

Universal scaling and the asymptotic behaviour of Fourier coefficients of the baryon-number density in QCD

C. Schmidt,^{a,*} D. A. Clarke,^b P. Dimopoulos,^c F. Di Renzo,^c J. Goswami,^d S. Singh,^a
V. V. Skokov^e and K. Zambello^f

^aUniversität Bielefeld, Fakultät für Physik, Universitätsstrasse 25, 33615 Bielefeld, Germany

^bDepartment of Physics and Astronomy, University of Utah, Salt Lake City, Utah 84112, United States

^cDipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma and INFN, Gruppo Collegato di Parma I-43100 Parma, Italy

^dRIKEN Center for Computational Science, Kobe 650-0047, Japan

^eDepartment of Physics, North Carolina State University, Raleigh, NC 27695, United States

^fDipartimento di Fisica dell'Università di Pisa and INFN-Sezione di Pisa, Largo Pontecorvo 3, I-56127 Pisa, Italy.

E-mail: schmidt@physik.uni-bielefeld.de

We discuss the scaling of the Yang-Lee singularity (YLS) and show how the universal scaling can be used to locate phase transitions in QCD. We describe two complementary methods to extract the location of the Yang-Lee singularity from lattice QCD data of the baryon-number density and higher order cumulants of the baryon number, obtained at imaginary chemical potential. The first method (multi-point Padé resummation) is used to determine the Roberge-Weiss phase transition temperature. Our continuum extrapolated result is $T_{RW} = 211.1 \pm 3.1$ MeV. The second method is based on the asymptotic behaviour of the Fourier coefficients of the baryon-number density. We discuss the derivation of a fitting function and demonstrate that the procedure can successfully locate the YLS in the Quark Meson model.

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*Speaker

1. Introduction

The QCD phase diagram is subject to active research since the introduction of the quark model. It is of utmost importance for cosmology, astrophysics and heavy ion phenomenology. Establishing the existence and location of the QCD critical point at nonzero temperature T and baryon chemical potential μ_B is considered a grand challenge in lattice QCD. Unfortunately, lattice QCD is hampered by the infamous sign problem such that direct lattice QCD calculations at $\mu_B > 0$ are impractical. We thus have to rely on extrapolation methods based on Taylor expansion [1] or analytic continuations from calculations at imaginary chemical potentials $\mu_B = i\theta$, $\theta \in \mathbb{R}$ [2, 3]. These methods are in principle sensitive to singularities in the complex chemical potential plane [4]. In particular, if the information from lattice QCD data is converted into a rational function form, it is straightforward to determine the roots of the denominator and thereby extract the positions of singularities.

In lattice QCD calculations at $T > 0$, and statistical physics in general, derivatives of the logarithm of the partition function Z are studied in order to investigate phase transitions. The scaling hypothesis dictates that these observables change with the reduced temperature (t) or symmetry breaking field parameter (h) as a power law, exposing the universal critical exponents. Thus sufficiently high derivatives diverge at $(t, h) = (0, 0)$. In a finite volume, Z can develop a countable number of zeros, or equivalently singularities of $\ln Z$. It is well known that for $t > 0$ the zeros move into the complex h -plane in a particular manner [5]. The Yang-Lee singularity (YLS), which is approximated by the first zero (up to finite size effects), moves along the imaginary h -axis and scales with temperature such that it takes a universal (constant) position in the scaling variable $z = t/h^{1/\beta\delta} \equiv z_c$. Here β, δ are critical exponents of the underlying universality class. The universal position of the YLS has been determined only very recently [6].

Here we use derivatives of $\ln Z$ w.r.t. μ_B as our input data. These observables characterize fluctuations of the conserved (net) baryon number, i.e. higher derivatives are the cumulants of the baryon-number distribution. It has been realized that tracking the YLS in the complex μ_B -plane, which have been determined from the baryon-number density, is a novel and possibly very robust method for the determination of phase transition in QCD [7–12]. We will discuss two methods that are used to extract the YLS from the lattice QCD data. The first method is the multi-point Padé method, which has been introduced in [7]. Using this method we will report on the status of the determination of the Roberge-Weiss transition temperature T_{RW} in QCD, extracted through the universal scaling of the YLS. Applying this method also in the vicinity of the QCD critical end point is very tempting and will be discussed elsewhere [8, 9]. For a discussion of finite size scaling using the multi-point Padé approach, see [10, 11]. As a second procedure to extract YLS from the lattice data, we will introduce and discuss the asymptotic behavior of the Fourier coefficients of the baryon-number density. We show that the first $O(20)$ Fourier coefficients might be sufficient to extract the position of the YLS, given the data is sufficiently precise. We demonstrate the efficiency of the method in the Quark-Meson Model [13].

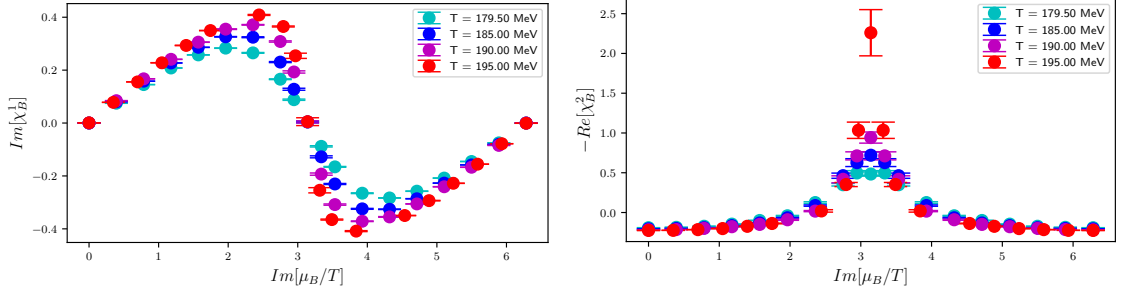


Figure 1: First- and second-order cumulants of the baryon number as a function of the imaginary chemical potential, calculated on $36^3 \times 6$ lattices.

2. The multi-point Padé method

We perform lattice QCD calculations with the highly improved staggered quark (HISQ) action using the SIMULATEQCD software [14, 15]. We are using (2+1) flavors with physical masses, using the scale setting procedure and line of constant physics as described by the HotQCD collaboration [16]. The observables we determine are the cumulants of the (net) baryon number, given as

$$\begin{aligned} \chi_n^B(T, V, \mu_B) &= \frac{1}{VT^3} \left(\frac{\partial}{\partial \hat{\mu}_B} \right)^n \ln Z(T, V, \mu_l, \mu_s) \\ &= \frac{1}{VT^3} \left(\frac{1}{3} \frac{\partial}{\partial \hat{\mu}_l} + \frac{1}{3} \frac{\partial}{\partial \hat{\mu}_s} \right)^n \ln Z(T, V, \mu_l, \mu_s). \end{aligned} \quad (1)$$

Here μ_l and μ_s are the chemical potentials of the two light flavors and of the strange quark, respectively. We also have introduced the dimensionless notation $\hat{\mu} = \mu/T$. For simplicity we use $\mu_l = \mu_s$, which corresponds to $\mu_B = 3\mu_l$ and zero strangeness chemical potential $\mu_s = 0$ ¹. The derivatives are expressed in space-time traces over operators, which are appropriate combinations of the inverse and the derivatives of the fermion matrix. We calculate the traces by the random noise method, using normally distributed volume sources. Moments of the traces are calculated in an unbiased manner [17]. For temperatures $T \lesssim 200$ MeV, we calculate on lattices of size $N_\sigma^3 \times N_\tau = 24^3 \times 4$, $36^3 \times 6$ and $48^3 \times 8$. The results for the first two cumulants from the $N_\tau = 6$ lattices are shown in Fig. 1. The statistics varies between 2000 and 6000 configurations per simulation point (μ_B, T) . From the data we determine the multi-point Padé of χ_1^B in $\theta = \text{Im}\hat{\mu}_B$ for each temperature T by the ansatz

$$\chi_1^B = R_n^m(\theta) = \frac{\sum_{i=0}^m a_i \theta^i}{1 + \sum_{j=1}^n b_j \theta^j}. \quad (2)$$

The coefficients a_i, b_i are determined by solving a set of linear equations, making use of χ_1^B and χ_2^B data [7]. Finally, we calculate the roots of the denominator to obtain the closest (uncanceled) singularity $\hat{\mu}_{YL}$, which approximates the position of the YLs in the infinite volume limit. To apply Yang-Lee scaling, we have to express the universal scaling fields t, h in terms of the QCD

¹For the conversion of the quark chemical potentials μ_u, μ_d, μ_s to the hadronic chemical potential μ_B, μ_Q, μ_S see e.g. Ref. [18].

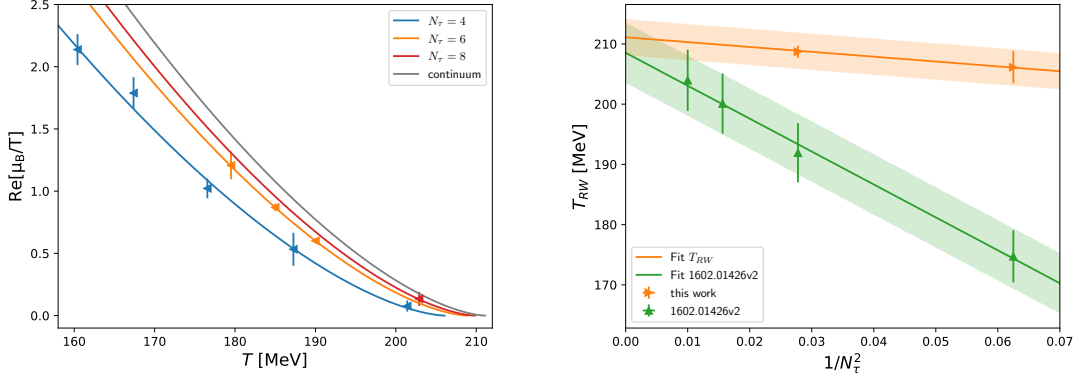


Figure 2: Scaling of the Yang-Lee singularity with temperature for three different lattice spacings (N_τ) and continuum extrapolation (left). The N_τ dependence of the Roberge-Weiss transition temperature $T_{RW}(N_\tau)$ from this work and from [20].

parameters T, μ_B . In the vicinity of the Roberge-Weiss transition [19], located at $\hat{\mu}_B = i\pi$, we have the following relations

$$t = t_0^{-1} \frac{T_{RW} - T}{T_{RW}}, \quad h = h_0^{-1} \frac{\hat{\mu}_B - i\pi}{i\pi}, \quad (3)$$

where t_0, h_0 are normalization constants and T_{RW} is the Roberge-Weiss phase transition temperature. Note that the imaginary direction of the symmetry breaking field is mapped onto the real direction in the chemical potential $\hat{\mu}_B$. We can now solve $t/h^{1/\beta\delta} = z_c$ to obtain $\hat{\mu}_{YL}(T)$. Here we use the ansatz

$$\hat{\mu}_{YL}(T) = a(N_\tau) \left(\frac{T_{RW}(N_\tau) - T}{T_{RW}(N_\tau)} \right)^{\beta\delta}, \quad (4)$$

where we assume the following cut-off dependence of the Roberge-Weiss transition and the amplitude: $T_{RW}(N_\tau) = T_{RW}^{(0)} + T_{RW}^{(2)}/N_\tau^2$ and $a(N_\tau) = a^{(0)} + a^{(2)}/N_\tau^2$. We thus have four fit parameters in total. In Fig. 2 (left) we show that the ansatz works well for the available data ($\chi^2 \approx 0.4$). We obtain the continuum result $T_{RW}^{(0)} = 211.1 \pm 3.1$ MeV. A comparison with the result from [20] is shown in Fig. 2 (right). Note that the two continuum extrapolations are in good agreement.

3. The Fourier coefficients

A complementary approach to the YLs is related to the Fourier coefficients b_k of the baryon-number density $\hat{n}_B = n_B/T^3 = \chi_1^B$, defined as

$$b_k = \frac{1}{i\pi} \int_{-\pi}^{\pi} d\theta \hat{n}_B(\hat{\mu} = i\theta) \sin(k\theta). \quad (5)$$

In order to evaluate the integral in Eq. (5) we deform the integration contour into the complex plane. This is valid as long as we do not cross any non-analyticities. It is important to notice that the YLs condense in the continuum limit to form branch-cuts in \hat{n}_B . We thus deform the integration contour to follow those branch cuts as shown in Fig. 3. We indicated here the branch cuts of the Roberge-Weiss (thermal) transition as well as the ones of the chiral phase transition. Note that they

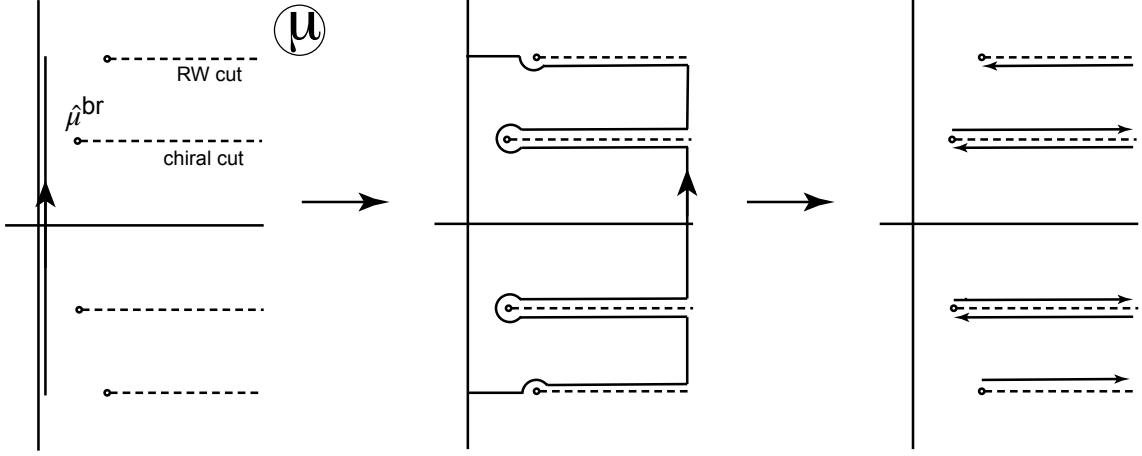


Figure 3: Deformation of the integration contour into the complex $\hat{\mu}_B$ plane along the Roberge-Weiss (thermal) cuts as well as the Yang-Lee cut of the chiral transition.

come in complex conjugate pairs. After the deformation, the first and the last segment cancel each other due to the periodicity in $\hat{\mu}_B$. The segments at infinity vanish due to the exponential decay of the integrand. Finally only the segments along the cuts remain.

As the next important step we express the baryon-number density by its universal behaviour in the vicinity of the branch point $\hat{\mu} \rightarrow \hat{\mu}^{\text{br}}$,

$$\hat{n}_B(\hat{\mu}) = A(\hat{\mu} - \hat{\mu}^{\text{br}})^\sigma (1 + B(\hat{\mu} - \hat{\mu}^{\text{br}})^{\theta_c} + \dots) + \sum_{n=0}^{\infty} a_n (\hat{\mu} - \hat{\mu}^{\text{br}})^n, \quad (6)$$

where σ denotes the leading order Yang-Lee edge critical exponent and θ_c the confluent critical exponent. The last term represents the regular contribution. It is interesting to note that the regular contribution exactly vanishes on the deformed integration contour. After injecting this expression for \hat{n}_B into Eq. (5) and performing the integrals, we obtain [13]

$$b_k = \tilde{A}_{\text{YLE}} \frac{e^{-\hat{\mu}^{\text{YLE}} k}}{k^{1+\sigma}} \left(1 + \frac{\tilde{B}_{\text{YLE}}}{k^{\theta_c}} + \dots \right) + \tilde{A}_{\text{RW}} \frac{e^{-\hat{\mu}^{\text{RW}} k}}{k^{1+\sigma}} \left(1 + \frac{\tilde{B}_{\text{RW}}}{k^{\theta_c}} + \dots \right) + \text{c.c.} \quad (7)$$

Dropping the sub-leading contribution and noting that $\text{Im} \mu^{\text{RW}} = \pi$, results in

$$b_k = |\tilde{A}_{\text{YLE}}| \frac{e^{-\hat{\mu}_r^{\text{YLE}} k}}{k^{1+\sigma}} \cos\left(\hat{\mu}_i^{\text{YLE}} k + \phi_a^{\text{YLE}}\right) + |\hat{A}_{\text{RW}}| (-1)^k \frac{e^{-\hat{\mu}_r^{\text{RW}} k}}{k^{1+\sigma}}, \quad (8)$$

which can be used as a fitting function to extract the position of the branch-cut singularity. Some remarks are in order: The exponential decay of the coefficients determines the real part of the branch-cut singularity μ_r , while the imaginary part μ_i is indicated by the oscillations. We usually assume that only one branch-cut singularity dominates, the one which has the smaller real part μ_r . The Roberge-Weiss branch cut is located at $\hat{\mu}_i^{\text{RW}} = \pi$ such that the oscillations are maximally $(-1)^k$, as long as the Roberge-Weiss branch cut is dominating.

In Fig. 4 we apply this fitting function to Fourier coefficients obtained in the mean-field approximation of the Quark Meson model at $T = 150$ and $T = 180$ MeV. Details of the model

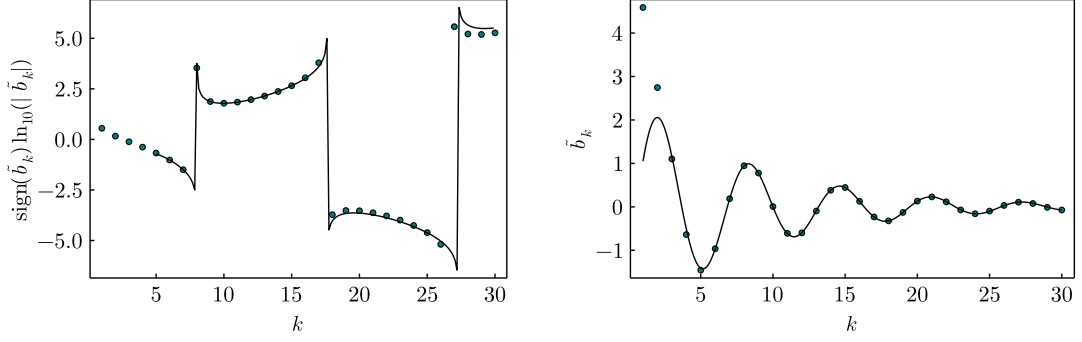


Figure 4: Mean-field Fourier coefficients $\tilde{b}_k = k^{1+\sigma} b_k$ ($\sigma_{\text{MF}} = 1/2$) for $T = 150$ MeV (left) and $T = 180$ MeV (right) and the corresponding fits.

are given in Ref. [21]. We see that the ansatz works very well and that the asymptotic behaviour already sets in at $k \gtrsim 5$. The fit reproduces the exact position of the branch-cut singularity within 7% precision.

We will apply this analysis to lattice QCD data in the future. The challenge is the precise calculation of the Fourier coefficients. To tackle this challenge we are currently exploring asymptotically correct quadrature rules designed for highly oscillatory integrals.

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