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Searching for the QCD critical point using Lee-Yang edge singularities

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Using $N_f = 2+1$ QCD calculations at physical quark mass and purely imaginary baryon chemical potential, we locate Lee-Yang edge singularities in the complex chemical potential plane. These singularities have been obtained by the multi-point Padé approach applied to the net baryon number density. We recently showed that singularities extracted with this approach are consistent with universal scaling near the Roberge-Weiss transition. Here we study the universal scaling of these singularities in the vicinity of the QCD critical endpoint. Making use of an appropriate scaling ansatz, we extrapolate these singularities on $N_\tau = 6$ and $N_\tau = 8$ lattices towards the real axis to estimate the position of a possible QCD critical point. We find an approach toward the real axis with decreasing temperature. We compare this estimate with a HotQCD estimate obtained from poles of a [4,4]-Padé resummation of the eighth-order Taylor expansion of the QCD pressure.

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1. Introduction

At sufficiently high T and/or μ_B, nucleons dissociate into their constituents, and nuclear matter changes phase from a gas of hadrons to quark-gluon plasma. At low enough temperature, one eventually encounters with increasing μ_B a first-order line, which is expected to terminate at a second-order critical endpoint (CEP) belonging to the 3-d, $\mathbb{Z}_2$ universality class. Unfortunately at $\mu_B > 0$, the Boltzmann factor becomes complex, and a direct estimate of the path integral through MCMC is no longer possible–this is the infamous sign problem. This limitation is a special hindrance when looking out for the possible CEP at nonzero μ_B mentioned above.

Nevertheless many approaches have been developed to at least partially circumvent this limitation, each with its own merits, drawbacks, and regions of applicability. One possibility is to carry out simulations at pure imaginary μ_B, where there is no sign problem. In this approach, observables calculated on the imaginary axis are then analytically continued to $\mu_B \in \mathbb{R}$ [1, 2]. Another common tactic is to expand the pressure P in μ_B/T about $\mu_B/T = 0$ [3, 4]. Both of these methods have been successfully employed to, for example, extract higher-order Taylor coefficients of P; unfortunately these quantities become prohibitively computationally expensive as the order increases, and state-of-the-art calculations only make it to order 8 [5, 6].

These difficulties motivate approaches that allow one to glean more information about the QCD phase diagram with fewer Taylor coefficients. The approach we study in these proceedings is the multi-point Padé [7], which allows one to construct high-order rational approximations using few Taylor coefficients. This approach has opened up a vibrant research campaign, facilitating our exploration of the QCD phase diagram at nonzero chemical potential [8–10].

2. Using rational approximations to locate the CEP

The Lee-Yang theorem [11] tells us that the zeroes of the partition function $\mathcal{Z}_{\text{QCD}}$ that approach the real axis as the physical volume $V \to \infty$ correspond to phase transitions; hence the pressure $P = (T/V) \log \mathcal{Z}_{\text{QCD}}$ is expected to be singular at a phase transition in the thermodynamic limit, and correspondingly, the closest singularity to the origin in the complex μ_B plane limits the radius of convergence of the pressure series.

The CEP is thought to belong to the 3-d Ising universality class. In that context there are two relevant couplings $t \sim T - T_{\text{c}}$ and h, the reduced temperature and symmetry-breaking coupling respectively, that parameterize the distance from the critical point. Away from T_{c}, the Lee-Yang singularity gets demoted to Lee-Yang edges (LYE), two branch cuts in the complex h-plane that pinch the real axis as $T \to T_{\text{c}}$ [12]. According to the extended analyticity conjecture [13], the LYE are the closest singularities to the origin. So the thinking goes that the convergence radius of the pressure is limited by the LYE corresponding to the CEP[1]. Switching from h to $z \equiv th^{-1/\beta\delta}$, with β and δ being universal critical exponents, the LYE is known to be located at

$$z_c = |z_c| e^{\pm i\pi/2\beta\delta}. \tag{1}$$

[1]This statement of course depends on the nearest phase transition. At high temperatures one needs to consider the Roberge-Weiss transition, and for small quark masses, the chiral phase transition has increasing importance.

Due to the sign problem, lattice calculations cannot be performed at real μ_B directly. But eq. (1) opens up the possibility of carrying out simulations at pure imaginary μ_B, following the scaling to learn something[2] about real μ_B. Since a phase transition must occur at pure real μ_B, one can follow the imaginary part until it hits zero, signalling the transition, and see what the real part is at that point. This requires us to find complex singularities.

Rational approximations are good candidates for approximating functions with singularities, as zeroes in their denominator mimic singular behavior. Given a generic function f of some variable x, we construct a rational approximation

$$R_n^m(x) \equiv \frac{\sum_{i=0}^m a_i x^i}{1+\sum_{j=1}^n b_j x^j}. \tag{2}$$

To connect the approximation closely to f, let f have a formal Taylor series

$$f(x) = \sum_{k=0}^{\infty} c_k x^k. \tag{3}$$

The Padé approximant of order $[m, n]$ is the rational approximation R_n^m with coefficients chosen such that R_n^m equals the Taylor series up to order $m+n$. This constraint yields a set of equations relating coefficients a_i, b_j, c_k. Some properties of Padé approximants are rigorously known; for instance a Padé approximant is unique when it exists, and the $[m, n]$ approximant converges to f exactly as $m \to \infty$ when f has pole of order n. Other properties must be deduced from numerical experiments; for instance if f has a branch cut, zeroes of the denominator tend to accumulate along the cut. Turning to P, we are faced with the difficulty mentioned in Sec. 1 that expansion coefficients are known only up to eighth order, which therefore limits the order of the corresponding Padé.

To mitigate this difficulty, we use the multi-point Padé. The problem to solve is that we only have information about the Taylor expansion to low order, say order $s-1$. The multi-point Padé is a rational function R_n^m satisfying for $0 \le l < s-1$

$$\left.\frac{\mathrm{d}^l R_n^m}{\mathrm{d}x^l}\right|_{x_i} = \left.\frac{\mathrm{d}^l f}{\mathrm{d}x^l}\right|_{x_i} \tag{4}$$

for N data points x_i. Thus the limited Taylor coefficient information is buttressed by constraints asking derivatives of the rational approximation to match the Taylor coefficients at multiple points x_i. In practice, if we have enough data points and a high enough order of the Taylor series, i.e. when $m+n+1 = Ns$, eq. (4) yields a system of equations that can be solved to obtain the coefficients a_i and b_i. When $m+n+1 < Ns$, one can fit the rational function coefficients, obtaining them through a maximum likelihood approach.

Unfortunately even less seems to be known about the multi-point Padé. To ensure that rational functions constructed in this way carry useful and robust information, we have carried out many numerical experiments. For example in the context of the 1-d Thirring model, it was shown the multi-point Padé captures the exact chiral condensate well [14] and outperforms an ordinary Padé for capturing the exact number density [7]. In the context of the 2-d Ising model, the

[2]Assuming we know the mapping from T and μ_B to t and h.

multi-point Padé was successfully employed to reproduce correct critical exponents and Lee-Yang finite size scaling [15, 16]. Most relevant to the QCD phase diagram, this multi-point Padé approach was used to find the Roberge-Weiss transition temperature[3] [7] in agreement with earlier determinations [18, 19], and Re μ_B obtained from this approach yields Lee-Yang finite size scaling that is consistent with expectations [20].

Since the QCD CEP is expected to be in the 3-d, $\mathbb{Z}_2$ universality class, $\beta\delta \approx 1.56$. Unfortunately the exact mapping from T and μ_B to the Ising model is not yet known. Sufficiently close to the CEP, a linear ansatz

$$\begin{aligned} t &= \alpha_t \Delta T + \beta_t \Delta\mu_B \\ h &= \alpha_h \Delta T + \beta_h \Delta\mu_B, \end{aligned} \tag{5}$$

where $\Delta T \equiv T - T^{\text{CEP}}$ and $\Delta\mu_B \equiv \mu_B - \mu_B^{\text{CEP}}$, should be reliable. This suggests [21]

$$\mu_{\text{LY}} = \mu_B^{\text{CEP}} + c_1 \Delta T + i c_2 |z_c|^{-\beta\delta} \Delta T^{\beta\delta} + c_3 \Delta T^2 + O\left(\Delta T^3\right). \tag{6}$$

Our strategy is then as follows: For each temperature ensemble, we use multi-point Padé approximations to find the signature of the closest singularity of χ_1^B to the origin in the complex μ_B plane. We fit the imaginary part of the singularity according to eq. (6), and since phase transitions exist at real μ_B, the point where this fit crosses the T-axis yields a T^{CEP} estimate. At the same time, we fit the real part of the singularity to eq. (6); plugging T^{CEP} into this fit yields μ_B^{CEP}.

3. Computational set up

We generate $36^3 \times 6$ lattices with $N_f = 2 + 1$ HISQ quarks [22] using `SIMULATeQCD` [23, 24]. We select bare parameters to maintain constant physical pion mass, i.e., $m_s/m_l = 27$. To overcome the sign problem, we conduct our simulations at pure imaginary chemical potentials. For simplicity, we set $\mu_l = \mu_s$. We generated a varying number of configurations (ranging from 1800 to 16000) at temperatures 166.6, 157.5, 145.0, and 136.1 MeV. Configurations are spaced by either 10 or 5 molecular dynamics time units, depending on the temperature. The HotQCD [4,4]-Padé chemical potentials [25] are computed from their parameters $c_{6,2}$ and $c_{8,2}$ along with the observables χ_2^B and χ_4^B. Error bars on these chemical potentials are obtained by a Gaussian bootstrap of size 24000 implemented in the AnalysisToolbox [26], which is also used to carry out the fits.

4. Results

In Fig. 1 we show the current status of our $(T^{\text{CEP}}, \mu_B^{\text{CEP}})$ estimate. The red data indicate singular μ_B estimated from HotQCD data that used a [4,4] Padé on $N_\tau = 8$ ensembles. Moreover the HotQCD data used aspect ratio $N_\sigma/N_\tau = 4$. Singular μ_B coming from the multi-point Padé are in blue. To one significant digit, extrapolations indicate approximate critical endpoints $(T^{\text{CEP}},\ \mu_B^{\text{CEP}})$ of (100 MeV, 600 MeV) and (70 MeV, 500 MeV) for the HotQCD and Bielefeld-Parma data, respectively. We currently do not have a strong reason to favor one estimate over the other, hence we average these quantities, yielding approximately

$$(T^{\text{CEP}}, \mu_B^{\text{CEP}}) \approx (85\text{ MeV}, 550\text{ MeV}) \quad \text{and} \quad \mu_B^{\text{CEP}}/T^{\text{CEP}} \approx 6.5. \tag{7}$$

[3] We are currently updating our continuum-limit estimate of T_{RW} [17].

Year	Method	$T^{\rm CEP}$ [MeV]	$\mu_B^{\rm CEP}$ [MeV]	$\mu_B^{\rm CEP}/T^{\rm CEP}$
2023	CP+LQCD [27]	≈ 100	≈ 580	≈ 5.8
2022	LQCD [25]			$\gtrsim 3$
2021	DSE [28]	≈ 130	≈ 500	≈ 3.8
2021	DSE [29]	109	610	5.59
2020	fRG [30]	107	635	5.54
2017	BHE [31]	89	724	8.1

Table 1: Some results and constraints on the CEP location from conformal Padé (CP) and lattice QCD (LQCD) along with Dyson-Schwinger equations (DSE), functional renormalization group (fRG), and black hole engineering (BHE).

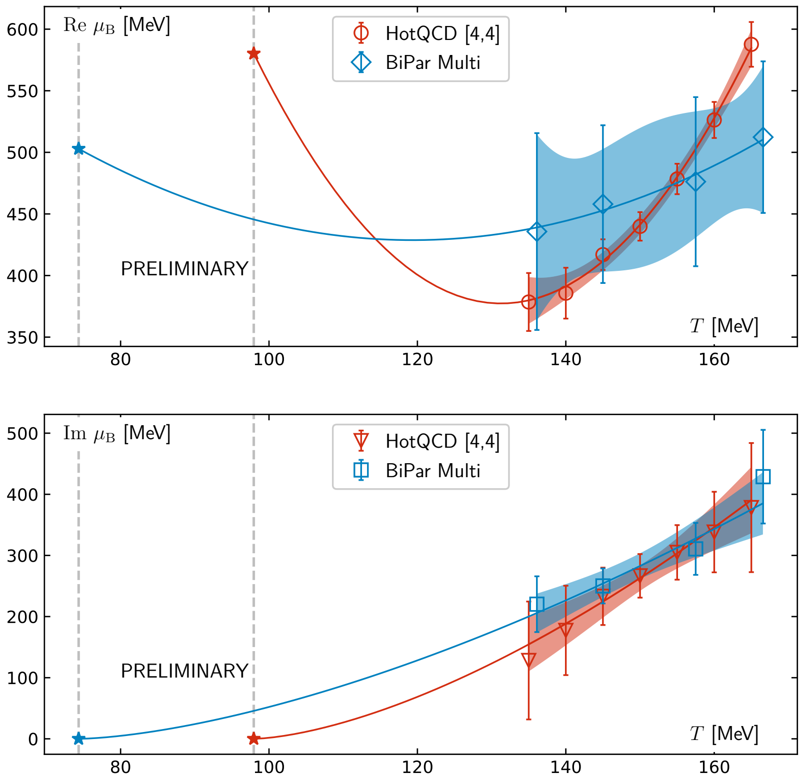

Figure 1: Projections of the location of $\mu_B^{\rm CEP}$ and $T^{\rm CEP}$ using the HotQCD [4,4] Padé and the present study's multi-point Padé. Data are fit using eq. (6). In the lower panel, the stars indicate where Im $\mu_B^{\rm CEP} = 0$, which estimates where the critical point should be. Following the dotted grey line upwards sets the cutoff for the fit to Re μ_B, whose corresponding star indicates our estimate for $\mu_B^{\rm CEP}$.

In Table 1 we collect several other estimates and constraints on the critical point from lattice data and effective models. Our preliminary result is in rough agreement with these other approaches, which consistently seem to find a temperature around 90-130 MeV and a chemical potential around 500-700 MeV. All approaches seem to be sensitive to some physical phenomenon there.

We stress that these results are still preliminary. The fit to singular Re μ_B obtained from the multi-point Padé currently suffers from having only 4 data points to fit 3 parameters. The fit should hence stabilize with lower temperature data, which is also crucial for the imaginary part, giving us more information on the approach to the T-axis. Our error analysis is still undergoing some refinement. Hence the picture we give in Fig. 1 is subject to change[4] slightly as we converge on our final estimate.

5. Summary and outlook

The multi-point Padé has been tested in a variety of situations, including for the Ising model, Thirring model, and near the Roberge-Weiss critical point, which gives us confidence in the approach. We observe a possible indication of the QCD CEP around $T \sim 85$ MeV, $\mu_B \sim 550$ MeV when $\mu_Q = \mu_S = 0$. We stress that, as of these proceedings, this result is preliminary. In the short term, we are adding a lower temperature point and refining our CEP estimate strategy. A long-term goal is an eventual continuum-limit extrapolation. Lower temperature ensembles are being generated to get a better handle on the CEP fit. Besides probing the QCD CEP, we are also investigating the chiral transition with this approach.

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