Nf=2 lattice QCD at finite density using canonical ensemble method

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JINR, Dubna,
Hadronic matter under extreme conditions
31.10.16-03.11.16

Outline:

- Introduction
- Canonical approach
- Results
- Conclusions

Introduction

This work is completed by joint
FEFU - ITEP - IHEP lattice group

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Vladimir Goy, Alexander Nikolaev, Denis Boyda

FEFU lattice QCD group (http://188.162.234.56)

Main project: Study of the quark-gluon plasma using lattice QCD

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)

$N_f = 2$ lattice QCD with improved Wilson fermions and Iwasaki improved gauge field action

Our approach to finite density QCD: canonical ensemble approach

Main goal of the project:
Phase diagram of QCD at finite baryon density

QCD phase diagram

The lattice QCD numerical simulations can provide results from the first principle calculations.
For vanishing quark chemical potential $\mu = 0$, the phase structure was satisfactorily investigated.
It is very hard to study QCD at finite baryon density by lattice QCD methods
Infamous “sign problem’: the fermionic determinant at nonzero chemical potential, $\det \Delta(\mu)$, which appears in the path integral

$$Z_{GC}(\mu_q, T, V) = \int \mathcal{D}U (\det \Delta(\mu_q))^{N_f} e^{-S_G}. \quad (1)$$

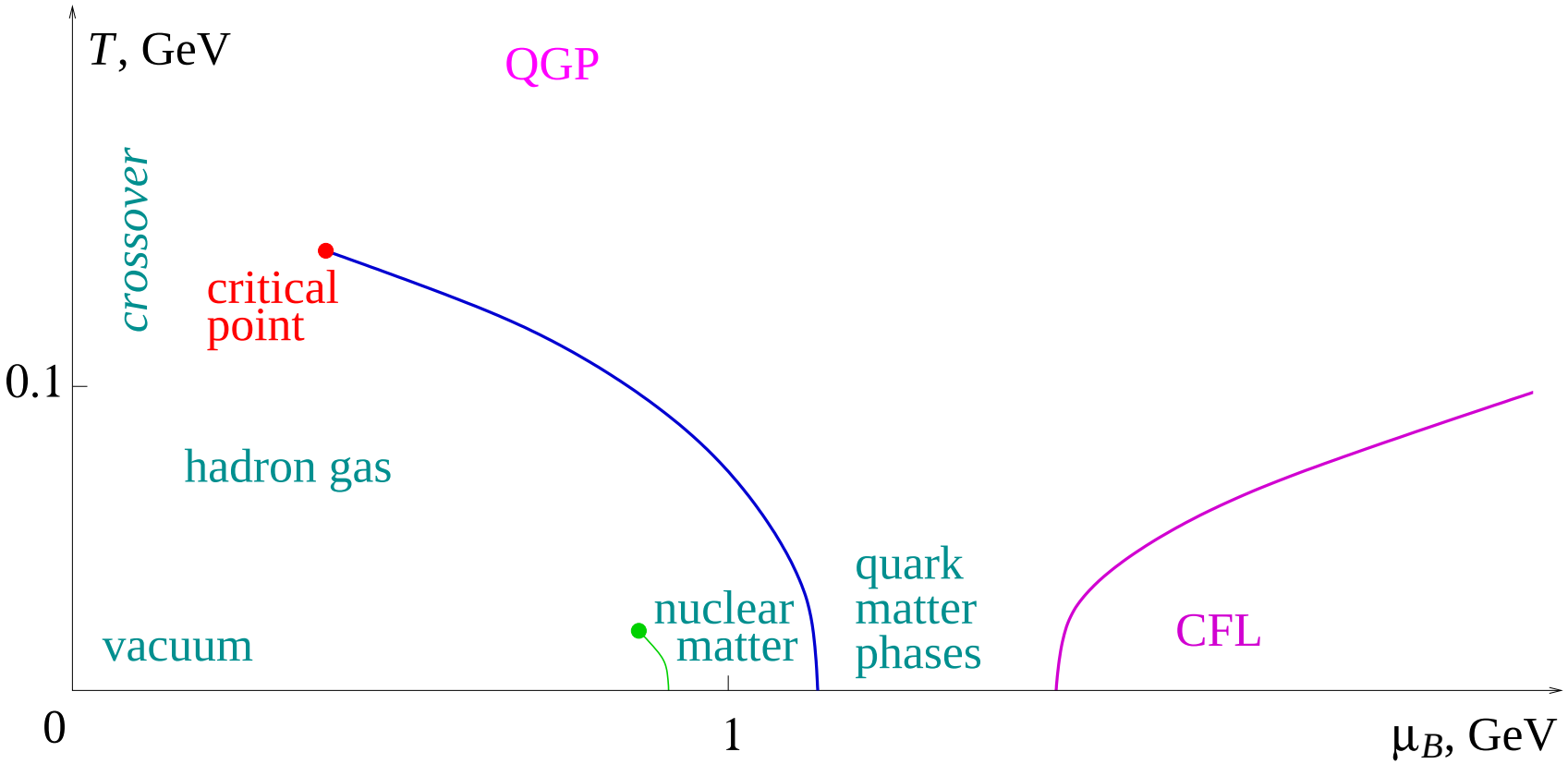
is in general not real
It cannot be included into the probability
Standard algorithms are not directly applicable

Numerical simulations of lattice QCD have convincingly shown that at $\mu = 0$ the transition is in fact a rapid crossover that takes place at temperatures around 160 MeV. For increasing μ the transition may

become a first-order phase transition, signaling the presence of a critical point on the QCD phase diagram.

This critical point is of great interest. The existence of a critical point would establish a remarkable universality link between QCD matter and condensed matter physics.

To reach the needed temperature and baryon density, two new facilities FAIR at GSI and NICA at JINR are being built.



Schematic QCD phase diagram.

Methods to solve sign problem:

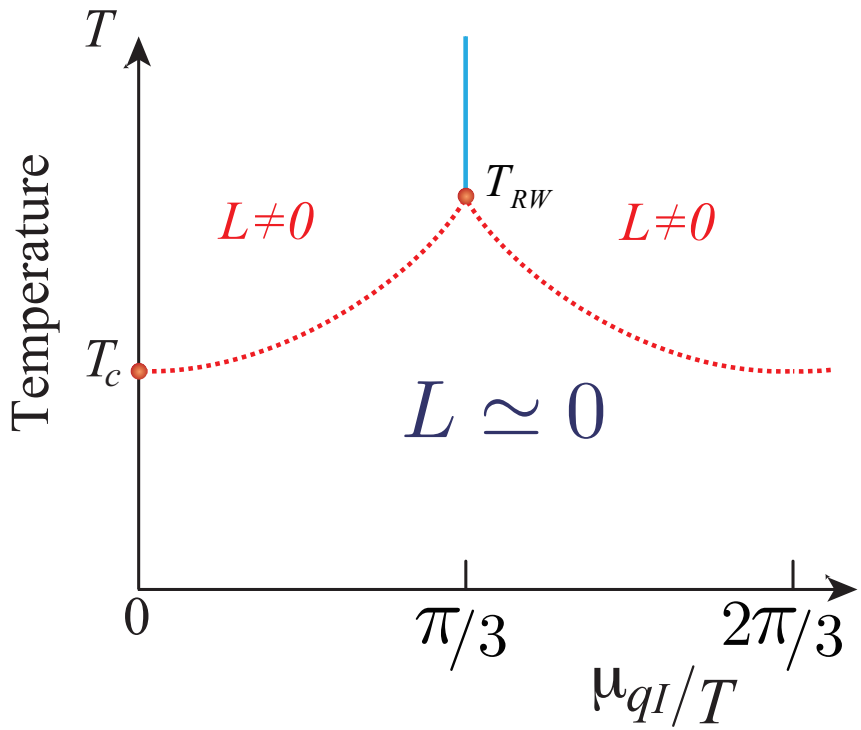
Multi-Parameter Reweighting	Z. Fodor, S. D. Katz, 2002
Taylor expansion	QCD-TARO Collaboration, 2002
Multi-Parameter Reweighting+Taylor Expansion	Bielefeld-Swansea, 2002
Imaginary Chemical Potential	DElia, Lombardo, 2002
canonical ensemble approach	de Forcrand, Philipseni, 2002

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?

Roberge,Weiss, 1986

QCD possesses rich phase structure at nonzero $\theta \equiv \mu_I/T$, which depends on the number of flavors N_f and the quark mass m_q

Study of QCD at nonzero θ can provide us with information about physical range: $\mu_q = 0$ and even about $\mu_q > 0$
- extrapolation to $\mu_q = 0$ or analytical continuation to nonzero real μ_q
- Canonical ensemble approach



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

$$Z_{GC}(\theta) = Z_{GC}(\theta + 2\pi/N_c) \tag{2}$$

1st order phase transitions at $\theta = (2k+1)\pi/3$ at $T > T_{RW}$
Roberge and Weiss, 1986

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 $Z_C(n, T, V)$

$$Z_{GC}(\mu_q, T, V) = \sum_{n=-\infty}^{\infty} Z_C(n, T, V)\xi^n, \tag{3}$$

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 $\mu_q/T = i\mu_I/T = i\theta$.
Standard Monte Carlo simulations are possible

Quark number density n_q defined by equation

$$\frac{n_q}{T^3} = \frac{1}{VT^2}\frac{\partial}{\partial \mu_q} \ln Z_{GC} \tag{5}$$

$$= \frac{N_f N_t^3}{N_s^3}\frac{1}{Z_{GC}} \int \mathcal{D}U e^{-S_G} (\det \Delta(\mu_q))^{N_f} \mathrm{tr}\left[\Delta^{-1}\frac{\partial \Delta}{\partial \mu_q / T}\right], \tag{6}$$

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 $Z_n = \frac{Z_C(n,T,V)}{Z_C(0,T,V)}$

$$\frac{n_{qI}}{T^3} = \frac{N_t^3}{N_s^3} \frac{\sum_n n Z_n \sin(n\theta)}{\sum_n Z_n \cos(n\theta)} \tag{7}$$

Our suggestion is to compute Z_n using this equation.

Using numerical data directly or fitted form of $n_{qI}(\theta)$ one can compute the grand canonical partition function by integration over imaginary chemical potential

$$P(\theta) \equiv \log \frac{Z_{GC}(\theta)}{Z_{GC}(0)} = -V \int_0^\theta d\tilde{\theta}\; n_{qI}(\tilde{\theta}). \tag{8}$$

Then Z_n can be computed

$$Z_n = \frac{\int_0^{2\pi} \frac{d\theta}{2\pi} e^{-in\theta} e^{P(\theta)}}{\int_0^{2\pi} \frac{d\theta}{2\pi} e^{P(\theta)}} \tag{9}$$

We obtained promising results for canonical partition functions Z_n.

We found most successful the following approach.
In the deconfining phase we fit the data for n_{ql} to a polynomial of θ

$$n_{ql}(\theta) = \sum_{n=1}^{n_{max}} a_n \theta^{2n-1} \tag{10}$$

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

$$n_{ql}(\theta) = \sum_{n=1}^{n_{max}} f_{3n} sin(3n\theta) \tag{11}$$

Similar fits were used in Takahashi et al, 2014
Gunther et al., 2016 arXiv:1607.02493

Simulation settings

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

To fix parameters (lattice spacing a, temperature T, quark mass m_q) we use $T = 0$ results of WHOT QCD collaboration

Currently quark mass is defined by ratio $m_\pi / m_\rho = 0.8$ ($m_\pi \approx 0.7$ GeV
Lattice size: $16^3 \times 4$
large lattice spacing: $a \approx 0.2$ fm
large volume: $L \approx 3.2$ fm
We simulate at imaginary chemical potential $\mu_q = i\mu_q^I$
At $T > T_c$ ($T/T_c = 1.08$; 1.35, 1.20)
at $T < T_c$ ($T/T_c = 0.84$; 0.93; 0.99)

Hopping parameter expansion

$$Z_{GC}(\mu_{qI}, T) = \int DU \det\Delta^{N_f}(\mu_q^0, U) \frac{\det\Delta^{N_f}(\mu_{qI}, U)}{\det\Delta^{N_f}(\mu_q^0, U)} e^{-S_G[U]}$$

It is not possible to calculate Z_{GC} itself but its ratio:

$$\frac{Z_{GC}(i\theta T, T)}{Z_{GC}(\mu_q^0, T)} = \left\langle \frac{\det \Delta^{N_f}(i\theta T, U)}{\det \Delta^{N_f}(\mu_q^0, U)} \right\rangle_{\mu_q^0}$$

$\mu_q^0 = 0$ or $\mu_q^0 = i\theta T$

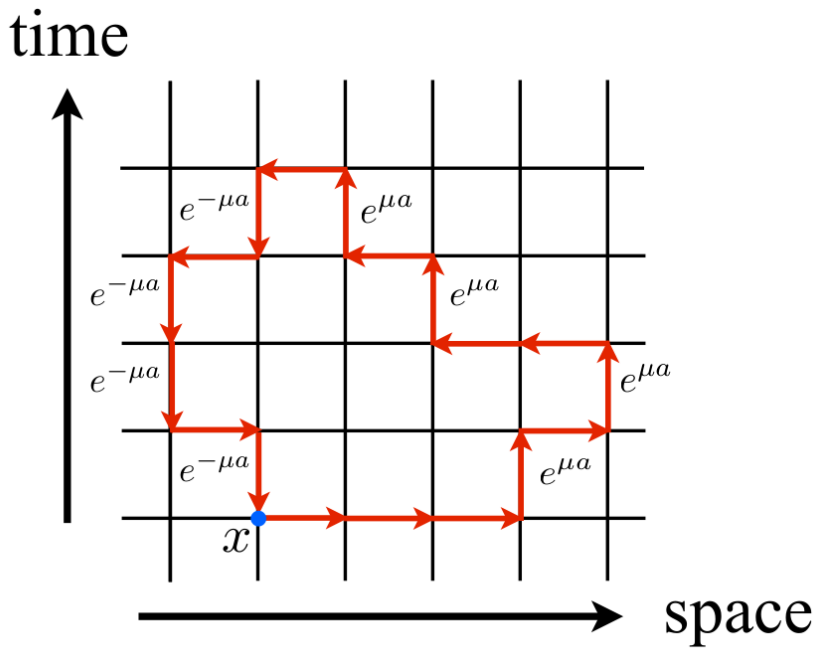
calculation of $\det \Delta(\mu_q, U)$ is required

We consider clover improved Wilson fermions:

$$\Delta(\mu_q) = I - \kappa \left[\sum_{i=1}^{3} \left(Q_i^+ + Q_i^- \right) + T \right] - \kappa e^{\mu_q a} Q_4^+ - \kappa e^{-\mu_q a} Q_4^-,$$

where

$$\begin{aligned} \kappa &= \frac{1}{2\left(ma+4\right)} \\ \left(Q_\mu^+\right)_{nm} &= \left(1-\gamma_\mu\right) U_{n,\mu} \delta_{m,n+\hat{\mu}} \\ \left(Q_\mu^-\right)_{nm} &= \left(1+\gamma_\mu\right) U_{m,\mu}^\dagger \delta_{m,n-\hat{\mu}} \\ T_{nm} &= \frac{1}{2} c_{SW} \sum_{\mu<\nu} \sigma_{\mu\nu} F_n^{\mu\nu} \delta_{nm} \end{aligned}$$



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

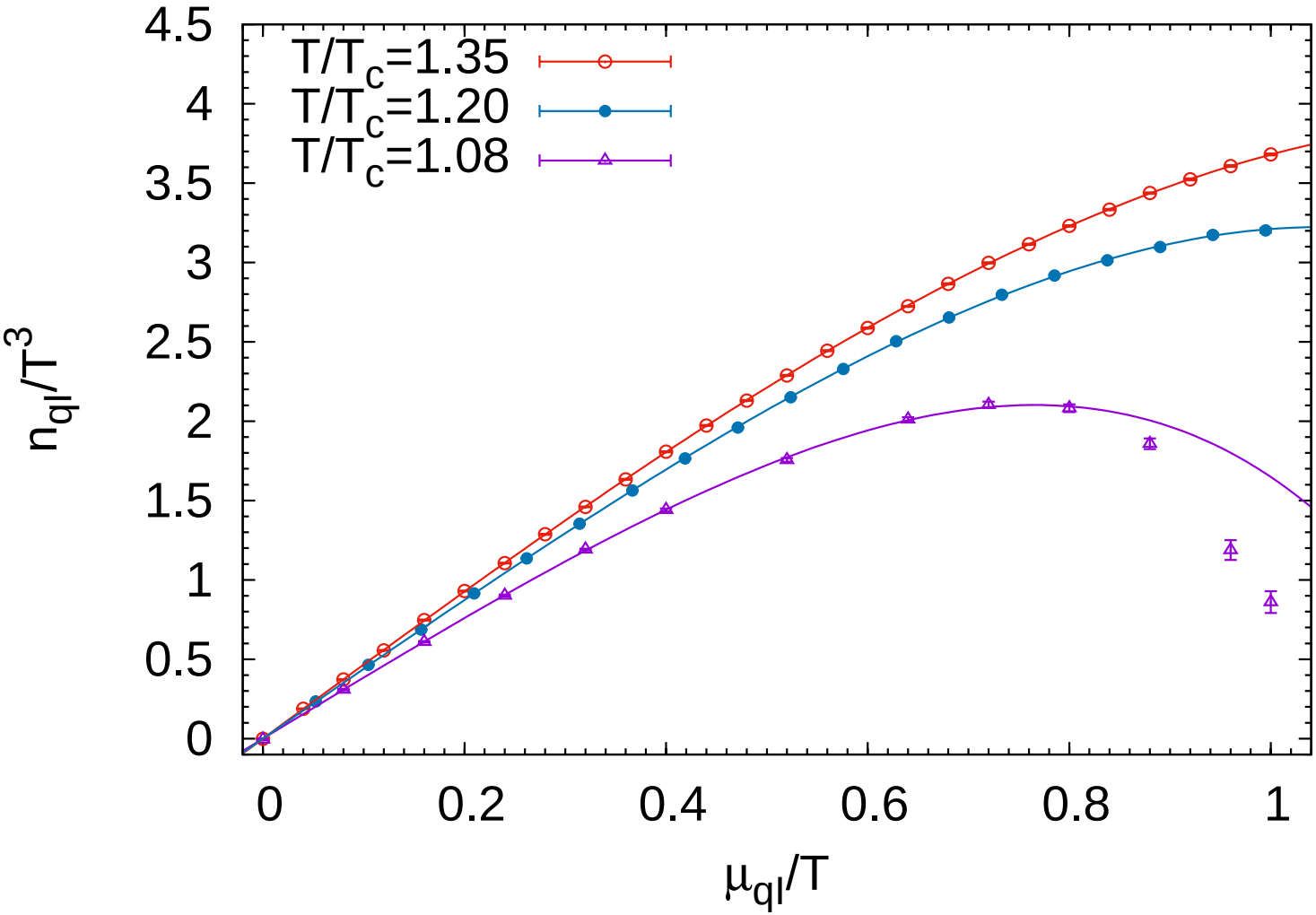
$$Tr\left[ln\,\Delta\right] = Tr\left[ln\left(I - \kappa Q\right)\right] = -\sum_{n=1}^{\infty} \frac{\kappa^n}{n} Tr\left[Q^n\right] = \sum_{n=-\infty}^{\infty} W_n \left(e^{\mu_B a N_\tau}\right)^n$$

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

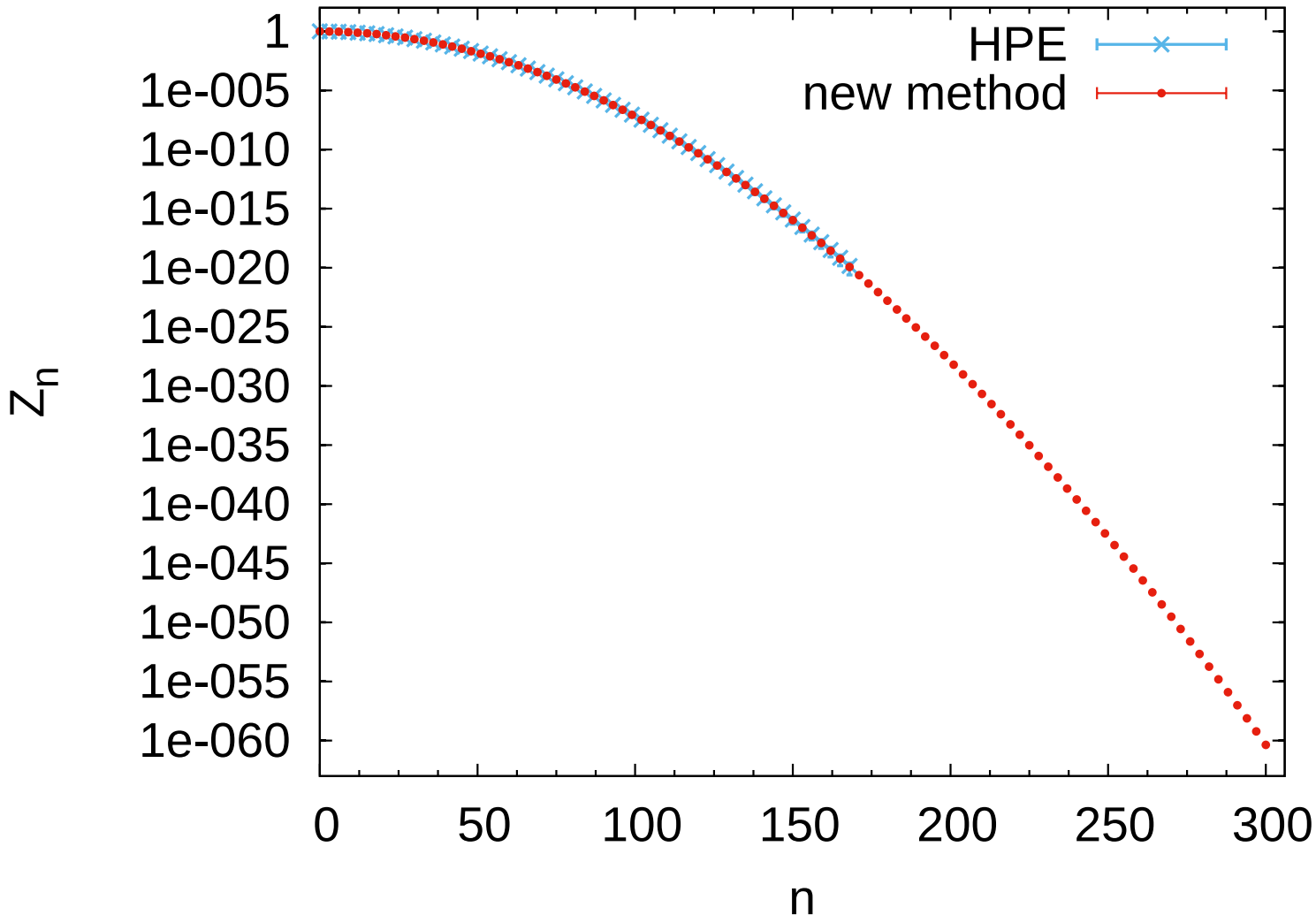
$W_n[U]$ may be calculated using stochastic estimators for $Tr\left[Q^n\right]$.

$$\det \Delta(U) = \sum_{n=-2N_x N_y N_z N_c}^{2N_x N_y N_z N_c} z_n[U]\xi^n$$

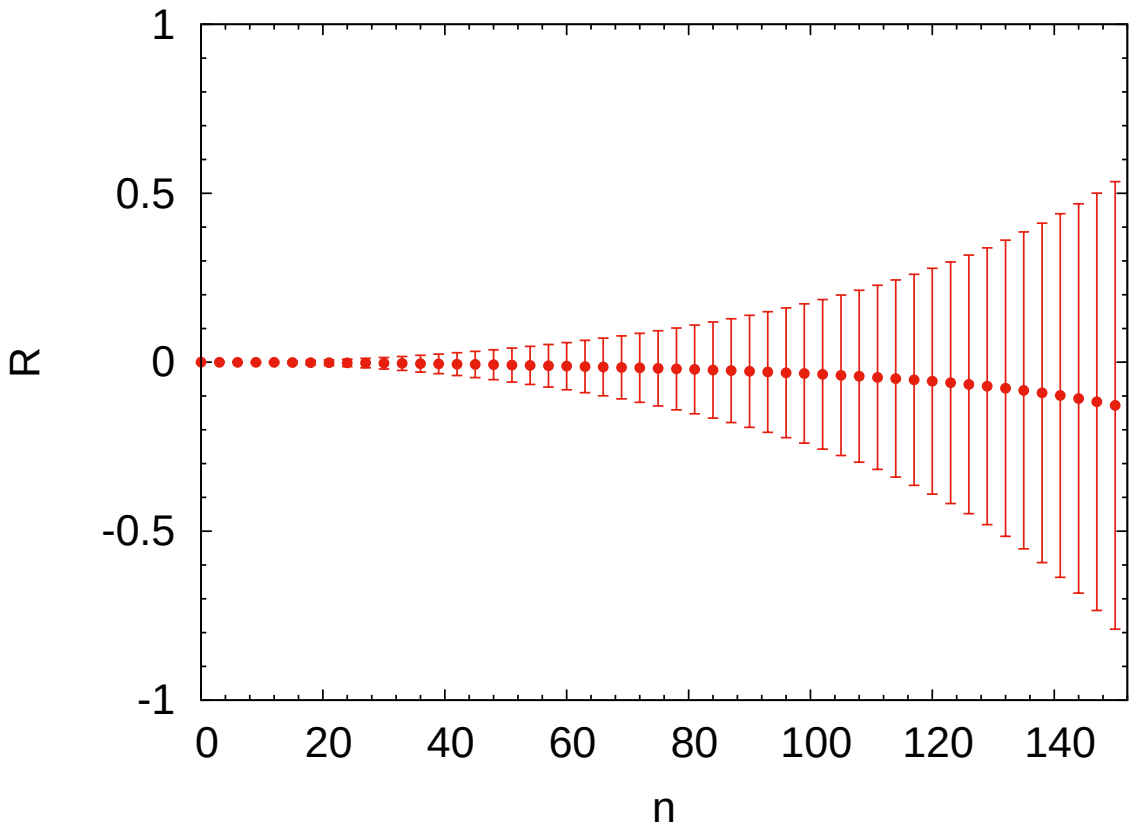
Results



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



Two methods show nice agreement.



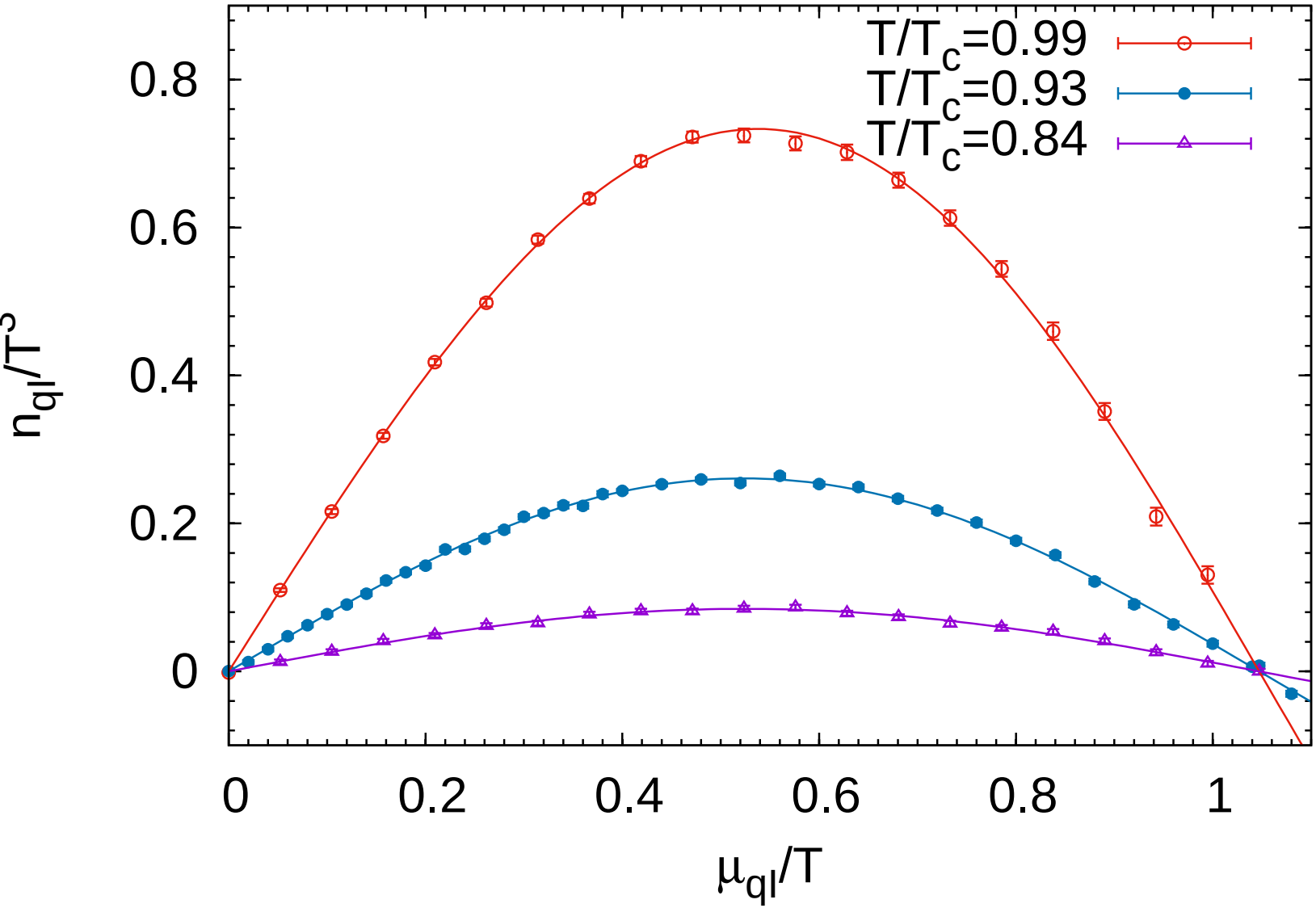
Relative deviation of results for Z_n obtained by two methods at $T/T_c = 1.35$

T/T_c	a_1	a_3	a_5	χ^2/N_{dof}	$2c_2$	$4c_4$
1.35	4.671(2)	-0.991(4)	-	0.67	4.68(1)	0.97(8)
1.20	4.409(6)	-1.03(3)	-0.17(3)	0.70	4.40(1)	1.3(1)
1.08	3.86(2)	-1.46(16)	-0.75(25)	0.91	3.88(2)	1.3(2)

Results of fitting of n_{ql}/T^3 in the deconfinement phase.

Comparison with Taylor expansion Ejiri et al., 2010

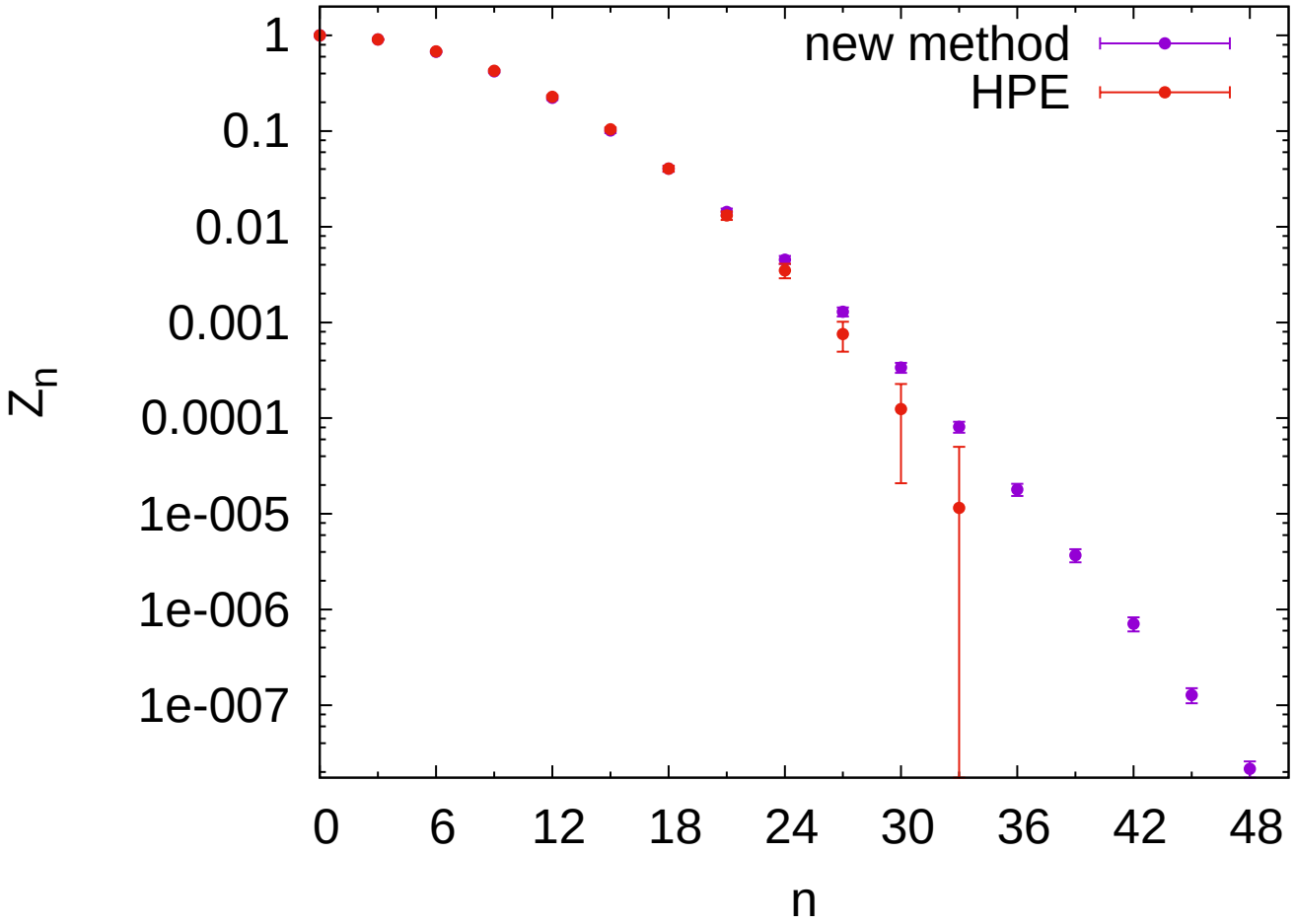
note, $a_1 = 2c_2; a_3 = -4c_4$


T/T_c=0.99
T/T_c=0.93
T/T_c=0.84
n_ql/T^3
μ_ql/T
0
0.2
0.4
0.6
0.8
1

Integral for Z_n can be computed exactly:

$$Z_{3n} = \frac{I_n(f_3 N_s^3/3)}{I_0(f_3 N_s^3/3)} \tag{12}$$

where $I_n(x)$ is the modified Bessel function of the 1st kind.



Agreement is not as good as in the deconfinement phase.
Reasons: insufficient statistics, overlap problem for the hopping parameter expansion method

T/T_c	f_3	f_6	$\chi^2/N_{dof}, N_{dof}$
0.99	0.7326(25)	-0.0159(21)	0.83, 18
0.93	0.2608(8)	-	0.93, 37
0.84	0.0844(7)	-	0.41, 18

Results of fitting data for n_{ql}/T^3 in the confinement phase

T/T_c	a_1	a_3	a_5	χ^2/N_{dof}	$2c_2$	$4c_4$
0.99	2.10(1)	-2.72(2)	0.45(6)	0.83	2.07(3)	2.90(8)
0.93	0.782(3)	-1.174(4)	0.528(2)	0.93	0.71(4)	0.33(5)
0.84	0.253(2)	-0.380(3)	0.171(2)	0.41	0.25(4)	0.0(37)

Taylor coefficients in the confinement phase.

We can get an asymptotics for Z_n at large n:

$$Z_{3n} = Ce^{-n\log(n)}. \tag{13}$$

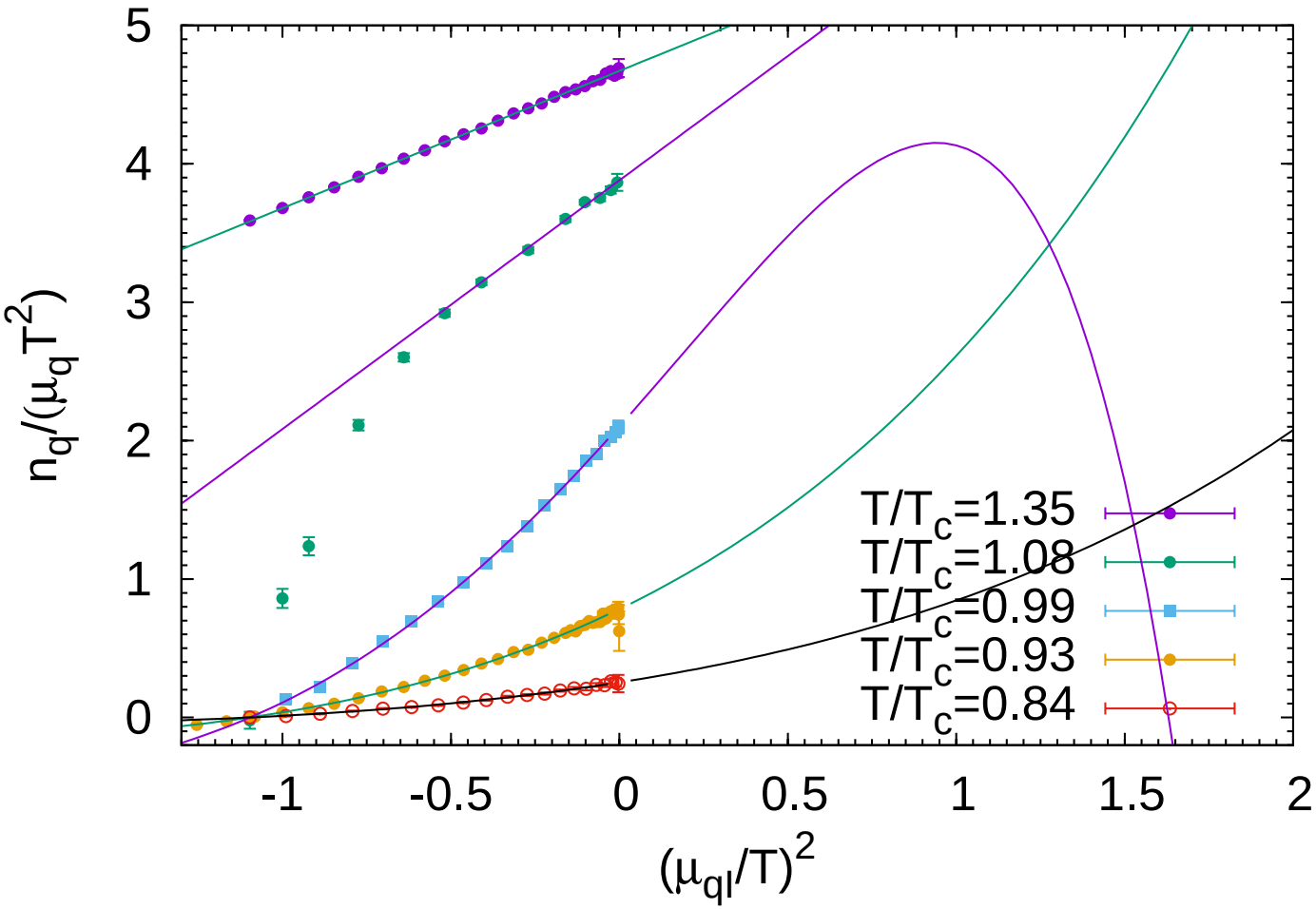
where C is some constant.
Recursion relation can be obtained for more general case with N terms in the fitting function:

$$f_3 sin(3\theta) + ... + f_{3N} sin(3N\theta) \tag{14}$$

Thus computation of Z_n is simplified

Asymptotics in this case can be derived

$$Z_{3n} = Ce^{-(n/N)\log(n)}. \tag{15}$$



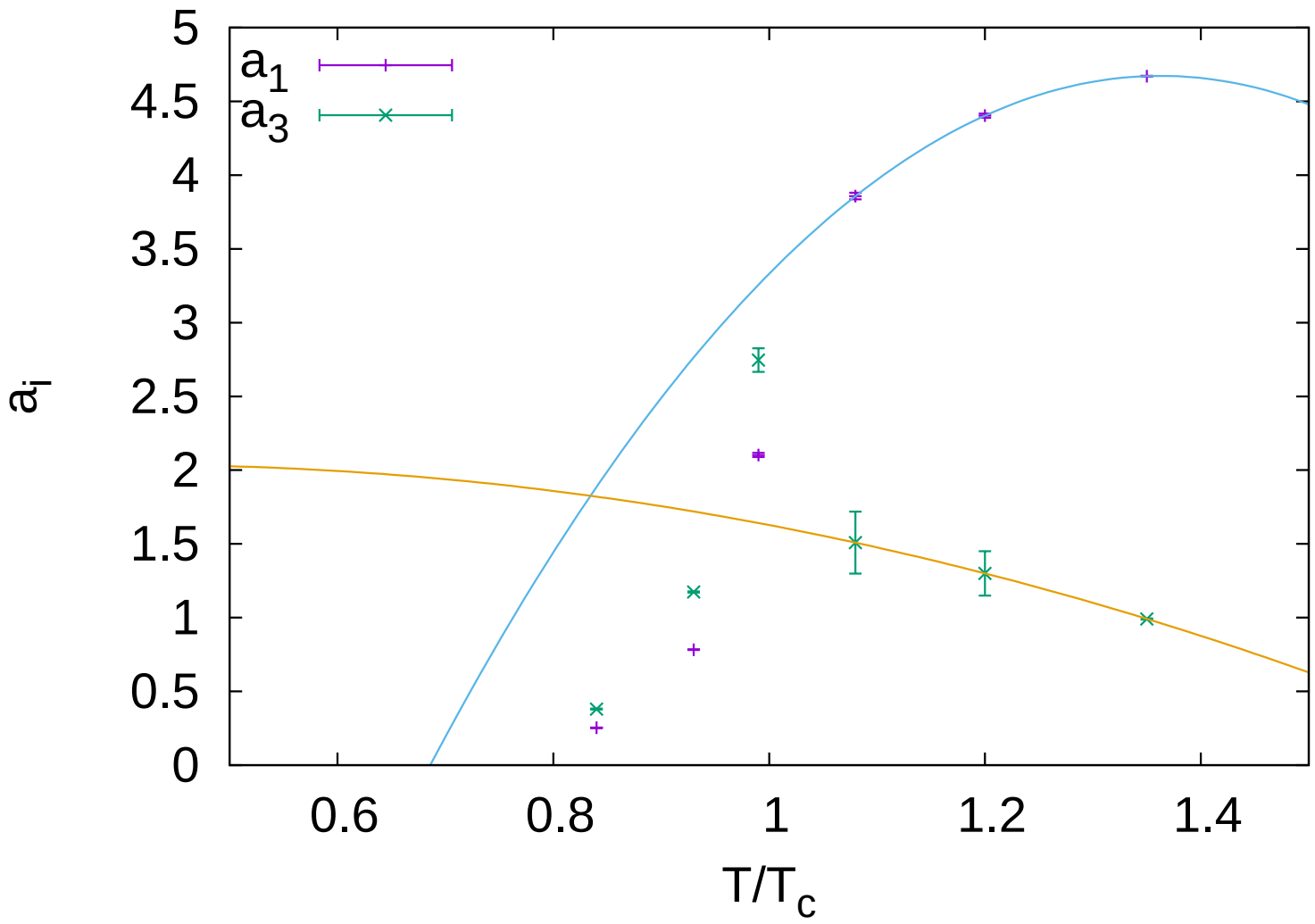
Analytical continuation for the number density.

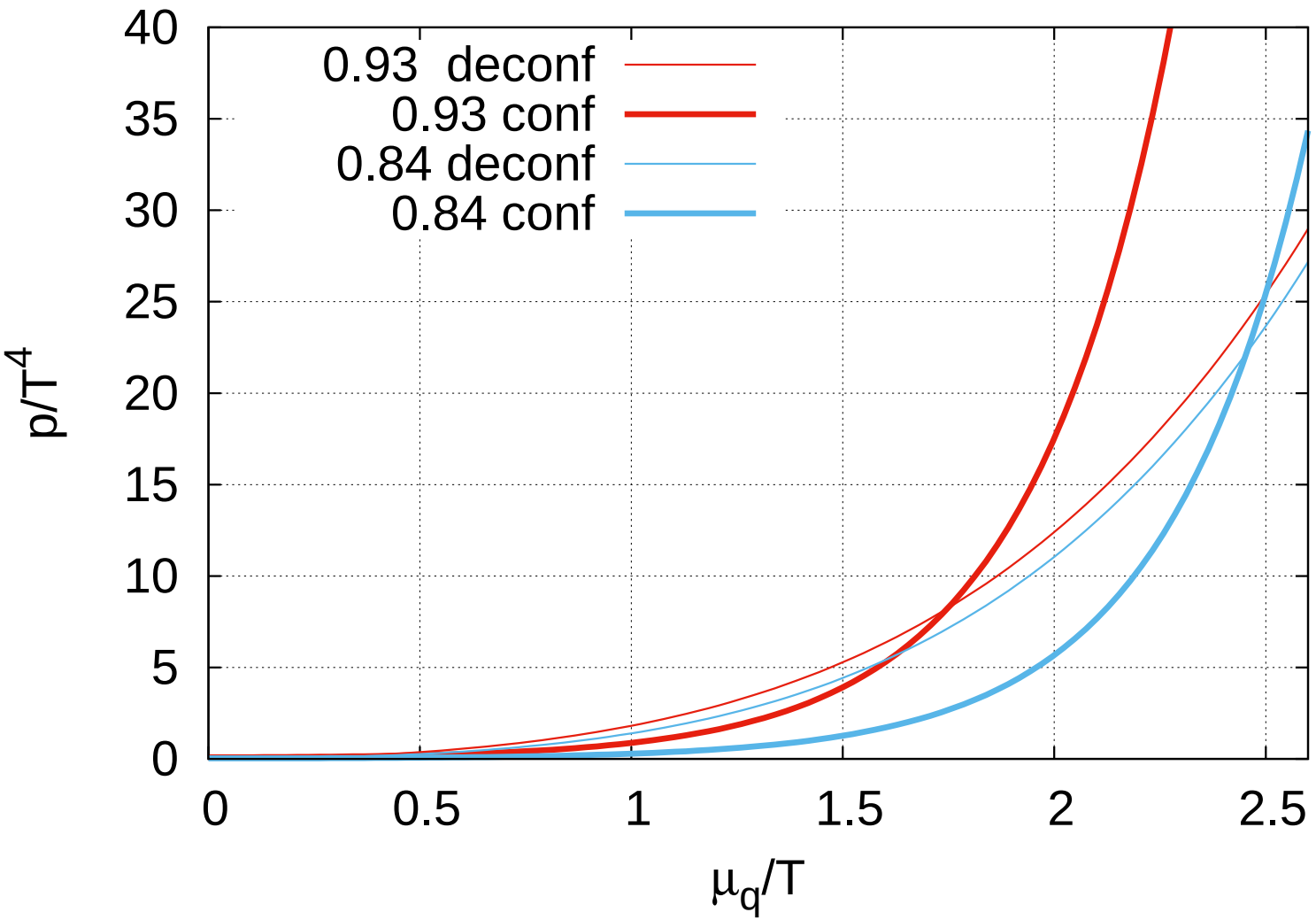
Conclusions

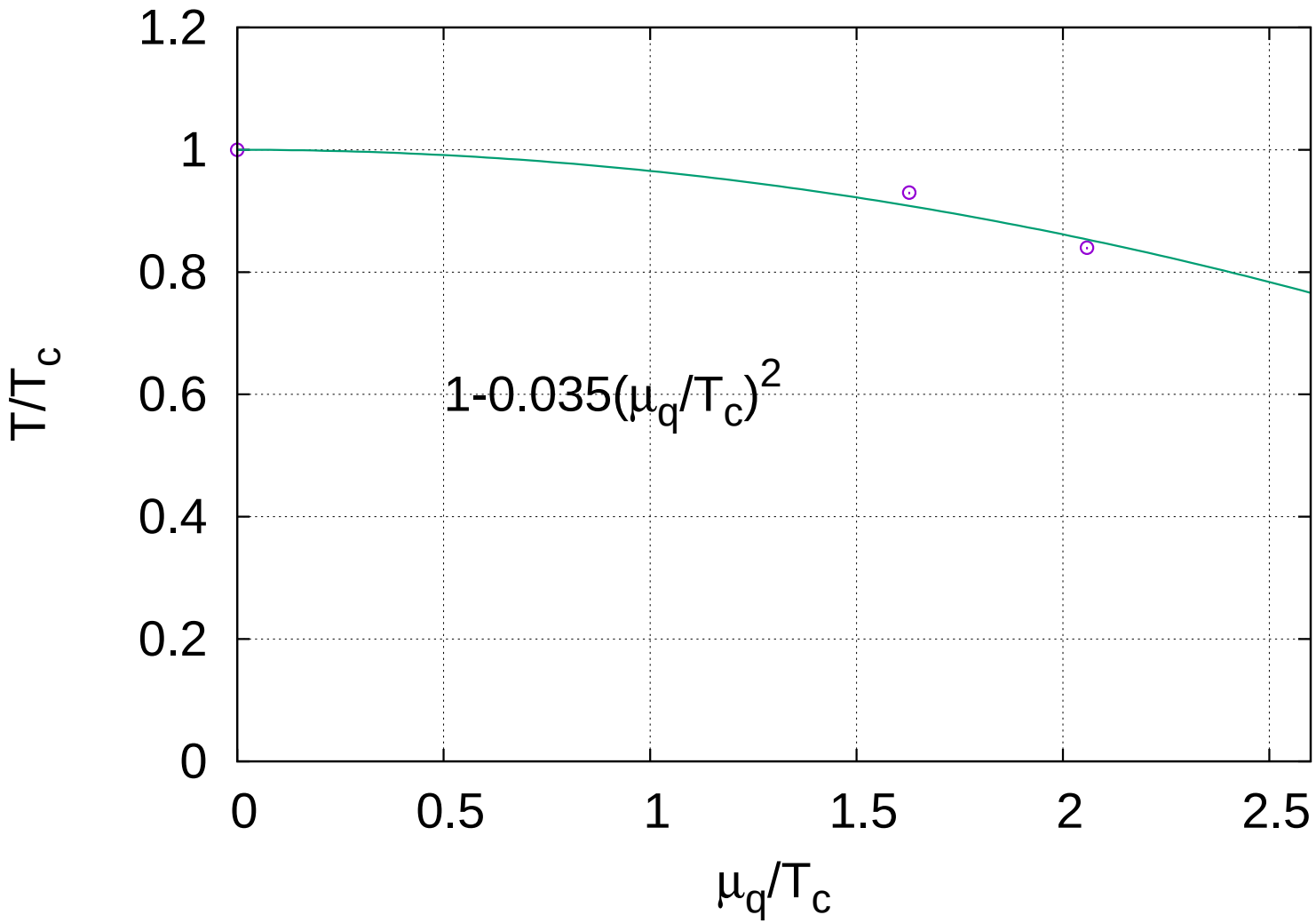
- new approach to compute Z_n has been tested
- coefficients of Taylor expansion agree with direct computation, smaller errors
- in the deconfining phase our results are in nice agreement with hopping parameter expansion
- in the confining phase agreement is not so good but there is hope for improvement
- 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

Future developments:

- to apply the method to smaller quark masses
- to understand the limits of validity over μ
- to solve the problem for $T_c < T < T_{RW}$


a_1
a_3
a_i
T/T_c
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
0.6
0.8
1
1.2
1.4


0.93 deconf
0.93 conf
0.84 deconf
0.84 conf
p/T^4
μ_q/T
0
5
10
15
20
25
30
35
40
0
0.5
1
1.5
2
2.5


1.2
1
0.8
0.6
0.4
0.2
0
T/T_c
1-0.035(μ_q/T_c)^2
0
0.5
1
1.5
2
2.5
μ_q/T_c