QC_2D as a Probe of the Analytic Continuation Methods

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Our goal:

To find the best parametrization of the quark density
for its analytical continuation
from imaginary to real quark chemical potential

Outline

1. Simulation settings
2. Analytical continuation of the quark density
3. Cluster Expansion Model (CEM) vs Rational Fraction Model (RFM)
4. Problem of negative probabilities and Lee-Yang zeroes
5. Lee-Yang zeroes and the Roberge-Weiss transition
6. Conclusions

Parameters of simulation

- Tree-level inproved Symanzik gauge action
- Staggered fermions

Sommer parameter $r_0 = 0.468\text{fm}$
Lattice spacing $a \approx 0.062$ fm
Lattice size $L \approx 1.74$ fm
$am_q = 0.0125$; $m_\pi \approx 800$ MeV

$N_c = 2, \quad N_f = 2$
$N_s^3 \times N_t$ lattices: $N_s = 28$;
$N_t = 20, 14, \quad 12$
$T = 159, 227, \; 265$ MeV

$$\theta = \frac{\mu_q}{T} = \frac{\mu_q' + \imath\mu_q''}{T} = \theta_R + \imath\theta_I$$

$$0 \le \theta_I \le \frac{\pi}{N_c}, \qquad 0 < \mu_q' < 600 \text{ MeV}$$

$$S_G = \beta\left(1.667\sum_{\square}\left(1-\frac{1}{2}\mathrm{Tr}\,\square\right) - 0.083\sum_{\square\square}\left(1-\frac{1}{2}\mathrm{Tr}\,\square\square\right)\right) \quad (1)$$

$$S_F = \sum_{x,y}\bar{\psi}_x D(\mu_q)_{x,y}\psi_y + \frac{\lambda}{2}\sum_x\left(\psi_x^T\tau_2\psi_x + \bar{\psi}_x\tau_2\bar{\psi}_x^T\right) \quad (2)$$

where $\bar{\psi}$, ψ are staggered fermion fields,

$$\begin{aligned} D(\mu_q)_{xy} &= ma\delta_{xy} + \frac{1}{2}\sum_{\nu=1}^{4}\eta_\nu(x)\Big[U_{x,\nu}\delta_{x+h_\nu,y}e^{\mu_q a\delta_{\nu,4}} \\ &\quad -U^\dagger_{x-h_\nu,\nu}\delta_{x-h_\nu,y}e^{-\mu_q a\delta_{\nu,4}}\Big], \end{aligned} \quad (3)$$

$\eta_1(x) = 1$, $\eta_\nu(x) = (-1)^{x_1+\ldots+x_{\nu-1}}$, $\nu = 2, 3, 4.$

$$\text{We use } B = \frac{n_q V}{N_c} \text{ instead of } n_q$$

B is the baryon number in the lattice volume,

$$\begin{aligned} B(\theta) &= \frac{1}{N_c} \frac{\partial \ \ln Z_{GC}(\theta)}{\partial \theta} \\ &= \frac{N_f}{4 N_c Z_{GC}} \int \mathcal{D}U e^{-S_G} (\det M)^{N_f/4} \mathrm{tr} \left[M^{-1} \frac{\partial M}{\partial \theta} \right] , \end{aligned}$$

where $M = Q^\dagger(\mu_q) Q(\mu_q) + (ma)^2$, $Q = D_{oe}$ and

$$Z_{GC}(\theta) = \int \mathcal{D}U e^{-S_G} (\det M)^{N_f/4} \tag{4}$$

is the Grand Canonical (GC) partition function.

Properties of the grand canonical partition function

$$Z_{GC}(\theta, T, V) = \sum_n \langle n| \exp\left(\frac{-\hat{H} + \mu\hat{Q}}{T}\right)|n\rangle \qquad (5)$$

meets the fugacity expansion, that is the Laurent series in $\xi = e^\theta$:

$$Z_{GC}(\theta, T, V) = \sum_{k=-\infty}^{\infty} Z_C(kN_c, T, V)e^{kN_c\theta}, \qquad (6)$$

it involves powers of ξ^{N_c} owing to the Roberge-Weiss symmetry

$$Z_{GC}(\theta_I, T, V) = Z_{GC}(\theta_I + 2\pi/N_c, T, V)\ , \qquad (7)$$

C−parity $\implies$ $Z_{GC}(\theta_I, T, V) = Z_{GC}(-\theta_I, T, V)$

- Problem:
  The baryon number $B(\theta)$ cannot be determined in lattice QCD at $\theta = \theta_R$ because of the sign problem.
- Solution:
  Find it at $\theta = \imath\theta_I$ and then employ analytical continuation in θ
- Problem in this way:
  Analytical continuation in θ depends on parametrization of $B(\theta)$
- Proposed solution:
  Test different parametrizations in the case of QC_2D, where $B(\theta)$ can be simulated at both $\theta = \theta_R$ and $\theta = \imath\theta_I$

Naive analytic continuation

Assuming that

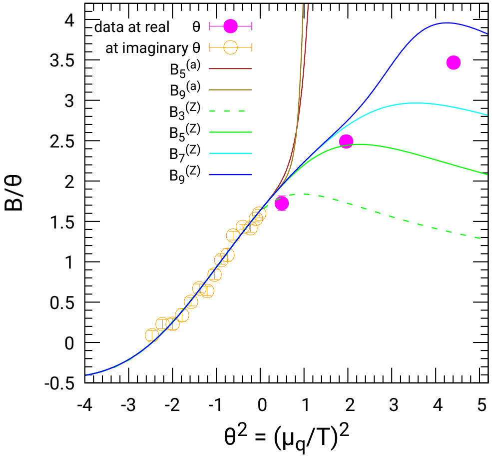
$$B(\theta)\Big|_{\theta_R=0} = \imath \sum_{n=1}^{\infty} a_n \sin\left(nN_c\theta_I\right), \qquad (8)$$

we arrive at

$$B(\theta)\Big|_{\theta_I=0} = \sum_{n=1}^{\infty} a_n \sinh\left(nN_c\theta_R\right) \qquad (9)$$

Limitatons:

- a_n are extracted from a fit over the segment $0 \le \theta_I \le \dfrac{\pi}{N_c}$
  $\Longrightarrow$ only a few of a_n can be determined.
- Series (9) converges only if $\lim\limits_{n\to\infty} \dfrac{|a_{n+1}|}{|a_n|} = r$ exists
  and $|\theta_R| < \dfrac{-\ln r}{N_c}$



$T = 227$ MeV

$$B_J^{(a)} = \frac{2\sum_{n=1}^{J} nZ_n \sin(nN_c\theta_I)}{1 + 2\sum_{n=1}^{J} Z_n \cos(nN_c\theta_I)}$$

Rational Fraction Model (RFM)

[G. A. Almasi, B. Friman, K. Morita, P. M. Lo, and K. Redlich 2019]

$$B(\theta_I)\Big|_{\theta_R=0} = \sum_{k=1}^{\infty} a_k^{\mathrm{RFM}} \sin\left(kN_c\theta_I\right) \tag{10}$$

$$a_n^{\mathrm{RFM}} = (-1)^{n+1}\, d\, \frac{1+\frac{\pi^2(N_c^2-1)}{6}n^2}{n^3(1+n\kappa)}\,. \tag{11}$$

$a_n^{\mathrm{RFM}} \sim \dfrac{(-1)^k}{k^2}$ as $k\to\infty \implies$ nonanalytic behavior:

$$B(\theta) \sim \left(\theta_I - \frac{\pi}{N_c}\right) \ln\left(\frac{\pi}{N_c} - \theta_I\right) \qquad \text{as} \qquad \theta_I \to \frac{\pi}{N_c} \tag{12}$$

$$
B_{RFM}(\theta) = d \left\{ \left(\frac{\pi^2 (N_c^2 - 1)}{6} + \kappa^2 \right) \left[\frac{\theta N_c}{2} - \right. \right. \tag{13}
$$

$$
\left. - \left(\beta\left(\frac{1}{\kappa}\right) - \frac{\kappa}{2} \right) \sinh\left(\frac{\theta N_c}{\kappa}\right) + \frac{1}{2} \int_0^{\theta N_c} dt \ \tanh\frac{t}{2} \sinh\frac{\theta N_c - t}{\kappa} \right]
$$

$$
\left. + \frac{\pi^2}{12} \left(\theta N_c + \frac{(\theta N_c)^3}{\pi^2} \right) - \kappa \int_0^{\theta N_c} \ln\left(2\cosh\frac{t}{2} \right) dt \right\}
$$

where

$$
\beta(z) = \frac{1}{2}\left(\psi\left(\frac{z+1}{2}\right) - \psi\left(\frac{z}{2}\right) \right), \qquad \psi(z) = \frac{1}{\Gamma(z)} \frac{d\Gamma(z)}{dz}
$$

Cluster Expansion Model (CEM)

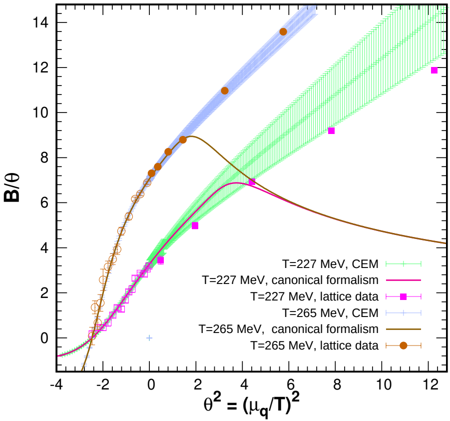
[V. Vovchenko, J. Steinheimer, O. Philipsen and H. Stoecker 2018]

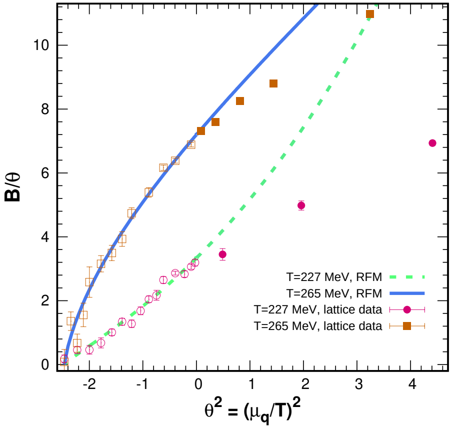
$$B(\theta_I)\Big|_{\theta_R=0} = \sum_{k=1}^{\infty} a_k^{\mathrm{CEM}} \sin\left(kN_c\theta_I\right) \tag{14}$$

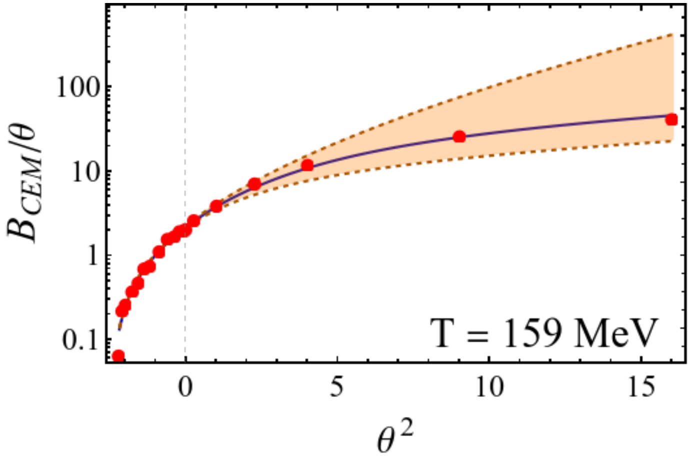
$$b_k \;=\; (-1)^{k+1}\, \frac{b\, q^{k-1}}{k} \left[1 + \frac{6}{\pi^2(N_c^2-1)k^2}\right] \tag{15}$$

$$B = \frac{b}{2q}\left\{\ln \frac{1+q\exp(\theta N_c)}{1+q\exp(-\theta N_c)} + \right.$$
$$\left. + \frac{6}{\pi^2(N_c^2-1)}\left[\mathrm{Li}_3\Big(-qe^{-\theta N_c}\Big) - \mathrm{Li}_3\Big(-qe^{\theta N_c}\Big)\right]\right\} \;. \tag{16}$$

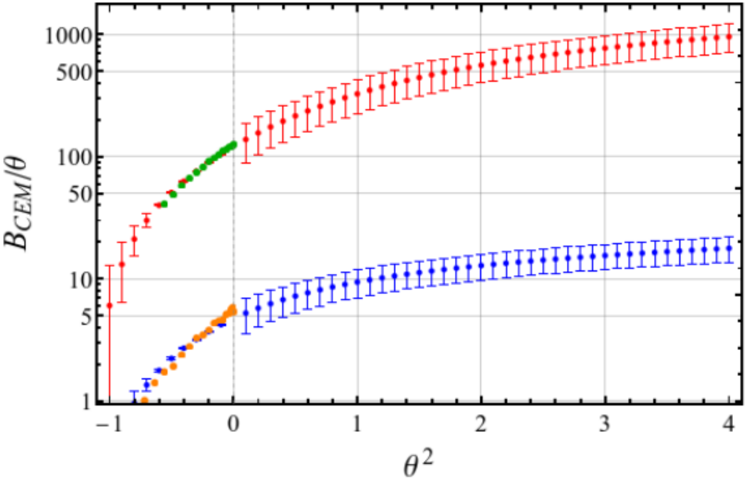
Comparison of the CEM and RFM with lattice data







$L = 3.5$ fm



$SU(3)$ $16^3 \times 4$ lattice,
lower curve $T = 0.8T_c$,
upper curve - $T = 1.8T_c$.

Fugacity expansion

$$\frac{Z_{GC}(\theta, T, V)}{Z_C(0, T, V)} = 1 + \sum_{n=1}^{\infty} Z_n \left(e^{nN_c\theta} + e^{-nN_c\theta} \right) \tag{17}$$

provides a natural parametrization of $B(\theta)$,

$$B(\theta) = \frac{-1}{N_c} \frac{\partial(T \ln Z)}{\partial \mu_q} = \frac{2\sum_{n=1}^{\infty} nZ_n \sinh(nN_c\theta)}{1 + 2\sum_{n=1}^{\infty} Z_n \cosh(nN_c\theta)} \tag{18}$$

$$B(\theta_I)\Big|_{\theta_R=0} = \imath \sum_{n=1}^{\infty} a_n \sin(nN_c\theta_I) \tag{19}$$

$$\sum_{n=1}^{\infty} a_n \sin(nN_c\theta_I) = \frac{2\sum_{n=1}^{\infty} nZ_n \sin(nN_c\theta_I)}{1 + 2\sum_{n=1}^{\infty} Z_n \cos(nN_c\theta_I)} \tag{20}$$

Problem: Given a_n, find Z_n

$$\text{Trigonometric identities} \implies a_i = \sum_{j=1}^{\infty} W_{ij} Z_j \ , \tag{21}$$

$$W_{jk} = 2j\delta_{jk} - a_{j+k} + a_{|j-k|} \cdot \mathrm{sign}(k-j) \qquad\qquad [\mathrm{sign}(0) = 0] \ . \tag{22}$$

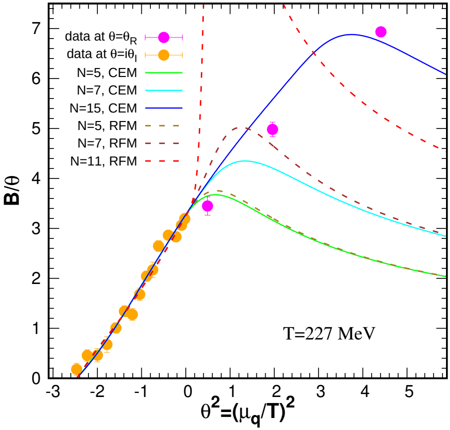
$$\mathbf{Z} = \mathbf{W}^{-1}\mathbf{a} \, . \tag{23}$$

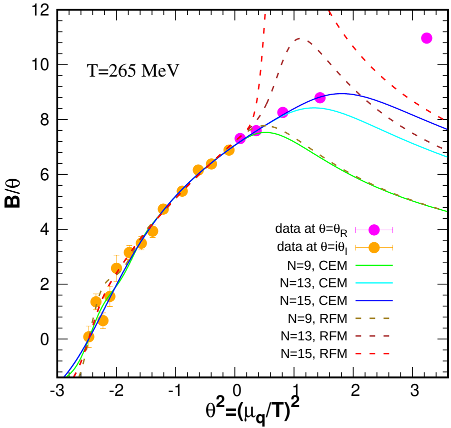
$$Z_{GC}(\theta_I) = \exp\left(N_c \sum_{n=1}^{N} \frac{a_n}{2n} \left(\cos(nN_c\theta_I) - 1 \right) \right) \tag{24}$$

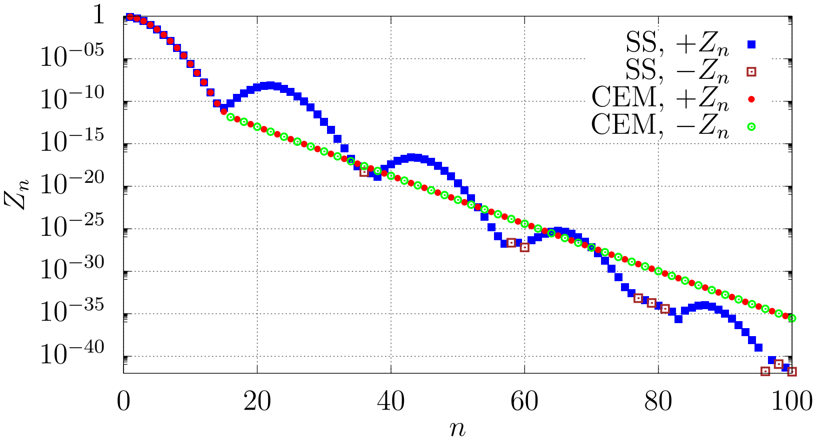
The inverse of the fugacity expansion has the form

$$Z_C\,(n, T, V) = \int_0^{2\pi} \frac{d\theta_I}{2\pi} e^{-in\theta_I} Z_{GC}(\theta_I, T, V) \ , \tag{25}$$

Comparison of the fugacity expansions using CEM and RFM







SS - Z_n from the truncared Fourier series;
CEM - Z_n found using analytic formula; Empty symbols: $Z_n < 0$

We prove numerically the following statement:

At certain values of b and q, the coefficients

$$b_k = (-1)^{k+1} \frac{b\,q^{k-1}}{k} \left[1 + \frac{6}{\pi^2(N_c^2-1)k^2}\right]$$

yeild negative values of Z_n.

$\Longrightarrow$ these values of b and q are unphysical.

$Z_n \geq 0$; $Z_n = 0 \implies$ absense of n-particle states.
To study limitations on the parameters in more detail, we consider a simplified formula,

$$b_k = (-1)^{k+1}\, b\,q^{k-1}$$

It is helpful to start from the other end:

to consider the simplest possible partition function

$$Z_{GC}(\theta) = (1 + qe^{\theta})(1 + qe^{-\ \theta}).$$

$Z_0 = 1 + q^2, \quad Z_1 = Z_{-1} = q\ .$

$$B = \frac{\partial \ln Z_{GC}(\theta)}{\partial \theta} = \frac{2q \sinh \theta}{1 + 2q \cosh \theta + q^2} \longrightarrow 2 \sum_{n=1}^{\infty} (-1)^{n+1} q^n \sin n\theta_I$$

Comparing this with the formula

$$b_k \ = \ (-1)^{k+1}\ b\, q^{k-1}$$

we arrive at $\boxed{\text{b=2q}}$

For example, $b = 4q$ results in the partition function

$$Z_{GC}(\theta) = (1 + qe^{\theta})^2 (1 + qe^{-\theta})^2$$

with

$$\begin{aligned} Z_0 &= 1 + 4q^2 + q^4 \\ Z_1 &= Z_{-1} = 2q(1 + q^2) \\ Z_2 &= Z_{-2} = q^2 \\ Z_k &= Z_{-k} = 0, \quad \text{if} \quad k > 2 \end{aligned}$$

$b = 2jq$ gives

$$Z_{GC}(\theta) = (1 + qe^{\theta})^j (1 + qe^{-\theta})^j$$

and at $j \in \mathbb{Z}$ we arrive at a finite number of positive Z_n $(n \leq j)$; $Z_n = 0$ at $n > j$.

$b = jq$ at $j \notin \mathbb{Z}$ gives rise to negative Z_n

As an example, let us consider $j = 0.5$:

$$Z_{GC}(\theta) = \sqrt{1+qe^{\theta}}\sqrt{1+qe^{-\theta}}$$

At $\ln q < \theta < -\ln q$ it can be expanded in the Taylor series in $\xi = e^{\theta}$.

$$\begin{aligned} \sqrt{1+q\xi} &= 1 + \frac{q\xi}{2} - \frac{q^2\xi^2}{8} + \frac{q^3\xi^3}{16} - \frac{5q^4\xi^4}{128} + \ldots \\ \sqrt{1+\frac{q}{\xi}} &= 1 + \frac{q}{2\xi} - \frac{q^2}{8\xi^2} + \frac{q^3}{16\xi^3} - \frac{5q^4}{128\xi^4} + \ldots \end{aligned}$$

$$Z_0 = 1 + \frac{q^2}{4} - \frac{q^3}{8} + \ldots; \qquad Z_1 = \frac{q}{2} - \frac{q^3}{16} + \frac{q^5}{128} - \ldots;$$

$$Z_2 = -\frac{q^2}{8} + \frac{q^4}{32} + \frac{5q^6}{1024} + \ldots$$

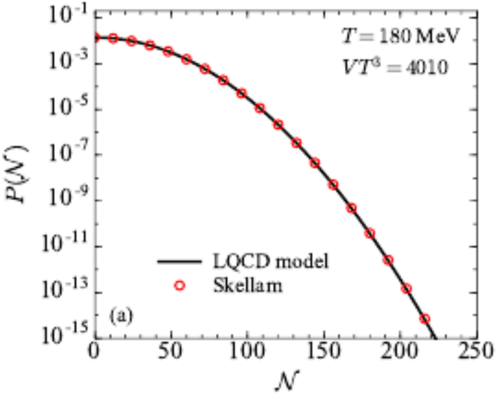
$b = jq$ at $j \notin \mathbb{Z}$ and $j \gg 1$

As an example, let us consider $j = 100.5$:

$$Z_{GC} = (1 + q\xi)^j \left(1 + \frac{q}{\xi}\right)^j$$

$$(1 + q\xi)^j = 1 + jq\xi + \frac{j(j-1)}{2!} q^2 \xi^2 + \frac{j(j-1)(j-2)}{3!} q^3 \xi^3 + ...$$

At $n < 100$ we obtain $Z_n > 0$



$\mathcal{P}(n) = \dfrac{Z_n}{Z_0 + 2\sum_{j=1}^{\infty} Z_j}$ from the paper Koch, Bzdak 2018

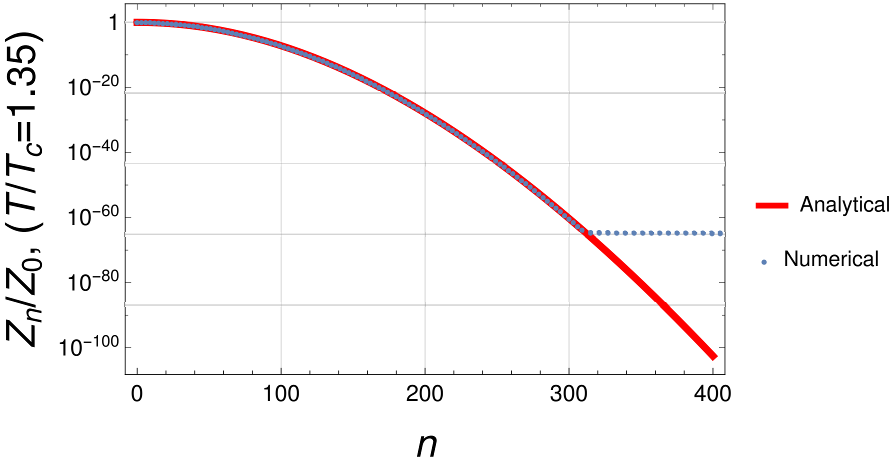
$$Z_{GC}(\theta) = \lim_{N\to\infty} \sum_{n=-N}^{N} Z_n \xi^n, \qquad \xi = e^{\theta}$$

$$Z_n = \frac{\int_0^{\pi/3} d\theta e^{-F_n(\theta)}}{\int_0^{\pi/3} d\theta e^{-F_0(\theta)}}$$

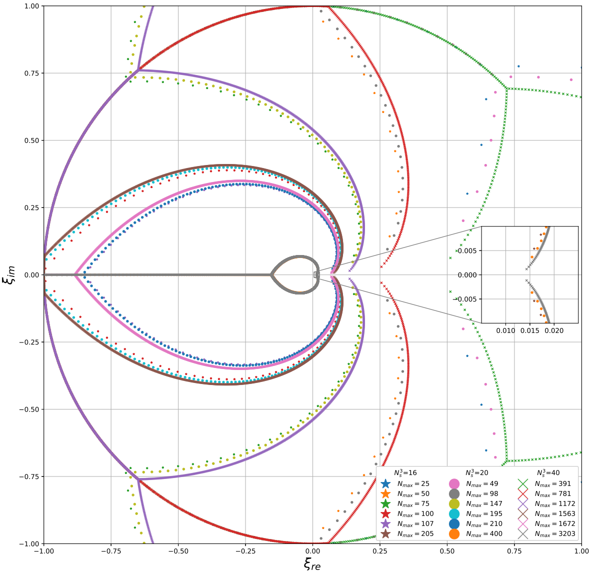
where

$$F_n(\theta) = -in\theta + VT^3 \left(\frac{1}{2} a_1 \theta^2 - \frac{1}{4} a_3 \theta^4 + \frac{1}{6} a_5 \theta^6 \right)$$

- Numerical high-precision evaluation: $Z_n \longrightarrow Z_{nN}$
- Asymptotic estimate: $Z_n \longrightarrow Z_{nA}$



Z_n/Z_0, $(T/T_c$=1.35)
1
10^{-20}
10^{-40}
10^{-60}
10^{-80}
10^{-100}
0
100
200
300
400
n
Analytical
Numerical



Distribution of Lee-Yang zeroes in the fugacity plane at $T > T_{RW}$ ($T = 1.35\,T_c$)

Conclusions

We have studied the analytical continuation of the quark density in QC_2D at $T < T_{RW}$ using various parametrizations. It was found

theoretical framework of parametrization	Agreement of the respective analytical continuation with lattice data at real μ_q
truncated Fourier series	bad
CEM	excellent
RFM	poor
the grand canonical approach with the CEM	good at $\lvert\mu_q\rvert < 320 \div 390$ MeV

Problem of negative canonical partition functions $Z_C(n, T, V)$ calls for further work