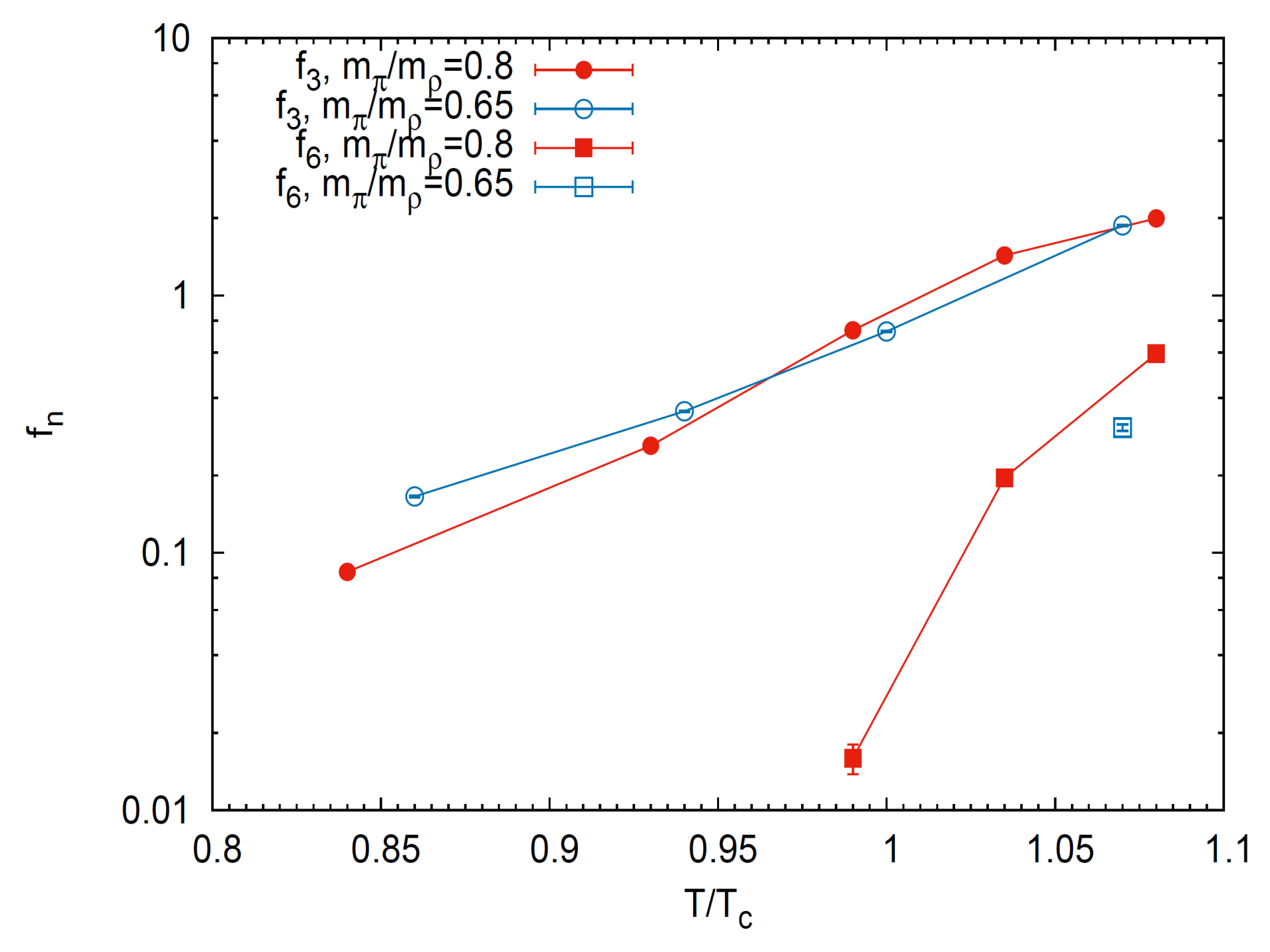
J. Gunther, R. Bellwied, S. Borsanyi , Z. Fodor, S.D. Katz, A. Pasztor, C. Ratti. EPJ Web Conf. 137 (2017) 07008

- 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

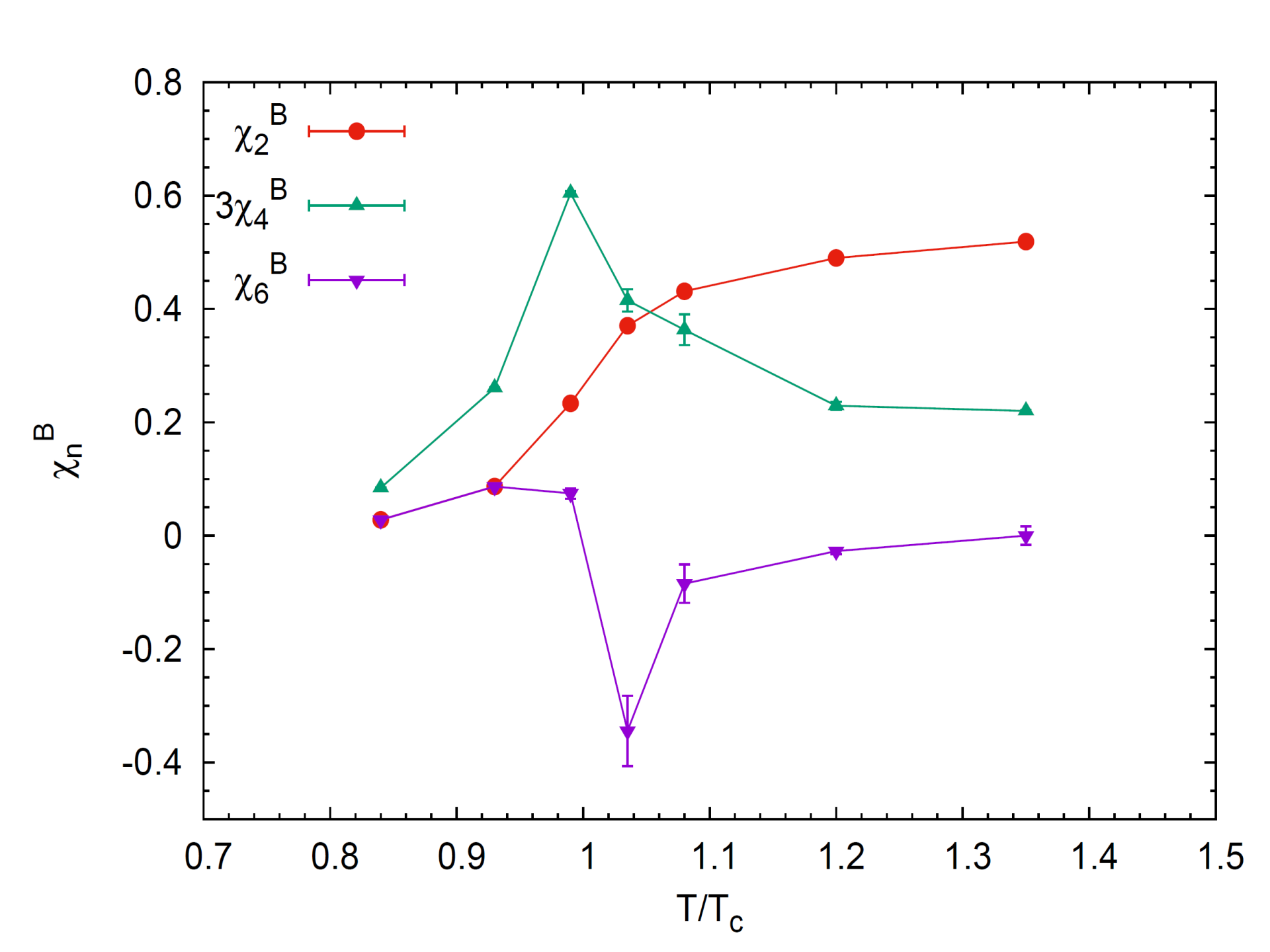

T/T_c=1.35
T/T_c=1.20
T/T_c=1.08
T/T_c=1.035
T/T_c=1.32
T/T_c=1.18
T/T_c=1.07
n_ql/T^3
μ_ql/T
0
0.5
1
1.5
2
2.5
3
3.5
4
0
0.2
0.4
0.6
0.8
1

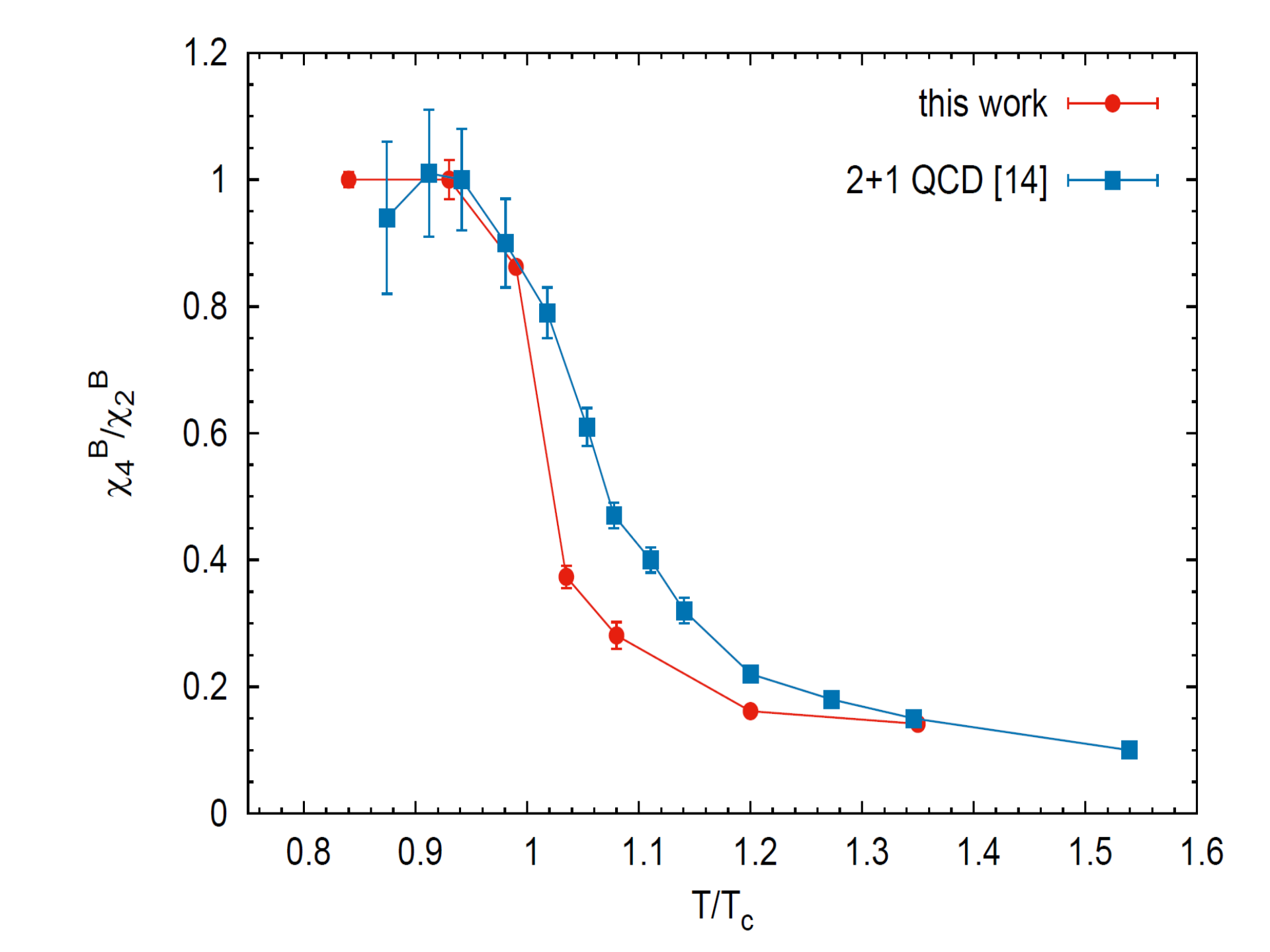

T/T_c=0.99
T/T_c=0.93
T/T_c=0.84
T/T_c=1.00
T/T_c=0.94
T/T_c=0.86
n_ql/T^3
μ_ql/T
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
0
0.2
0.4
0.6
0.8
1

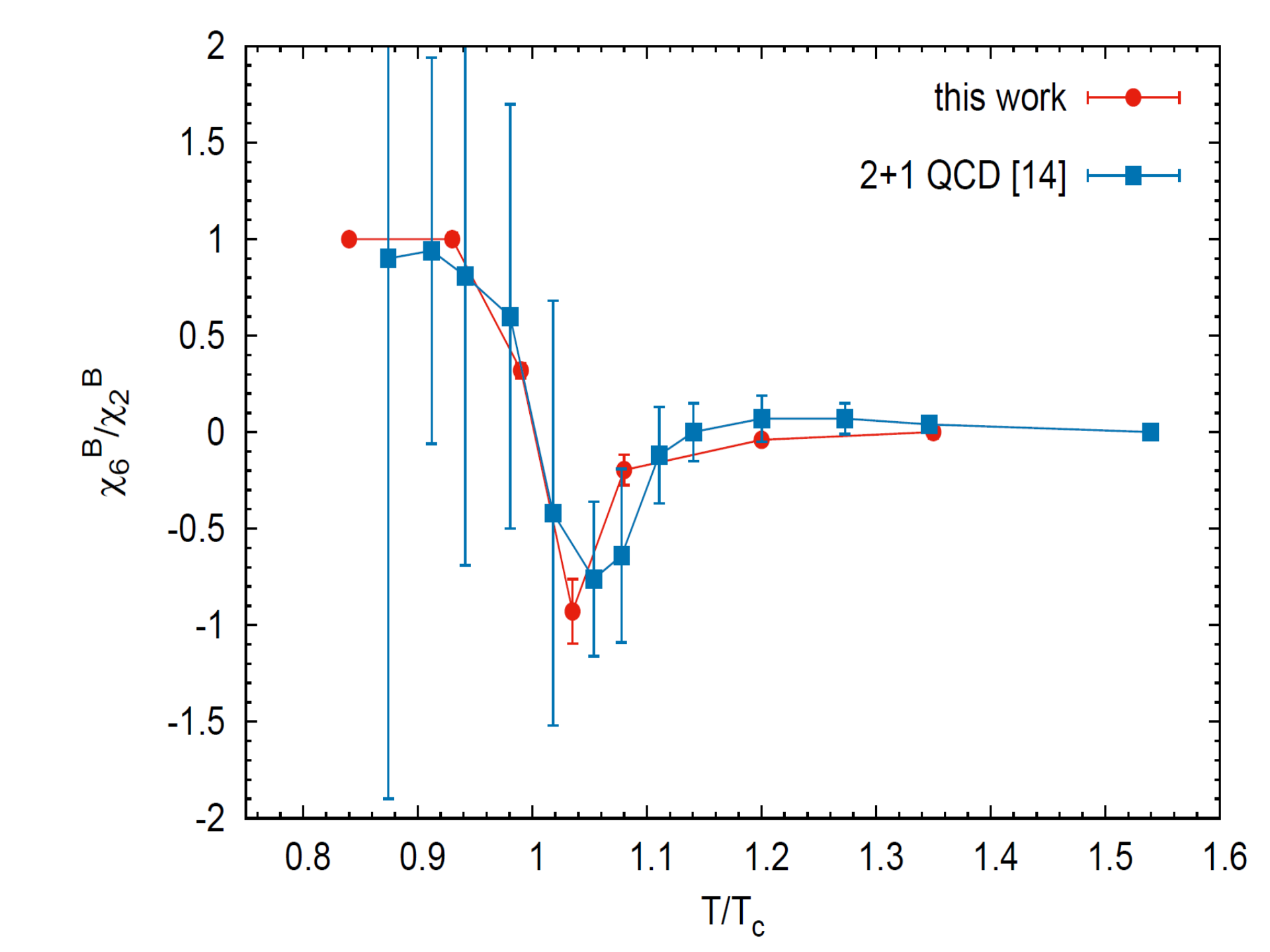

10
1
0.1
0.01
f_n
0.8
0.85
0.9
0.95
1
1.05
1.1
T/T_c
f_3, m_π/m_ρ=0.8
f_3, m_π/m_ρ=0.65
f_6, m_π/m_ρ=0.8
f_6, m_π/m_ρ=0.65

Taylor expansion:

$$\frac{p(T,\mu_B) - p(T,0)}{T^4} = \sum_{n=1}^{\infty} \frac{\chi_{2n}(T)}{(2n)!} \left(\frac{\mu_B}{T}\right)^{2n}$$


0.8
0.6
0.4
0.2
0
-0.2
-0.4
χ_n^B
χ_2^B
$3\chi_4^B$
χ_6^B
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
T/T_c


this work
2+1 QCD [14]
χ_4^B/χ_2^B
T/T_c
1.2
1
0.8
0.6
0.4
0.2
0
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
1.6


this work
2+1 QCD [14]
χ_6^B/χ_2^B
T/T_c
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
1.6

- Results for two quark masses do not differ substantially

- We found unexpectedly good agreement for ratios χ_4^B / χ_2^B and χ_6^B / χ_2^B with results obtained in 2+1 QCD with physical quark masses

1d QCD

1d QCD is solvable at finite μ

Bilic, Demeterfi, 1988

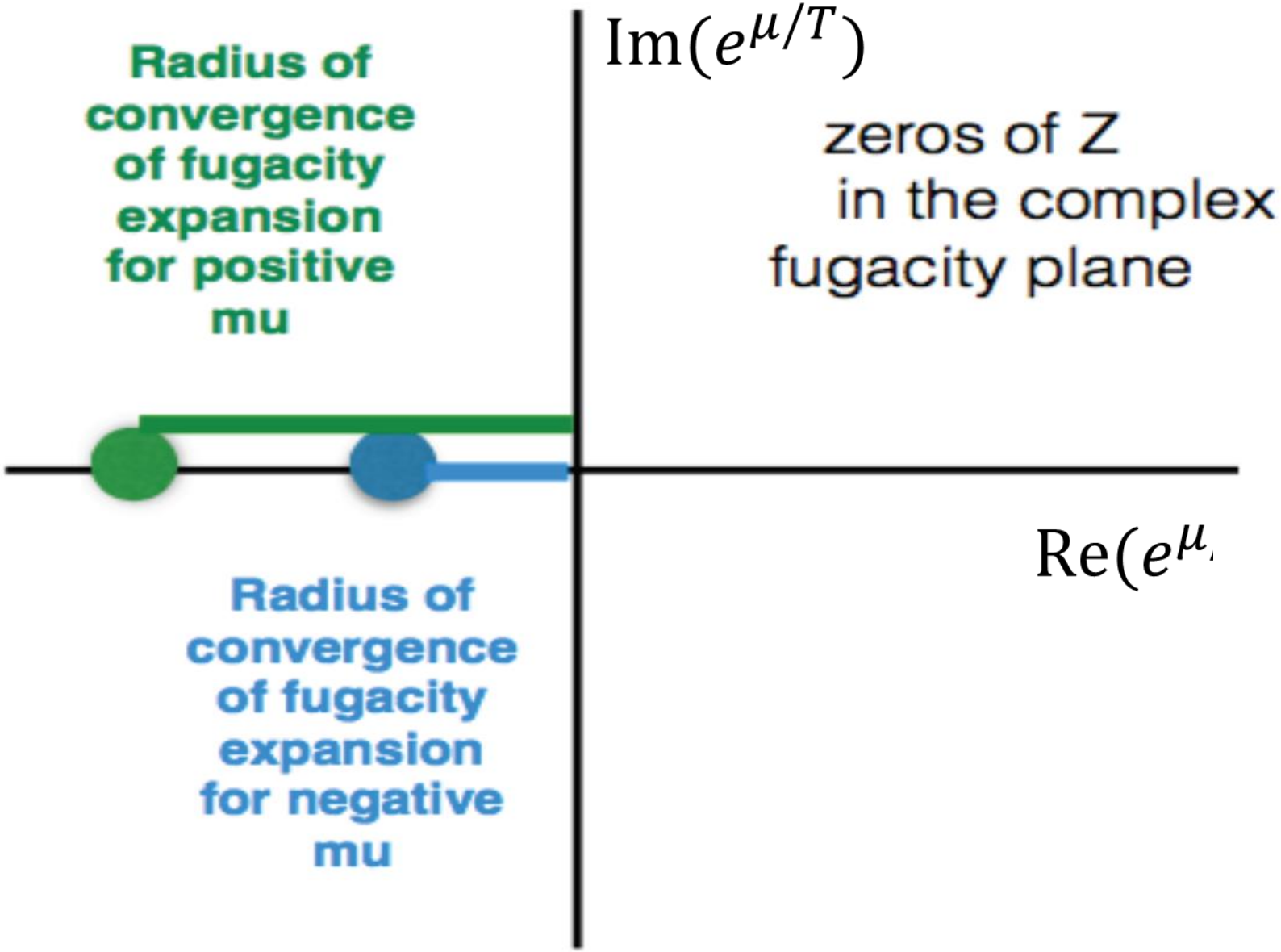
For any $T=1/aN$ and varying μ there is a crossover to a baryon reach phase which turns into 1st order phase transition at $T=0$.

GCPF $$Z(\mu, T) = 2\cosh\left(\frac{\mu}{T}\right) + A$$
$$= \sum Z_n(T)\,\xi^n,$$

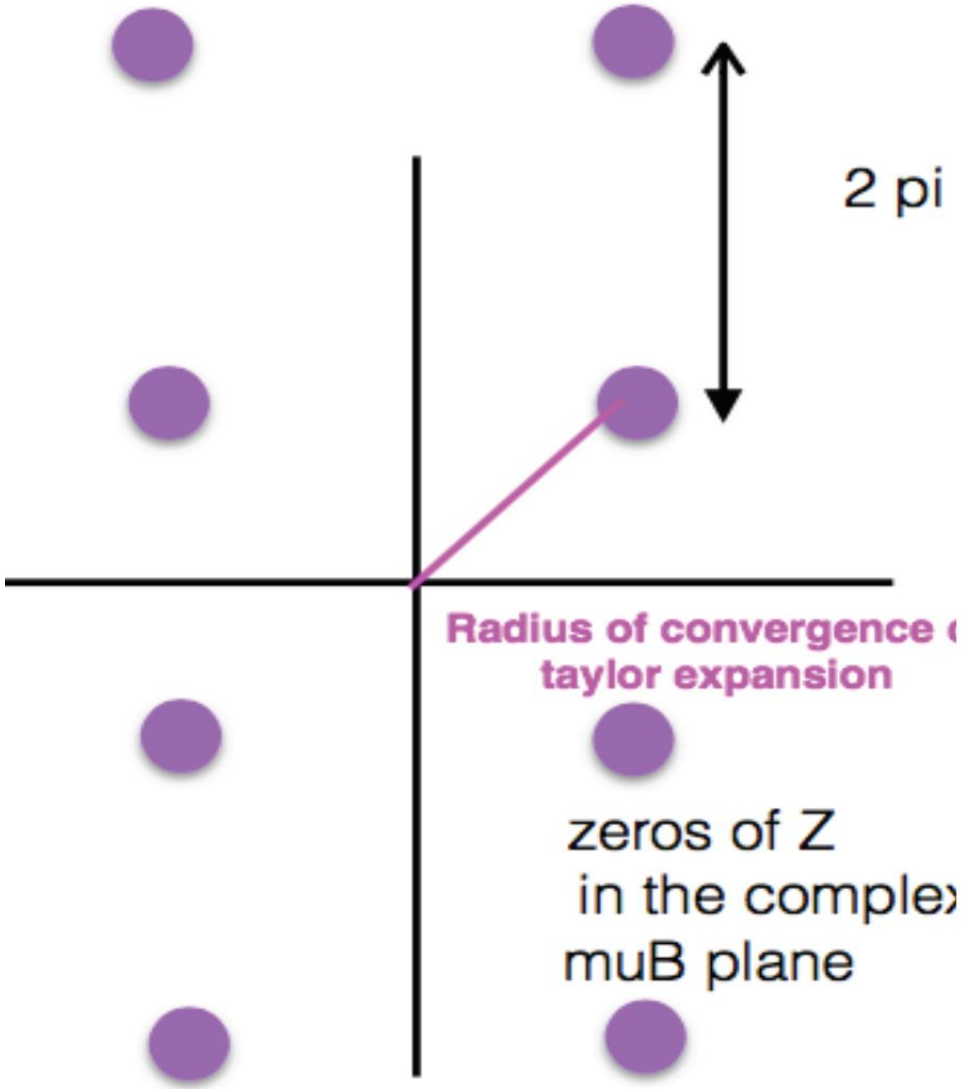
$$A = \sinh(4m'/T) \,/\, \sinh(m'/T), \qquad 4 \leq A < \infty$$
$$m' = \sinh^{-1}(m)$$

$$Z_0 = A, \quad Z_1 = Z_{-1} = A$$

Density $$n(\mu, T) = \frac{2}{Z}\sinh(\frac{\mu}{T})$$



$$Z = 0 \; at \qquad e^{\mu/T} = \frac{1}{2}\left(A \pm \sqrt{A^2 - 4}\right) = y_{1,2}$$

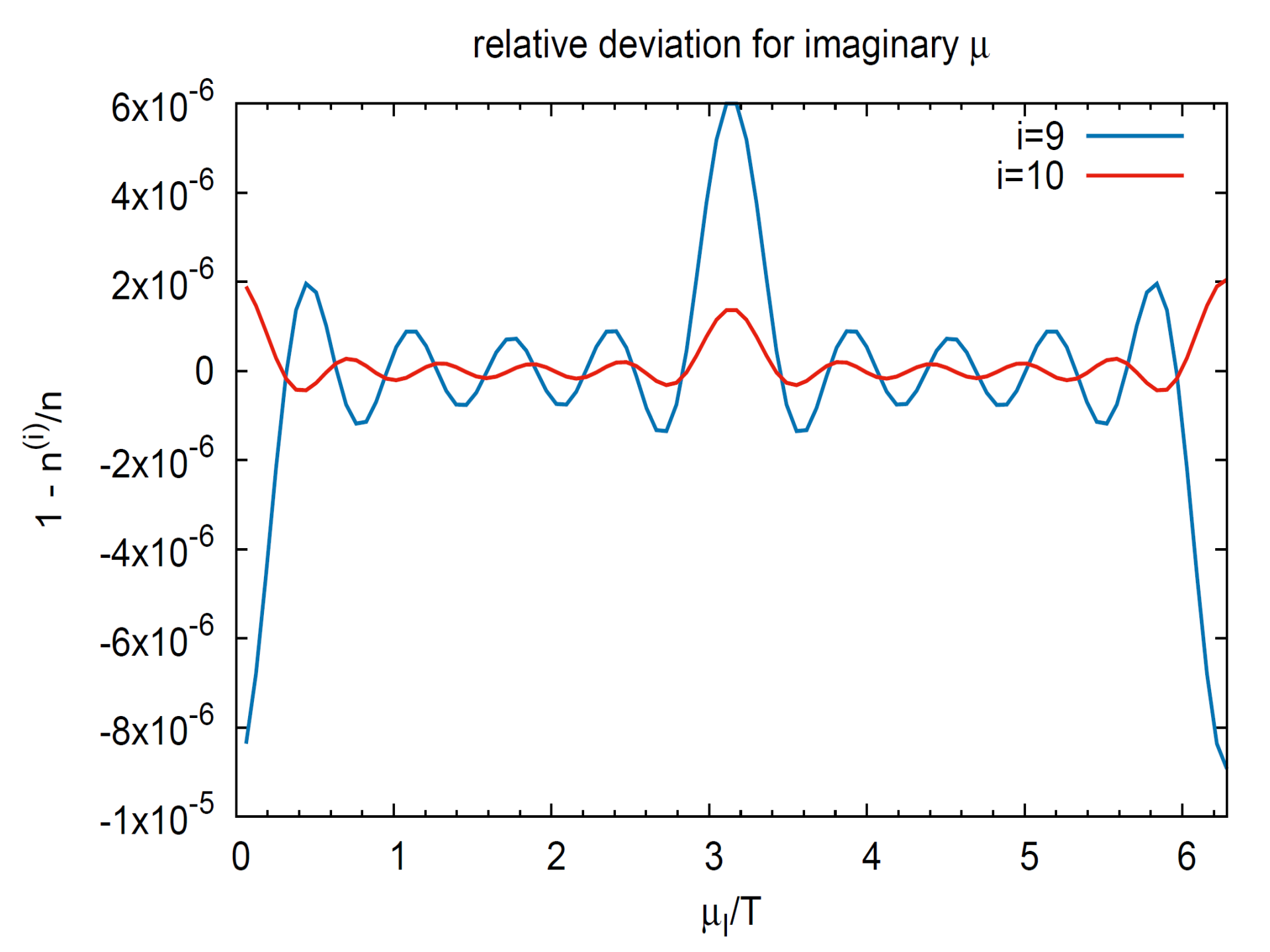


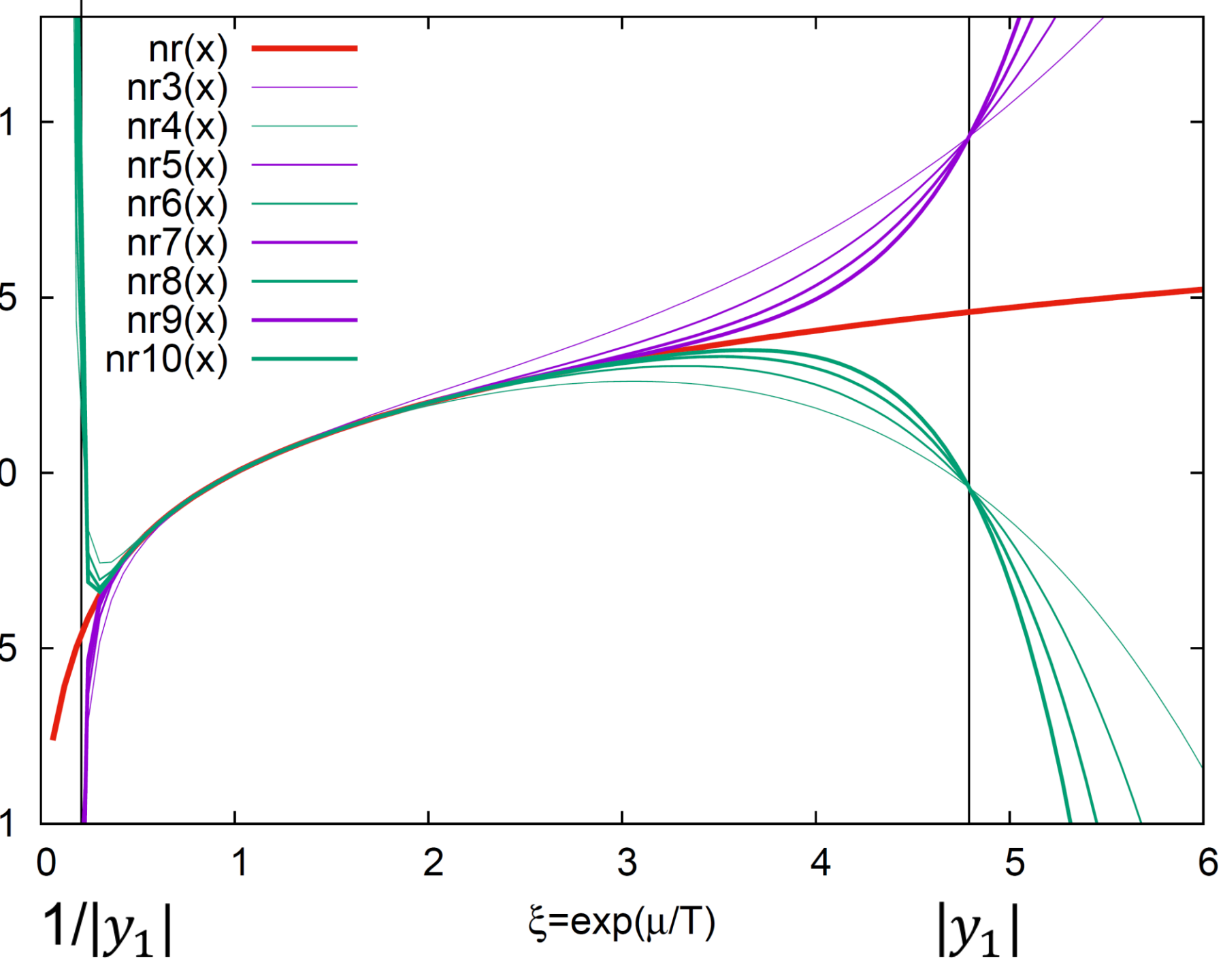
$$\mu = \pm T(log|y_1|) + i(2k+1)T\pi$$

Virial expansion for density

$$n^{(i)} = \sum_{k=1}^{i} a_k \sinh(k\frac{\mu}{T})$$

a_k are computed at imaginary μ as Fourier coefficients of exact $n(\mu)$.

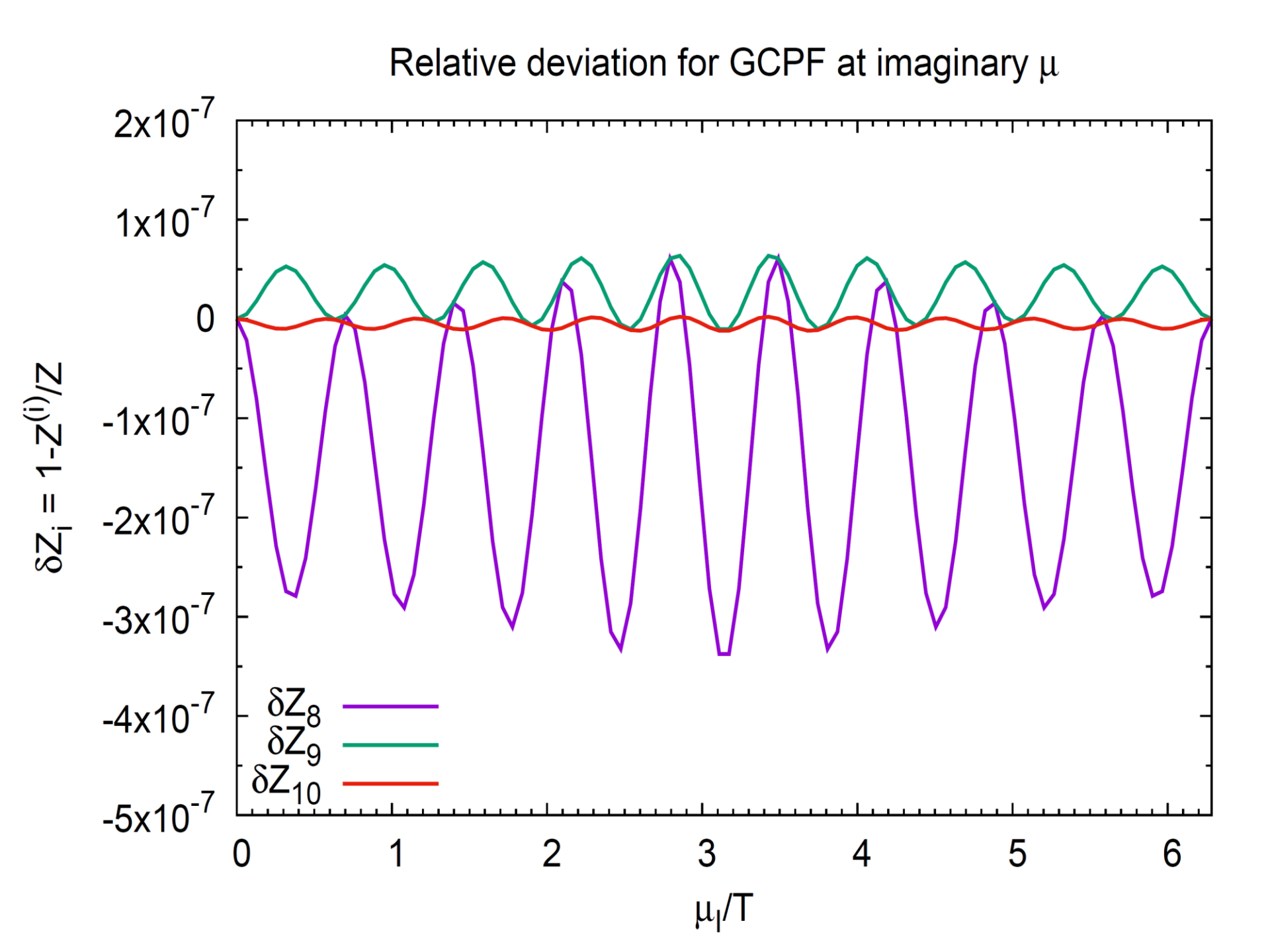

relative deviation for imaginary μ
6x10-6
4x10-6
2x10-6
0
-2x10-6
-4x10-6
-6x10-6
-8x10-6
-1x10-5
1 - n(i)/n
0
1
2
3
4
5
6
μI/T
i=9
i=10

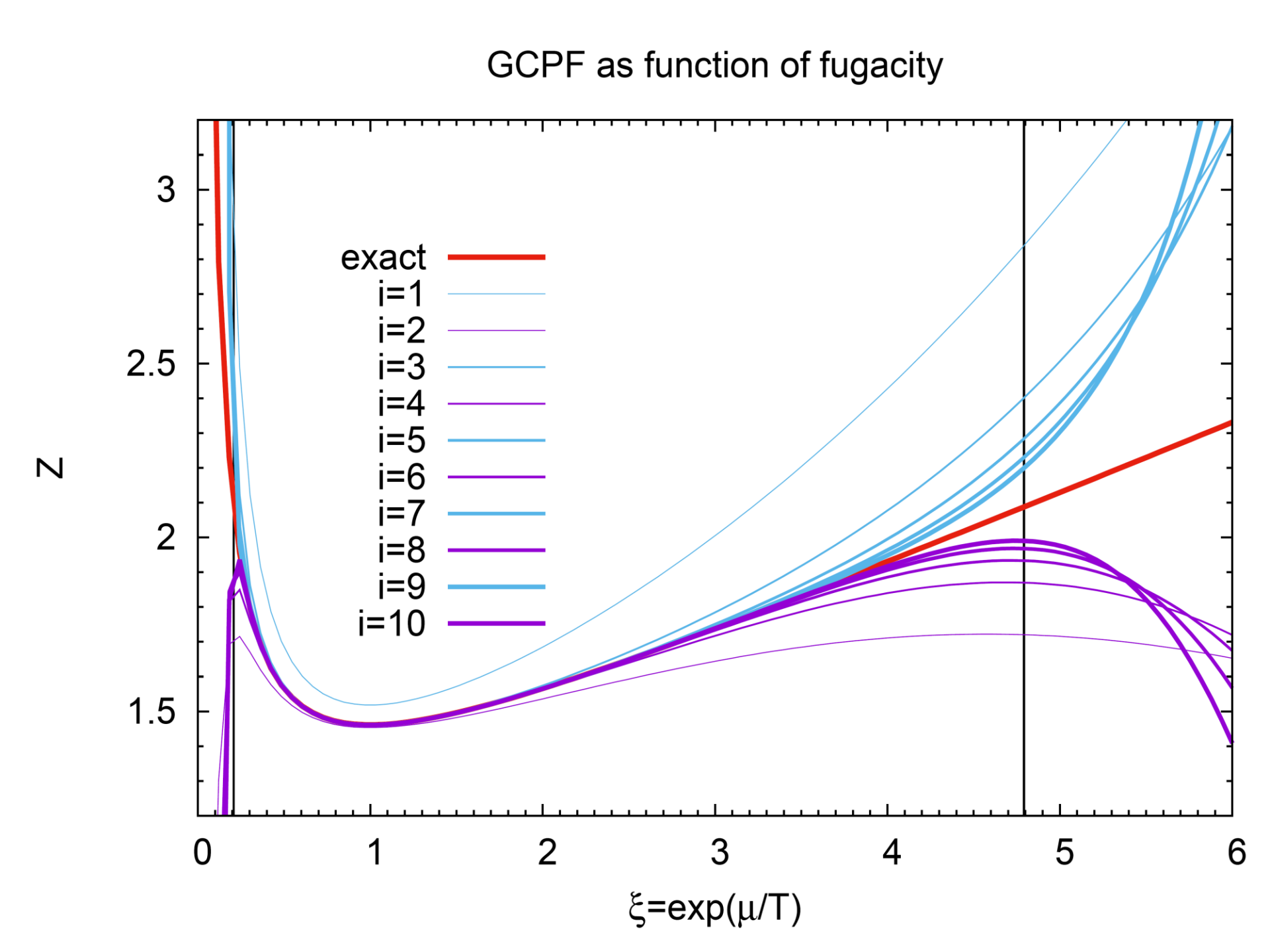

nr(x)
nr3(x)
nr4(x)
nr5(x)
nr6(x)
nr7(x)
nr8(x)
nr9(x)
nr10(x)
1
5
0
5
1
0
1
2
3
4
5
6
$1/|y_1|$
ξ=exp(μ/T)
$|y_1|$

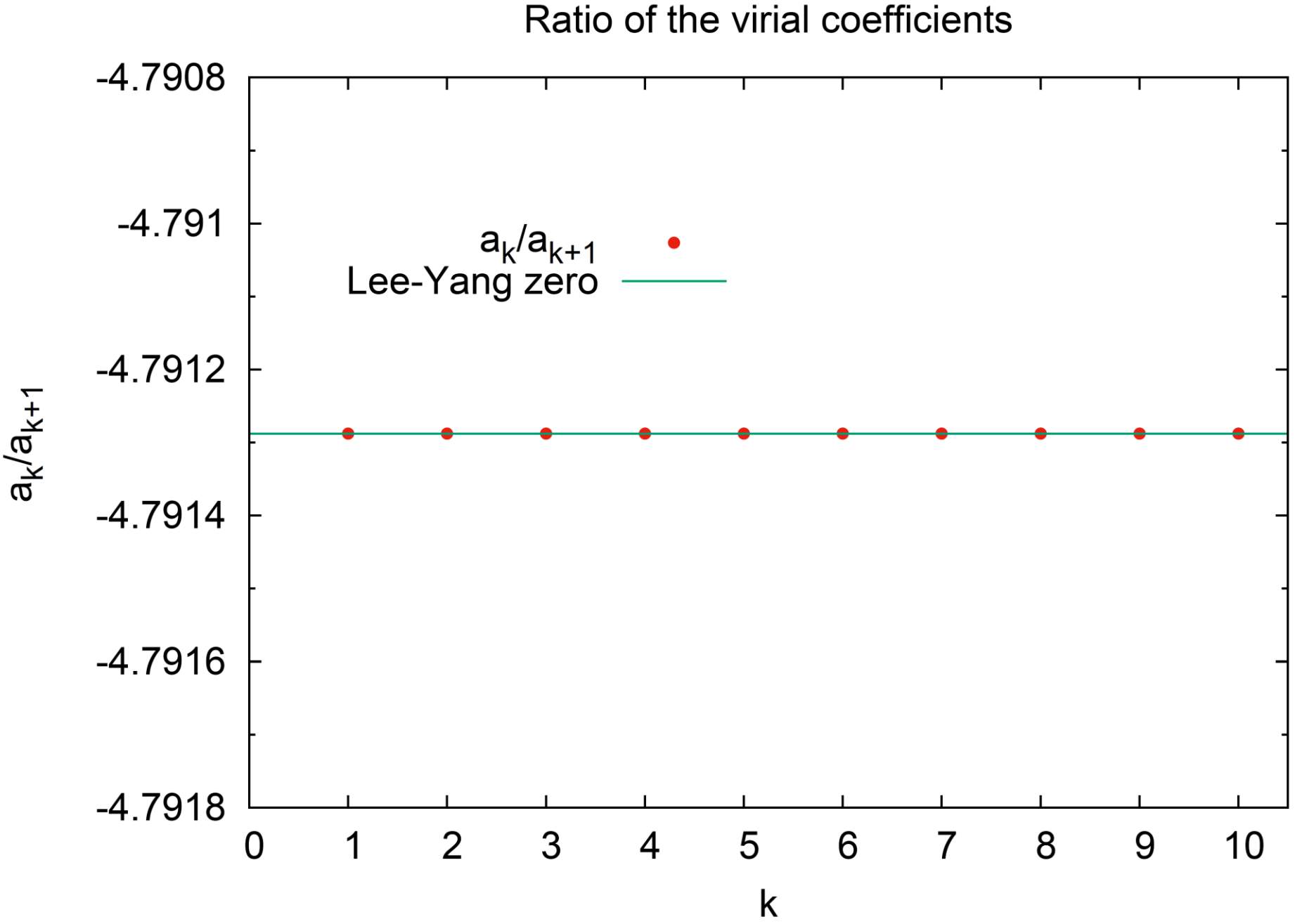
Virial expansion converges to exact solution within interval

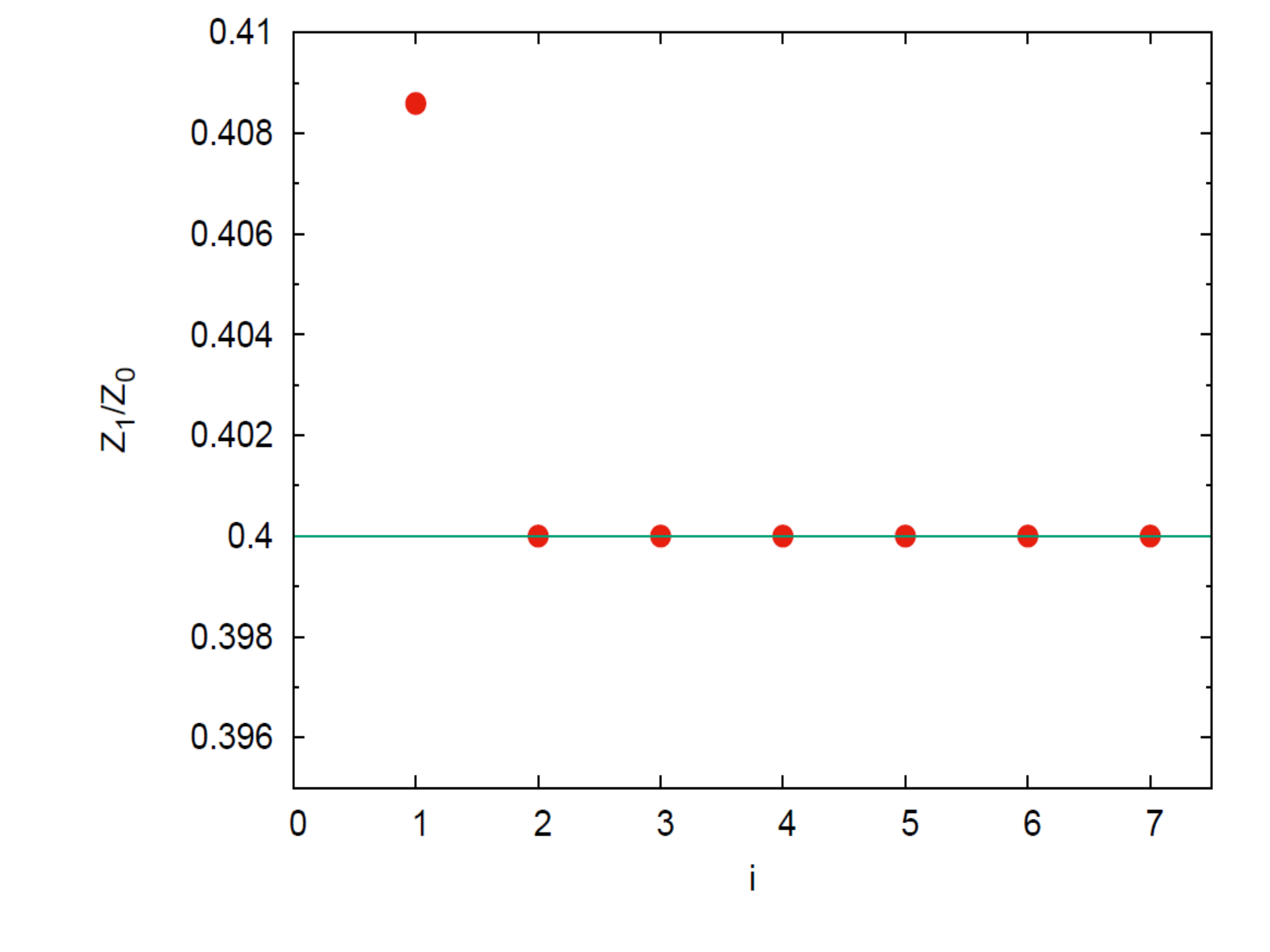
$$1/|y_1| < \xi < |y_1|$$

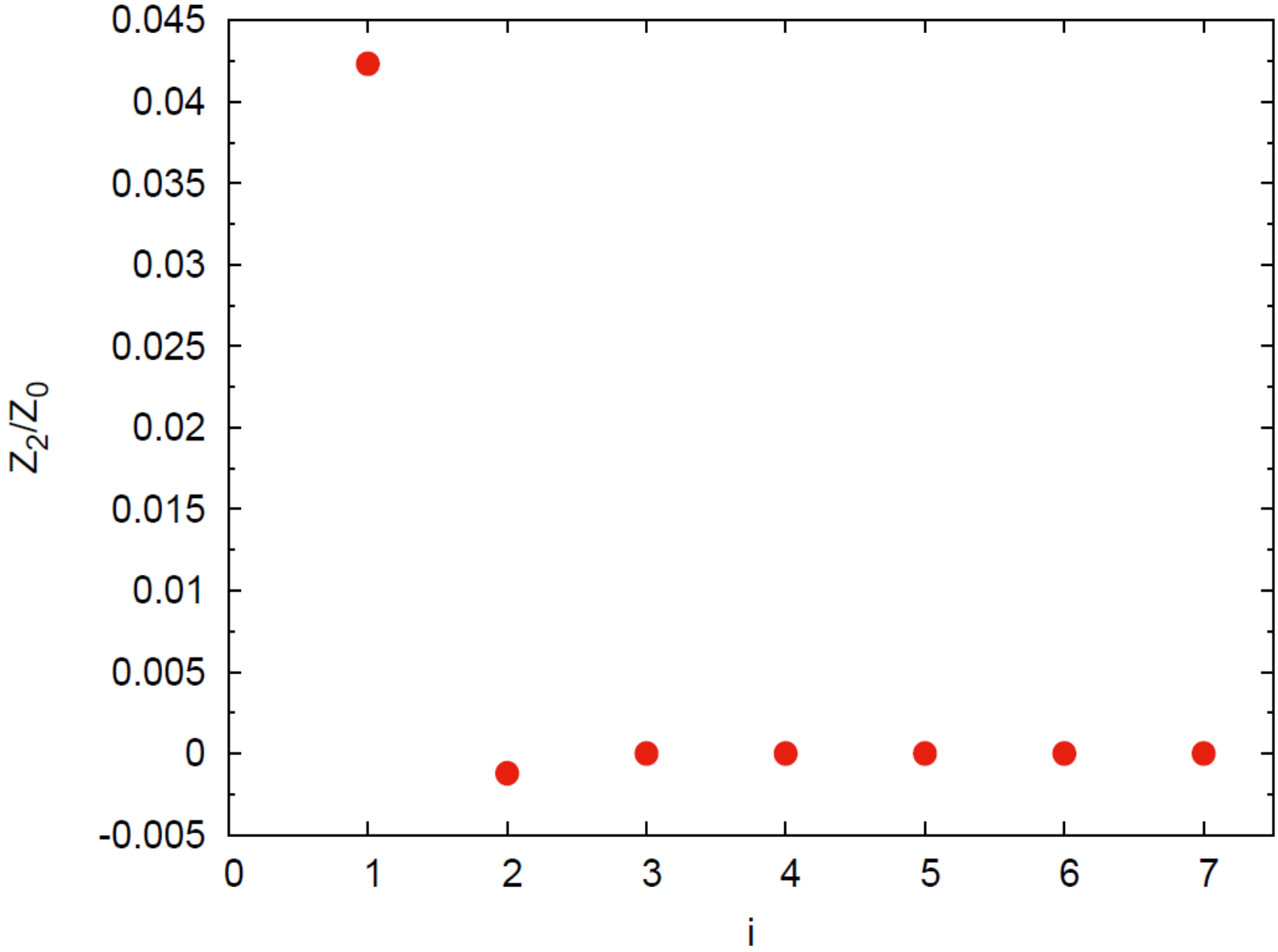
determined by analyticity

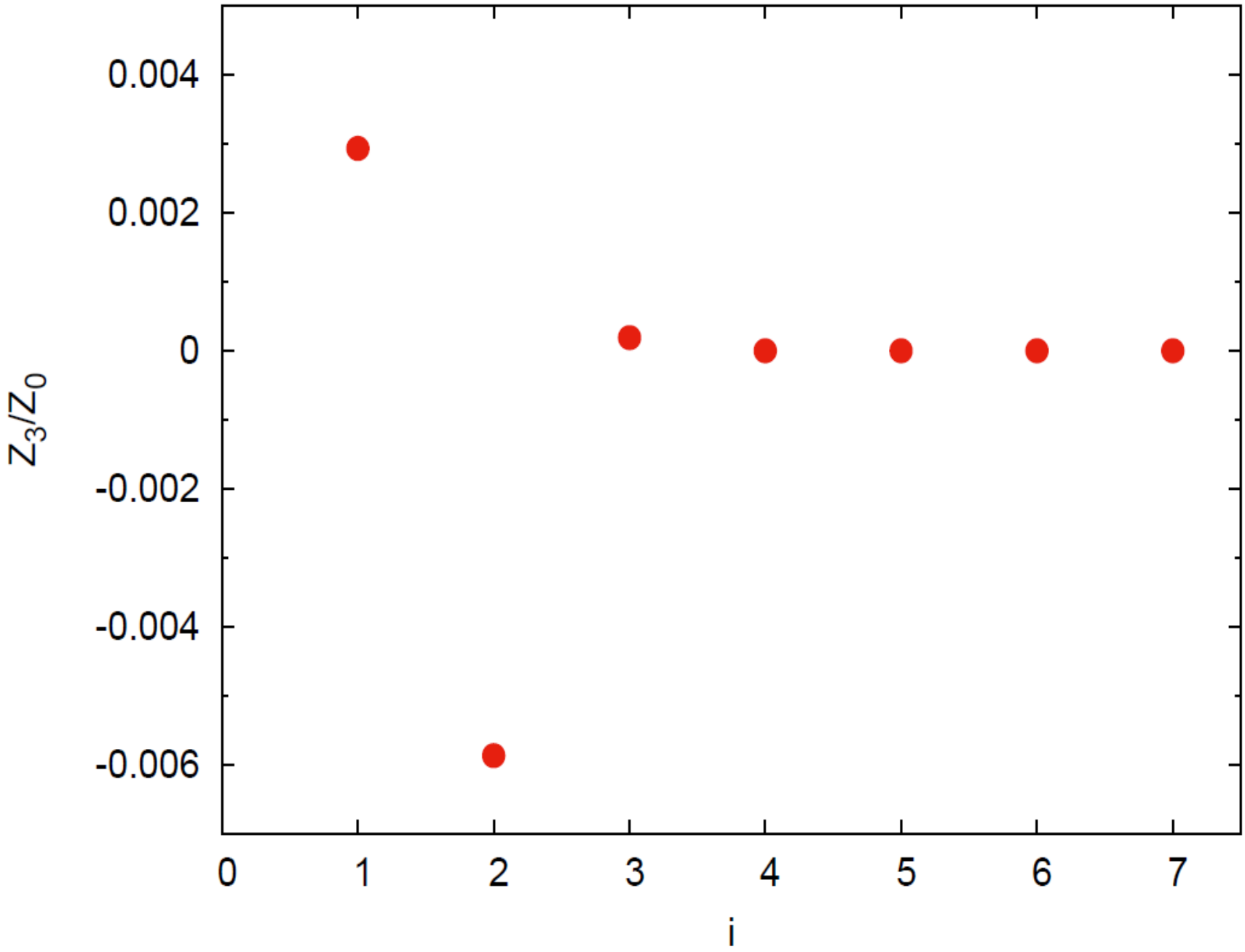

Relative deviation for GCPF at imaginary μ
2x10^-7
1x10^-7
0
-1x10^-7
-2x10^-7
-3x10^-7
-4x10^-7
-5x10^-7
δZ_i = 1-Z^(i)/Z
δZ8
δZ9
δZ10
0
1
2
3
4
5
6
μ_I/T


GCPF as function of fugacity
Z
ξ=exp(μ/T)
exact
i=1
i=2
i=3
i=4
i=5
i=6
i=7
i=8
i=9
i=10
3
2.5
2
1.5
0
1
2
3
4
5
6


Ratio of the virial coefficients
-4.7908
-4.791
-4.7912
-4.7914
-4.7916
-4.7918
a_k/a_{k+1}
a_k/a_{k+1}
Lee-Yang zero
0
1
2
3
4
5
6
7
8
9
10
k


0.41
0.408
0.406
0.404
0.402
0.4
0.398
0.396
Z_1/Z_0
0
1
2
3
4
5
6
7
i


0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
-0.005
Z_2/Z_0
0
1
2
3
4
5
6
7
i


0.004
0.002
0
-0.002
-0.004
-0.006
Z_3/Z_0
0
1
2
3
4
5
6
7
i

Lessons:

- The radius of converegence can be computed from the ratio of the virial coefficients
- The virial expansion provides good approximations for density and GCPF within radius of convergence. How to move beyond this region?
- In this model the GCPF can be reconstructed beyond radius of convergence via computation of CPF. Is it general?

Cluster Expansion Model for QCD Baryon Number Fluctuations: No Phase Transition at $\mu_B/T < \pi$

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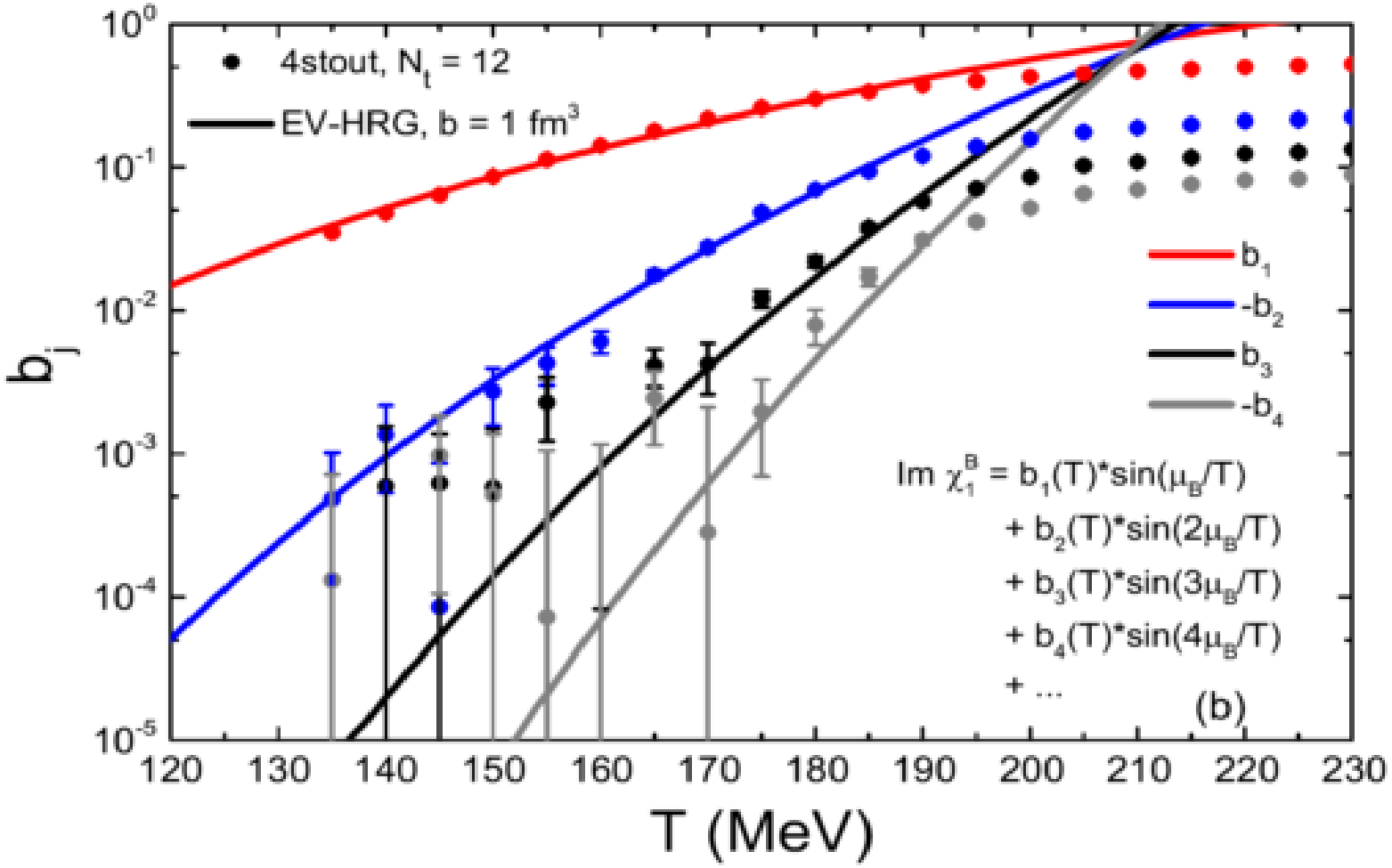
[2] *Frankfurt Institute for Advanced Studies, Giersch Science Center, Ruth-Moufang-Str. 1, D-60438 Frankfurt am Main, Germany*

GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstr. 1, D-64291 Darmstadt, Germany

Cluster Expansion Model (CEM), representing a relativistic extension of Mayer's cluster expansion, is constructed to study baryon number fluctuations in QCD. The temperature dependent first two coefficients, corresponding to the partial pressures in the baryon number $B = 1$ and $B = 2$ sectors, are the only model input, which we fix by recent lattice data at imaginary baryochemical potential. All other coefficients are constructed in terms of the first two and required to match the Stefan-Boltzmann limit at $T \to \infty$. The CEM allows calculations of the baryon number susceptibilities χ_k^B to arbitrary order. We obtain excellent agreement with available lattice data for the baryon fluctuation measures χ_2^B, χ_4^B, χ_6^B and predict higher order susceptibilities, that are not yet available from Lattice QCD. The calculated susceptibilities are then used to extract the radius of convergence of the Taylor expansion of the pressure. The commonly used ratio test fails due to the non-trivial asymptotic behavior of the Taylor coefficients. At the same time, a more elaborate estimator provides finite convergence radii at all temperatures and in agreement with the singularities of Padé approximants. The associated singularities lie in the complex μ_B/T-plane and appear smoothly connected to the Roberge-Weiss transition at high temperatures and imaginary chemical potential. No evidence for a phase transition at $\mu_B/T \lesssim \pi$ is found.

$$\frac{\rho_B}{T^3} = \frac{\partial(p/T^4)}{\partial(\mu_B/T)} = \sum_{k=1}^{\infty} b_k(T)\ \sinh\left(\frac{k\,\mu_B}{T}\right)$$



The temperature dependence of the first four Fourier coefficients b_k and within the EV-HRG model with baryonic eigenvolume parameter $b = 1$ fm^3

For high temperature (SB) limit:

$$b_k^{\mathrm{SB}} = \frac{(-1)^{k+1}}{k} \frac{4\left[3 + 4\left(\pi k\right)^2\right]}{27\left(\pi k\right)^2}.$$

CEM assumptions:

- The first coefficient $b_1(T)$ – the QCD partial pressure in the $|B| = 1$ sector – is taken as input. It is interpreted as a temperature dependent density of "free" excitations with $B = \pm 1$.
- The second coefficient, $b_2(T)$, is also taken as input. In the spirit of a cluster expansion it parametrizes the baryon-baryon interactions. In the HRG-EV model b_2 is rewritten as

$$b_2(T) = -b(T)\, T^3\, [b_1(T)]^2, \qquad (3)$$

where $b(T)$ is a temperature dependent "coupling" parameter.

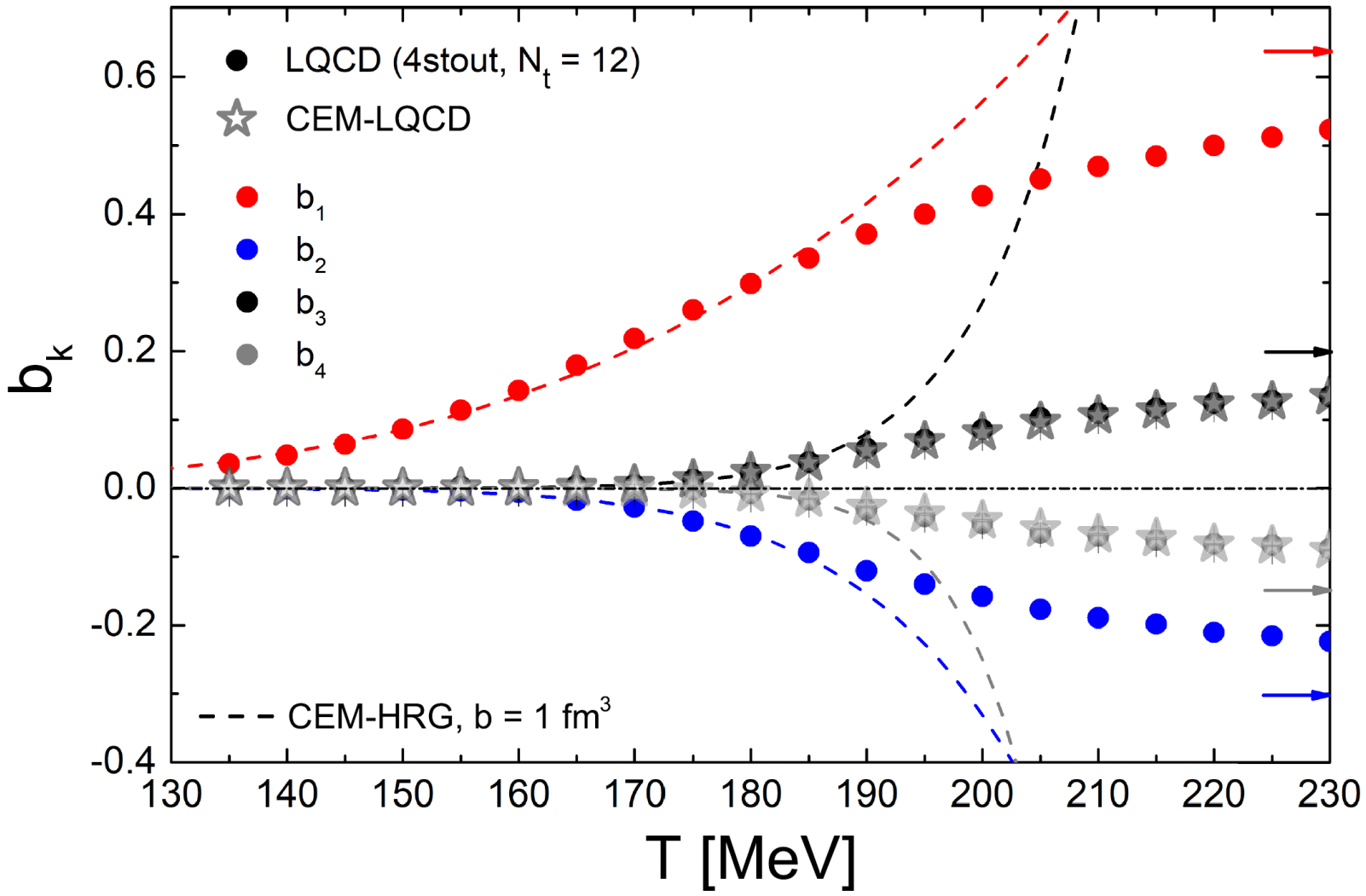
- Mayer's cluster expansion assumes two-particle interactions only, expected to be a good approximation at sufficiently low density or high temperature. The higher-order coefficients $b_k(T)$ can then be expressed in terms of the first two using the HRG-EV-type expression [10]: they are proportional to the k-th power of the "free" density $b_1(T)$ and to the $(k-1)$-th power of the "coupling" parameter $b(T)$, i.e.

$$b_k(T) = \alpha_k \left[-b(T)\, T^3\right]^{k-1} \left[b_1(T)\right]^k = \alpha_k \frac{\left[b_2(T)\right]^{k-1}}{\left[b_1(T)\right]^{k-2}}, \tag{4}$$

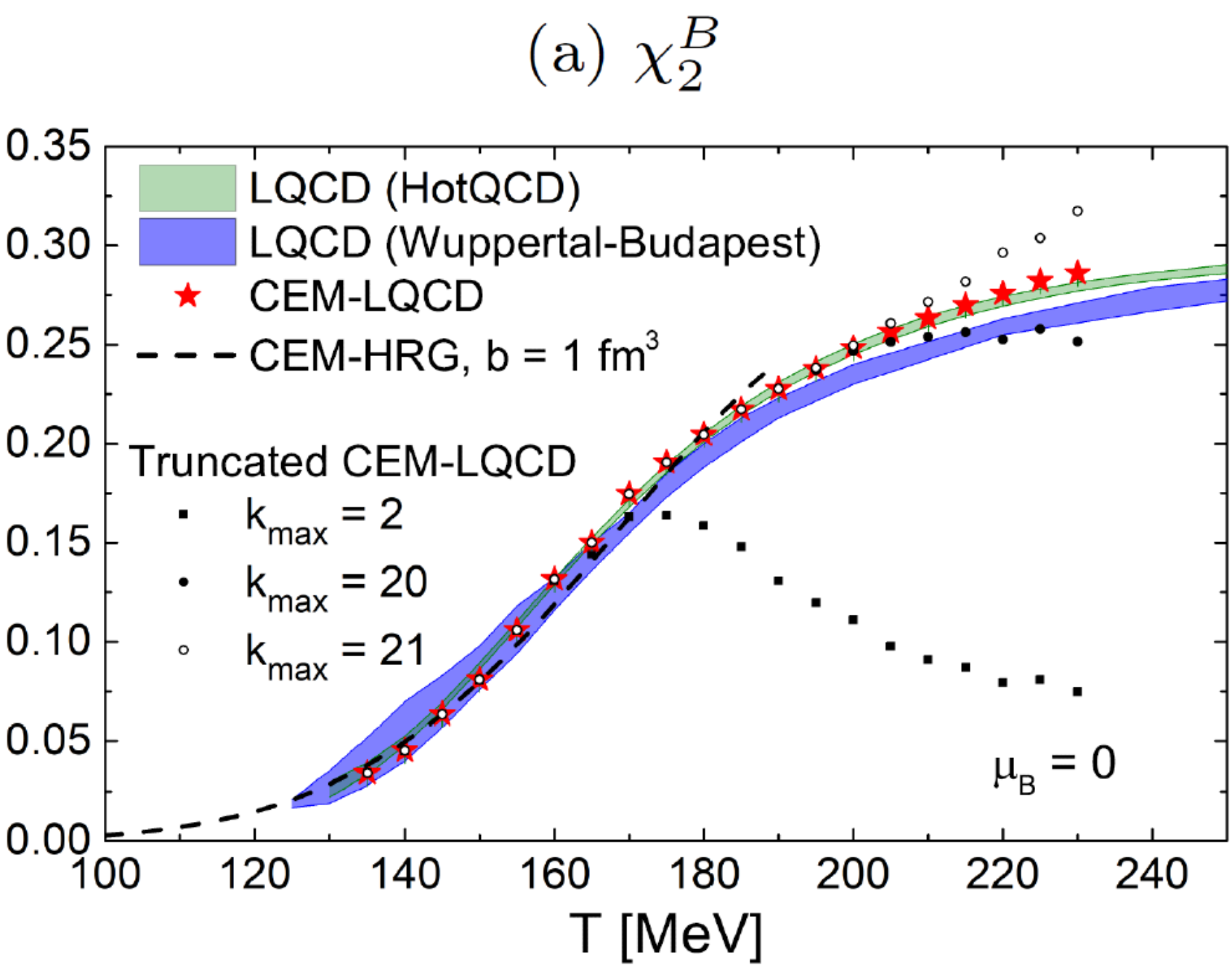
where α_k are temperature *independent* parameters.

- The model is constrained by the SB limit (2) of massless quarks and gluons at high temperatures, i.e. $b_k(T) \to b_k^{\rm SB}$ as $T \to \infty$. Assuming $b_1(T) \to b_1^{\rm SB}$ and $b_2(T) \to b_2^{\rm SB}$, this condition yields the coefficients α_k:

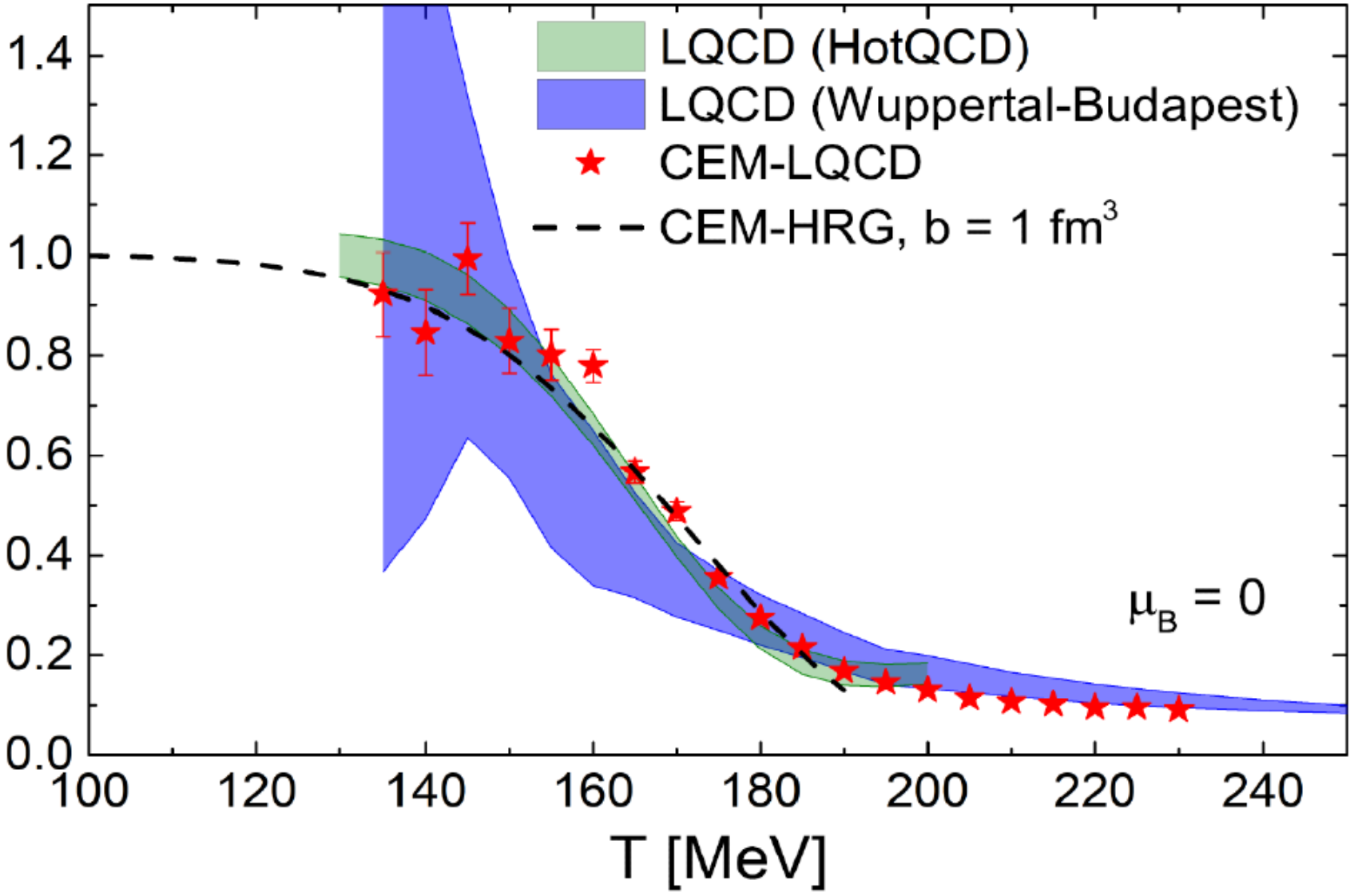
$$\alpha_k = \frac{[b_1^{\rm SB}]^{k-2}}{[b_2^{\rm SB}]^{k-1}}\, b_k^{\rm SB}\,. \tag{5}$$

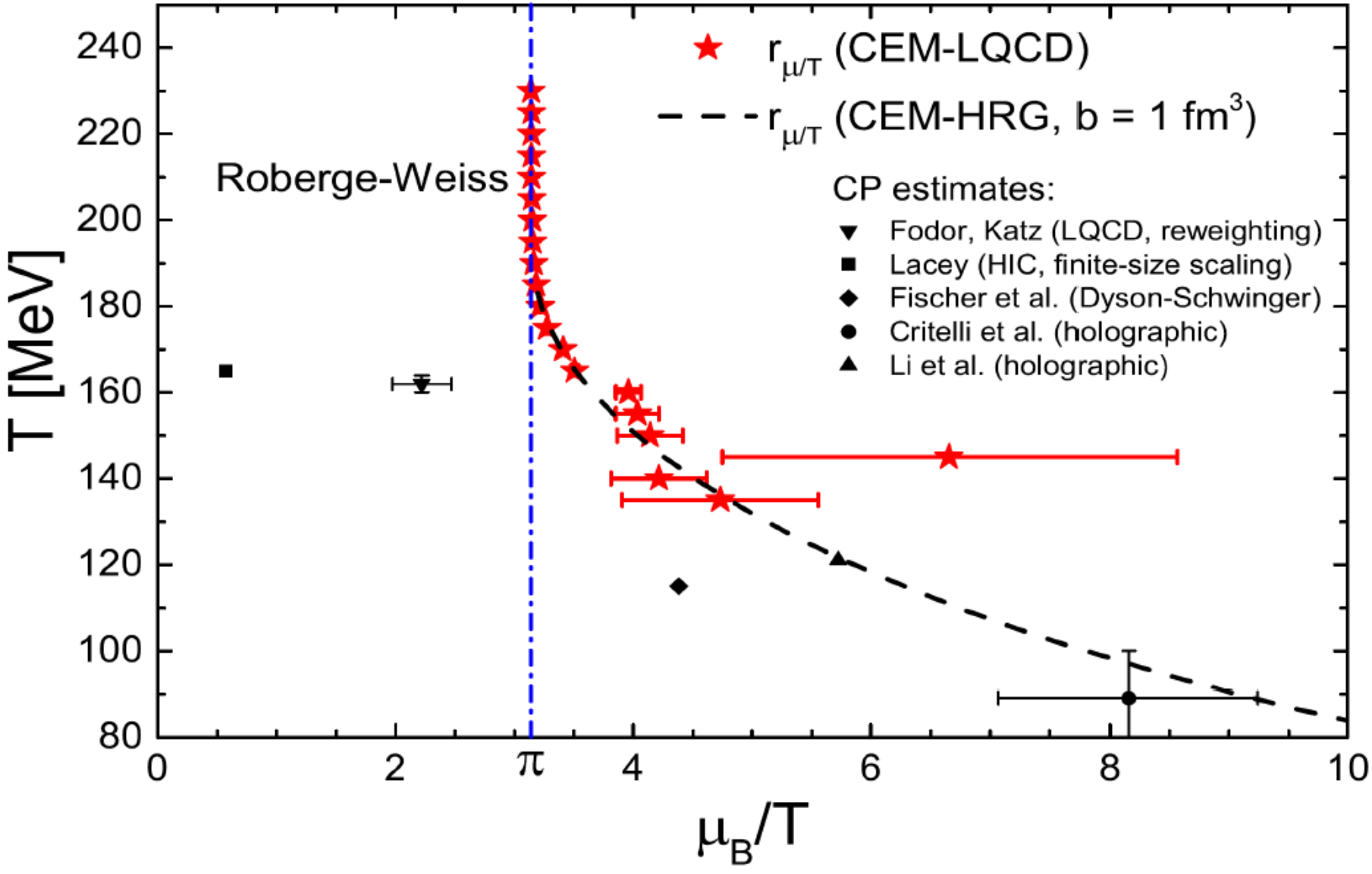


Lattice results (circles), CEM-LQCD (stars), CEM-HRG (dashed lines)


(a) χ_2^B
LQCD (HotQCD)
LQCD (Wuppertal-Budapest)
CEM-LQCD
CEM-HRG, b = 1 fm^3
Truncated CEM-LQCD
k_{max} = 2
k_{max} = 20
k_{max} = 21
μ_B = 0
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
100
120
140
160
180
200
220
240
T [MeV]

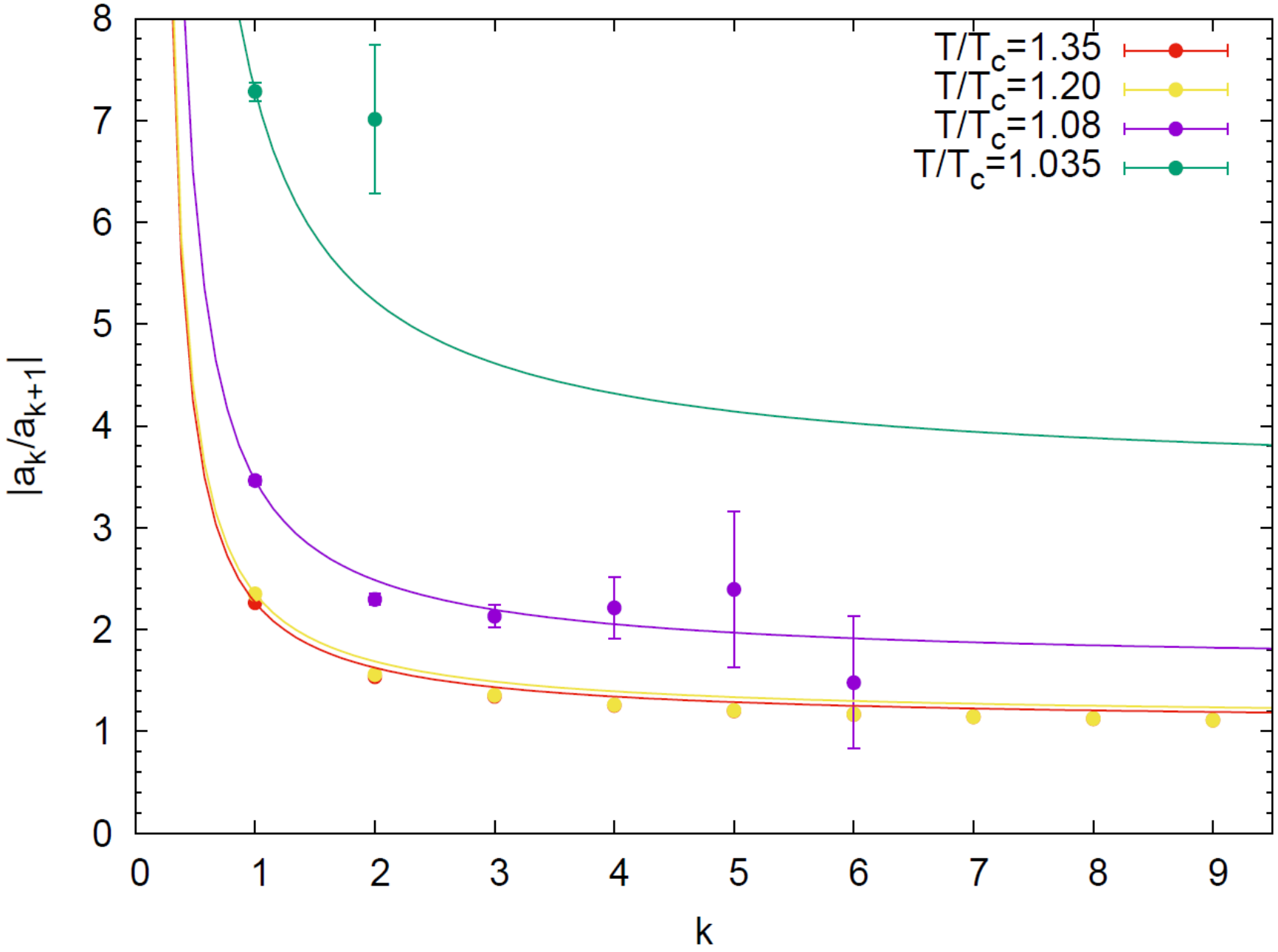
(b) χ_4^B/χ_2^B

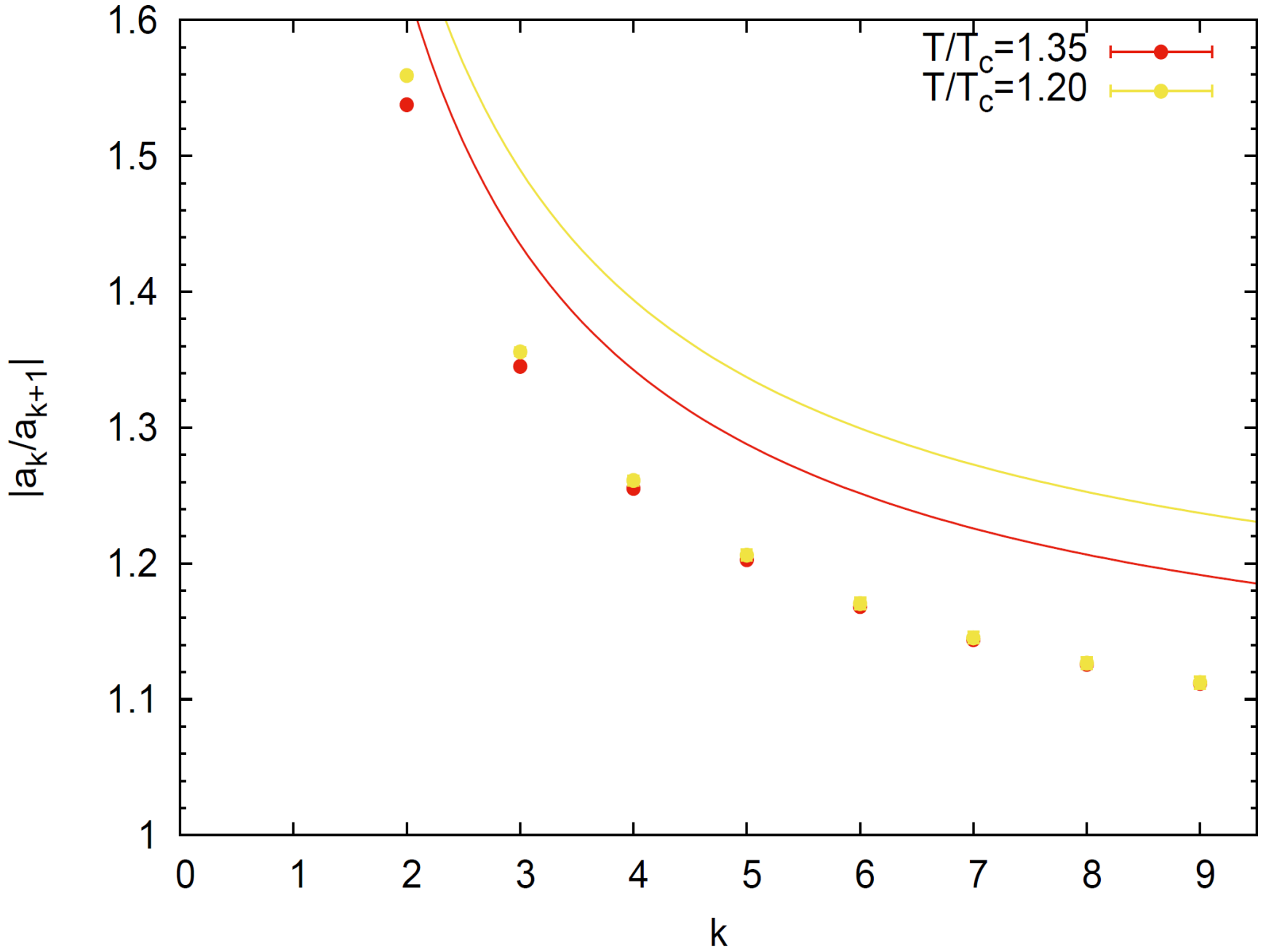




Radius of convergence

tial. The analysis within CEM shows no evidence for the existence of a phase transition or a critical point at real values of the baryochemical potential at $\mu_B/T \lesssim \pi$ for temperatures above 135 MeV.


T/T_c=1.35
T/T_c=1.20
T/T_c=1.08
T/T_c=1.035
$|a_k/a_{k+1}|$
k
0
1
2
3
4
5
6
7
8
9


1.6
1.5
1.4
1.3
1.2
1.1
1
0
1
2
3
4
5
6
7
8
9
k
|a_K/a_K+1|
T/T_c=1.35
T/T_c=1.20

Fourier coefficients of the net–baryon number density and chiral criticality

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We investigate the Fourier coefficients $b_k(T)$ of the net–baryon number density in strongly interacting matter at nonzero temperature and density. The asymptotic behavior of the coefficients at large k is determined by the singularities of the partition function in the complex chemical potential plane. Within a QCD-like effective chiral model, we show that the chiral and deconfinement properties at nonzero baryon chemical potential are reflected in characteristic k– and T– dependences of the Fourier coefficients. We also discuss the influence of the Roberge-Weiss transition on these coefficients. Our results indicate that the Fourier expansion approach can provide interesting insights

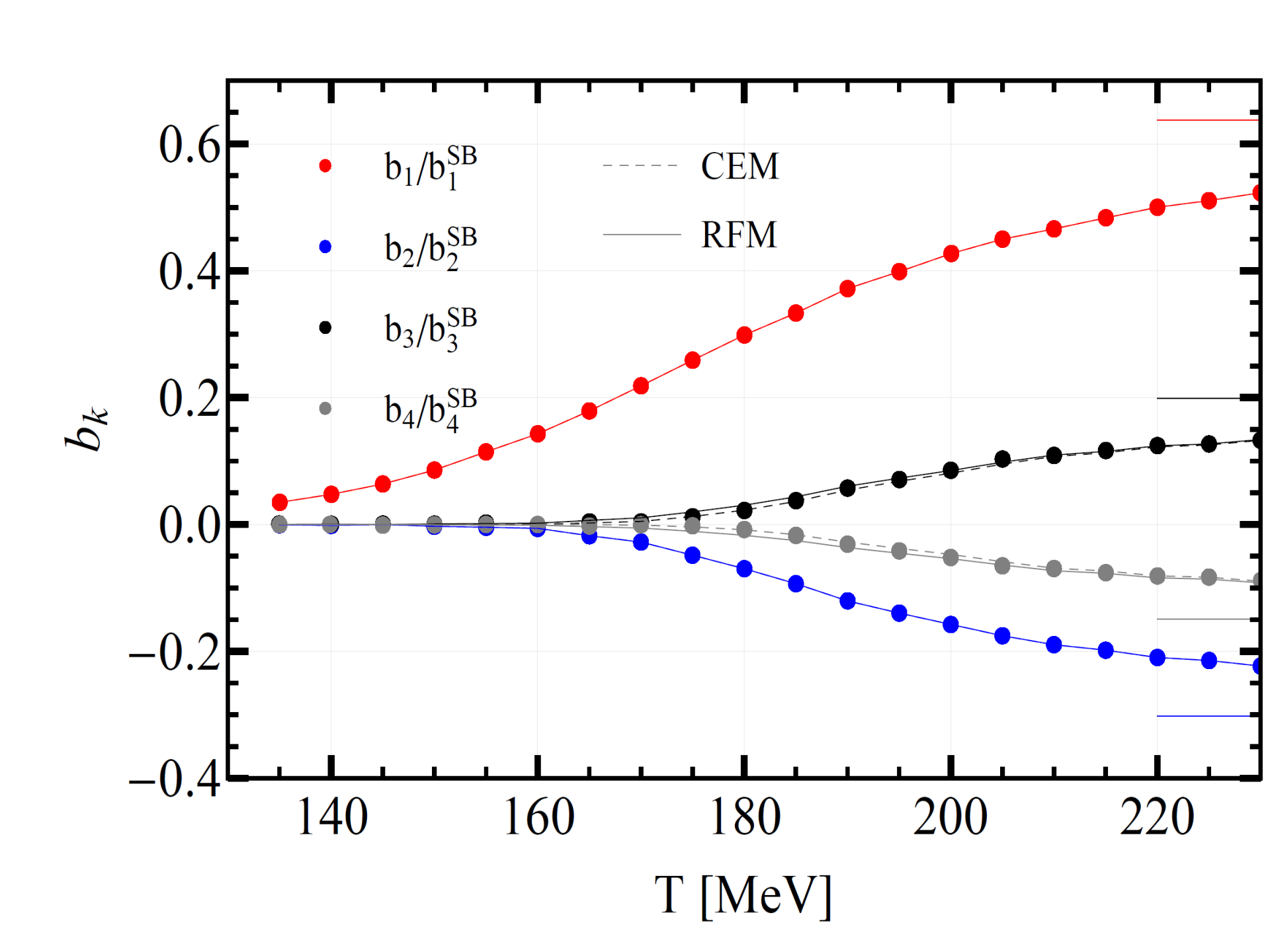
More generally, it is of interest to assess to which extent the modeling of Fourier coefficients is unique, when only the first two coefficients are provided as input. In order to illustrate these points, we introduce an alternative model for $b_k(T)$, which we dub the *Rational Fraction Model* (RFM)

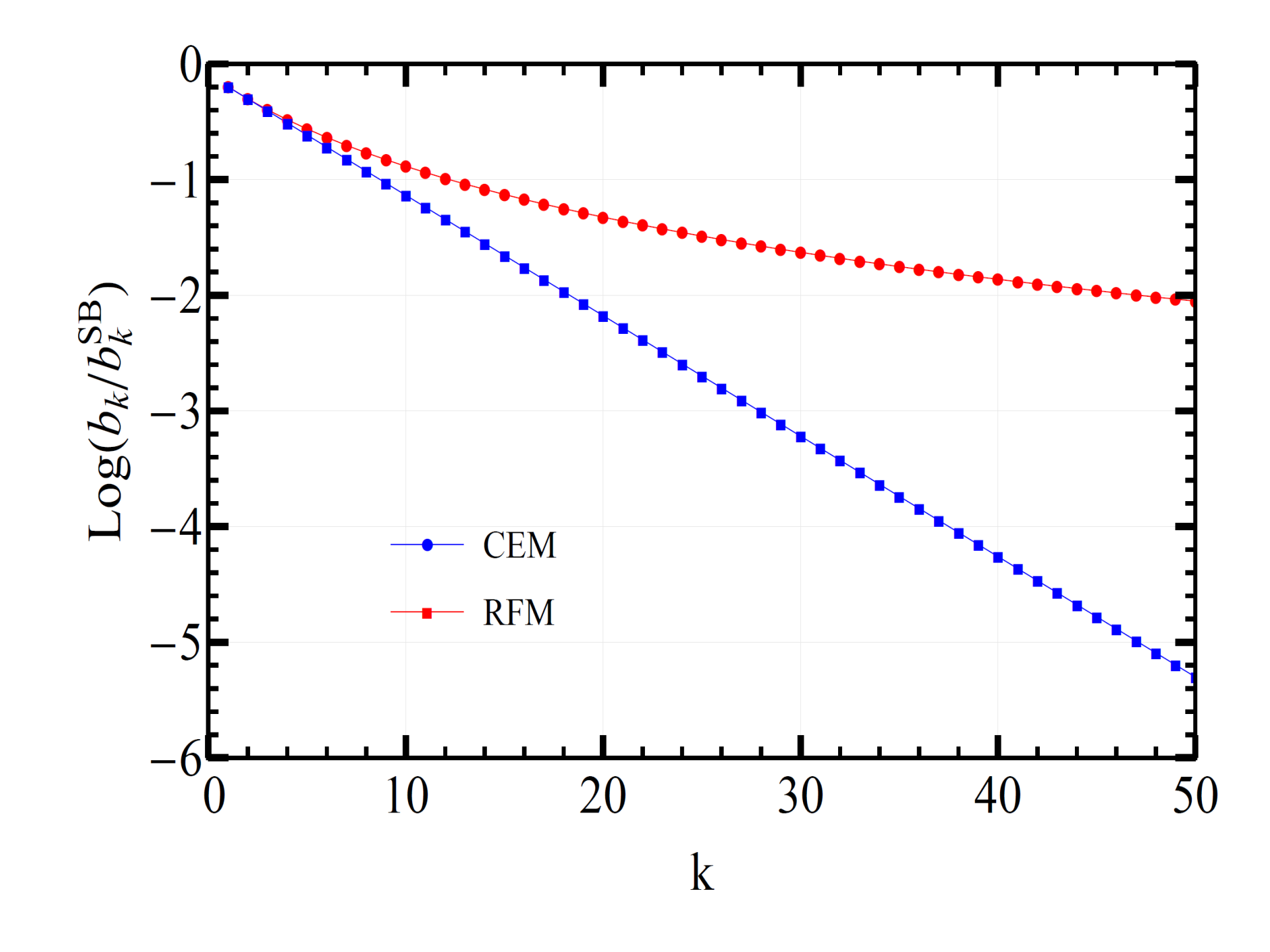
$$b_k^{\mathrm{RFM}}(T) = \frac{c(T)}{1 + k/k_0(T)} b_k^{SB}$$

with

$$k_0(T) = \left[\frac{b_1(T) b_2^{SB}}{b_2(T) b_1^{SB}} - 1 \right]^{-1} - 1,$$

$$c(T) = \frac{b_1(T)}{b_1^{SB}} \left(1 + \frac{1}{k_0(T)} \right).$$


0.6
0.4
0.2
0.0
−0.2
−0.4
b_k
b_1/b_1^{SB}
b_2/b_2^{SB}
b_3/b_3^{SB}
b_4/b_4^{SB}
CEM
RFM
140
160
180
200
220
T [MeV]


0
−1
−2
−3
−4
−5
−6
0
10
20
30
40
50
k
$\mathrm{Log}(b_k/b_k^{\mathrm{SB}})$
CEM
RFM

Conclusions

- CEM and RFM provide examples of modeling of the virial coefficients
- Lattice results are used as input and as check
- Would be good to find a model with CEP