Canonical partition functions, virial expansion and the critical point(s) of QCD

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Series expansions are useful tools to study the phase diagram in the region which is not directly accessible to MonteCarlo simulations due to the sign problem.

Typical parameters for the expansion are the the chemical potential μ and the fugacity $e^{\mu/T}$, while the observables to be expanded include the Grand Canonical Partition Function or the associated thermodynamic quantities, derivatives of the GCPF [1].

Which choice is most convenient depends on the thermodynamic region [2]: at high temperatures the pressure in the massless limit is a closed polynomial, hence Taylor expansion of any observable should work well. Deep in the hadronic phase the GCPF is well approximated by a simple trigonometric form, which suggests to use a virial expansion for the thermodynamics. Moreover, Cluster Model Expansions provide a phenomenological guidance for the value of coefficients, which constrain the position of the hypothesized critical point of QCD [3].

Series for thermodynamic quantities are limited by the position of the singularities, if any. This property has been exploited for instance in the search of a critical point by use of the Taylor expansion. On the other hand, series for the GCPF do not have this limitation: GCPF has zeros, not critical points!

Recently a strategy has been proposed which begins from the virial expansion at imaginary chemical potential - with a limited radius of convergence - and reconstruct the canonical partition functions, hence the GCPF, which is valid everywhere [4]. In this note we show how this is realized in a simple model. Further, we present preliminary results from realistic simulations of QCD where higher order virial coefficients determine the radius of convergence, and contrast the results with the predictions of the Cluster Expansion.

A simple model : QCD in 1d

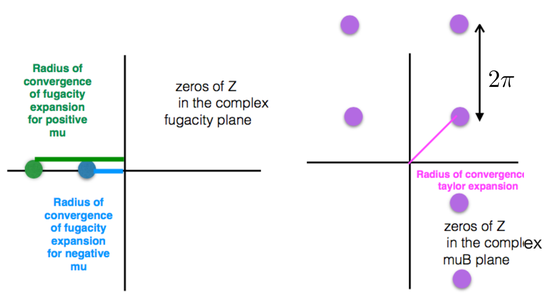
One dimensional QCD is a an interesting, exactly solvable model. There is no spontaneous symmetry breaking, but there are baryons. Its partition function is formally the same as the one obtained in 4d QCD at strong coupling, once an explicit mass term is identified with the 4d dynamically generated mass. For any temperature T and varying μ there is a crossover to a baryon rich phase, which turns into a first order transition at zero temperature.
The partition function reads

$$\mathcal{Z}(\mu,T) = 2\cosh(\mu/T) + \sinh(4m'/T)/\sinh(m'/T) = \sum_{n=-1,0,1} A_n \xi^n$$

$A_0 = \sinh(4m'/T)/\sinh(m'/T) \equiv A, A_1 = A_{-1} = 1$, μ is understood to be μ_B, $m' = sh^{-1}m$, with m the quark mass.

Virial expansion, zeros of the GCPF and radius of convergence

The zeros for the GCPF determine the radius of convergence of the expansion of $n(\mu) = \frac{\partial \log Z}{V \partial \mu}$



$4 < A < \infty \rightarrow y_1 = 1/y_2$ are two negative real roots.

$\Re e^{\mu/T} = (-A + / - \sqrt{A^2-4})/2 \equiv y_{1/2}$

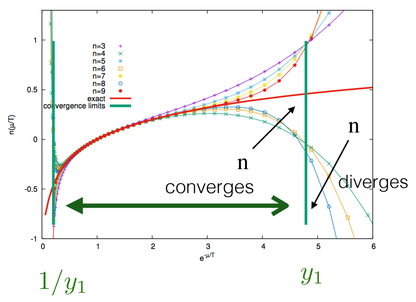
$\mu = \pm T(log|y_1|) + i(2k+1)T\pi.$

The fugacity series converges for:

$1/y_1 < e^{\mu/T} < y_1,$

Setting A=5.
$y_{1/2} = -4.79, -0.208.$

Virial expansion for $n(\mu)$



$1/y_1$ y_1

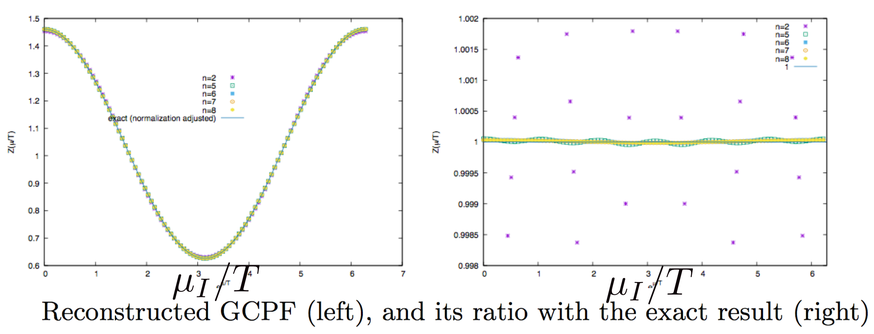
$$n^n(\mu) = \sum_1^n a_k \sinh(\mu/Tk)$$

The virial-like expansion is the typical outcome of analytic continuation from imaginary μ and its radius of convergence depends on the zeros of the GCPF in complex fugacity

The GCPF in QCD 1d beyond the radius of convergence

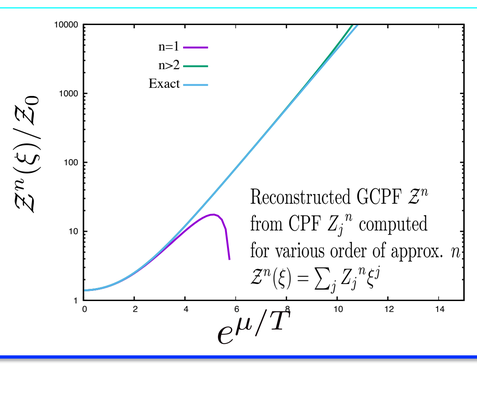
First, for μ_I

$\mathcal{Z}^n(\mu_I/T) = e^{-\int_0^{\mu_I/T} n^n(x)dx}$



Reconstructed GCPF (left), and its ratio with the exact result (right)

Then, for μ



Comments on QCD1d:

- The radius of convergence can be read off the virial coefficients
- A negative Zn may appear and signals an insufficient order of the virial expansion.
- The fugacity series is a double series with two radii of convergence
- The GCPF can be reconstructed beyond the radius of convergence

Beating the Sign problem by Canonical Approach (Hasenfraz-Toussant,1992)

Calculation in pure μ_I regions, where no sign problem.

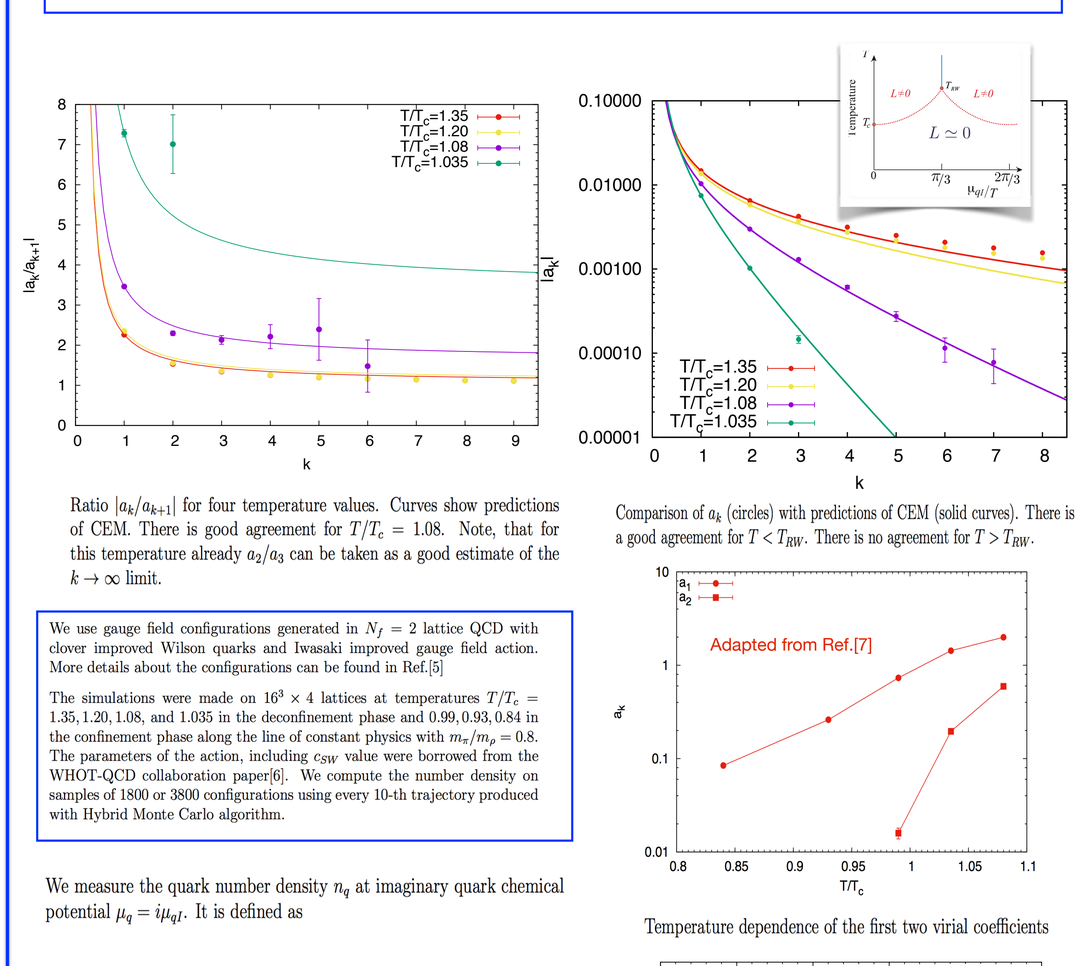
$$Z_n = \int \frac{d\theta}{2\pi} e^{in\theta} Z(T, \theta \equiv \frac{Im\,\mu}{T})$$

Then calculate Z in real μ regions.

$$Z(\xi, T) = \sum_n Z_n(T)\,\xi^n$$

$\xi \equiv e^{\mu/T}$

QCD - preliminary results . Virial expansion, radius of convergence, CEM



Ratio $|a_k/a_{k+1}|$ for four temperature values. Curves show predictions of CEM. There is good agreement for $T/T_c = 1.08$. Note, that for this temperature already a_2/a_3 can be taken as a good estimate of the $k \to \infty$ limit.

Comparison of a_k (circles) with predictions of CEM (solid curves). There is a good agreement for $T < T_{RW}$. There is no agreement for $T > T_{RW}$.

We use gauge field configurations generated in $N_f = 2$ lattice QCD with clover improved Wilson quarks and Iwasaki improved gauge field action. More details about the configurations can be found in Ref.[5]

The simulations were made on $16^3 \times 4$ lattices at temperatures $T/T_c = 1.35, 1.20, 1.08$, and 1.035 in the deconfinement phase and $0.99, 0.93, 0.84$ in the confinement phase along the line of constant physics with $m_\pi/m_\rho = 0.8$. The parameters of the action, including c_{SW} value were borrowed from the WHOT-QCD collaboration paper[6]. We compute the number density on samples of 1800 or 3800 configurations using every 10-th trajectory produced with Hybrid Monte Carlo algorithm.

Temperature dependence of the first two virial coefficients

We measure the quark number density n_q at imaginary quark chemical potential $\mu_q = i\mu_{qI}$. It is defined as

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

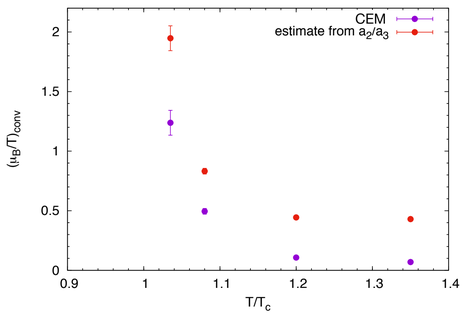
We then fitted the number density to functions

$$n_{qI}(\theta)/T^3 = \sum_{k=1}^{k_{max}} a_k \sin(3k\theta)$$

for $T < T_{RW}$ and

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

for $T > T_{RW}$ ($\theta = \mu_{qI}/T$). In this case we used Fourier transform to compute the virial coefficients a_k.



Radius of convergence of the virial expansion $(\mu_B/T)_{conv}$ computed using CEM and estimated from the ratio a_2/a_3.

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