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Lee-Yang singularities, series expansions and the critical point

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Determining the existence and the location of the QCD critical point remains a major open problem, both theoretically and experimentally. In this talk, I present a new way of reconstructing the equation of state in the vicinity of the nearest thermodynamic singularity (the Lee-Yang edge singularity in the crossover region) from a truncated Taylor series expansion for small μ. This is done by using a combination of Padé resummation and a conformal map. Then, I show that this information can be used to (i) determine the location of the critical point and (ii) constrain the non-universal mapping parameters between the Ising and QCD equations of state. I explicitly demonstrate these ideas in the 2d Gross-Neveu model whose phase diagram shares the key aspects of the conjectured QCD phase diagram including the existence of a critical point.

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1. Introduction

One of the major outstanding questions regarding the phase diagram of QCD is whether there is a critical point along the transition curve between the hadronic and Quark Gluon Plasma phases. It is now well established that for physical quark masses, the deconfinement transition overlaps with the chiral transition and is a smooth crossover at zero quark chemical potential, μ [1]. Various plausibility arguments and model calculations indicate, albeit less robustly, that the transition between nuclear and quark matter phases at zero temperature and nonzero μ_B is first order [2]. A natural conclusion of these two arguments is that at some point in the phase diagram, the smooth crossover must end on a second order critical point and into a first order transition. The search for this conjectured critical point is the focus of ongoing theoretical and experimental effort [3].

General symmetry arguments imply that, if it exists, the critical point is in the same static universality class as the 3d Ising model [2]. From the universality argument one can determine the values of the critical exponents. However neither the location of the critical point nor the relation between the thermodynamic parameters of the Ising model, the reduced temperature and the magnetic field (r, h), and those of QCD, temperature and chemical potential (T, μ), are universal. They have to be determined directly from QCD. Unfortunately our current theoretical knowledge of the QCD phase diagram at nonzero μ is severely limited due to the sign problem that prevents first-principle lattice computations at finite densities. One way to deal with this problem is to expand the equation of state around zero μ where Taylor coefficients can be computed on the lattice without the sign problem since they are evaluated at $\mu = 0$ (see [4, 5] for recent reviews). In this work I introduce a framework of extracting the underlying singularities of the equation of state from the coefficients of a truncated Taylor series [6]. These singularities carry information about the critical point and the aforementioned non-universal parameters.

2. Lee Yang edge singularities

In their seminal work phase transitions, Lee and Yang showed that the thermodynamic properties of a system is encoded in the distribution of the zeroes of the partition function $Z(\zeta)$ as a function of fugacity, $\zeta = e^{\mu/T}$ [7, 8]. In general, $Z(\zeta)$, has zeroes for complex values of μ and T. In the thermodynamic limit the zeroes coalesce into branch cuts emanating from branch points known as the Lee-Yang (LY) edge singularities. When the LY singularities pinch the real axis, the system exhibits a second order phase transition. Likewise the branch cut associated with a LY singularity crosses the real line when there is a first order phase transition.

At the critical point, (T_c, μ_c), the equation of state of a thermodynamic system exhibits singular behavior where the susceptibility diverges. At the same time, in general, even for temperatures away from T_c, the equation of state exhibits *complex* singularities at $\mu = \mu_{LY}(T)$. Now, consider the equation of state near a critical point, (T_c, μ_c), of system which is in the Ising universality class. From universality one can relate it to that of the Ising model via a linear map [9, 10]

$$\begin{pmatrix} r \\ h \end{pmatrix} := \mathbb{M} \begin{pmatrix} T - T_c \\ \mu - \mu_c \end{pmatrix} = \begin{pmatrix} r_T & r_\mu \\ h_T & h_\mu \end{pmatrix} \begin{pmatrix} T - T_c \\ \mu - \mu_c \end{pmatrix}. \tag{1}$$

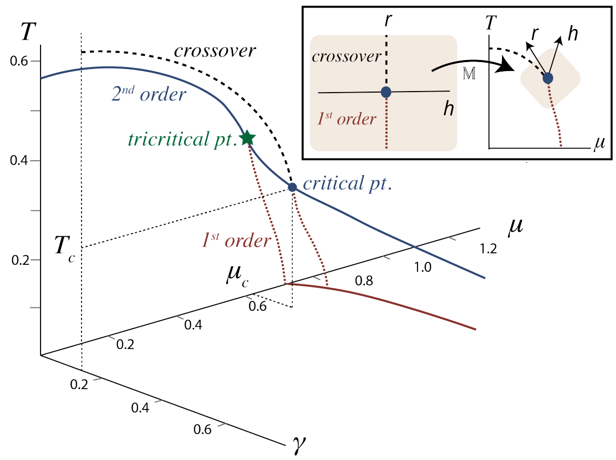

Figure 1: The phase diagram of the Gross-Neveu model. Inset: The mapping to the Ising model near the critical point.

This relation then leads to the following expression for the trajectory of the LY singularities [11]:

$$\mu_{LY}(T) \approx \mu_c - c_1(T-T_c) \pm i\frac{2}{3\sqrt{3}}c_2(T-T_c)^{\beta\delta} \quad \text{where } c_1 := \frac{h_T}{h_\mu} \quad c_2 := \frac{r_\mu{}^{\beta\delta}}{h_\mu}\left(\frac{r_T}{r_\mu}-\frac{h_T}{h_\mu}\right)^{\beta\delta}. \quad (2)$$

This expression follows from the fact that in the Ising model the LY singularities occur at $hr^{-3/2} = \pm 2i/(3\sqrt{3})$ [12, 13]. Notice that c_1 is the slope of the crossover line, whereas c_2 depends on the relative angle between the h and r axes [9, 10]. Therefore the trajectory in Eq. (2) depends on not only the location of the critical point, but also on the non-universal mapping parameters. In the context of QCD critical point, the Lee Yang singularities has been discussed in, for example, [11, 14–23]. In what follows I will introduce an effective way of reconstructing the LY trajectory give in Eq. (2) from a series expansion.

3. The Gross-Neveu Model

I will illustrate the resummation technique via the Gross-Neveu model which has been used as a toy model for QCD for a long time [24]. Similar to QCD, it exhibits asymptotic freedom, chiral symmetry breaking (in the massless limit) and dimensional transmutation. Furthermore its phase diagram (assuming that translational symmetry remains unbroken) qualitatively mirrors the conjectured QCD phase diagram including the existence of a critical point (see Fig. 1). In this work I will not discuss crystalline phases [25–27]. The Gross-Neveu model is defined by the action

$$S = \int d^2x \left(i\bar{\psi}(\partial\!\!\!/ - m_q)\bar{\psi} + \frac{g^2}{2}(\bar{\psi}\psi)^2 \right), \quad (3)$$

where ψ is a Dirac fermion with N_f flavors. The theory enjoys a $\mathbb{Z}_2$ chiral symmetry, $\psi \to \gamma_5\psi$, for $m_q = 0$. I will work in the limit $N_f \to \infty$ with fixed $g^2 N_f$ where the fluctuations are suppressed and the mean field solution is exact. The physical spectrum the theory consists of a free fermion whose mass is determined via the vacuum gap equation [25]. All the dimensionful parameters in this work are expressed in units of the dynamically generated vacuum fermion mass. The phase diagram of the theory follows from minimizing the effective potential

$$\Omega(\phi,T,\mu) \;=\; \frac{\phi^2}{2\pi}\left(\log\phi-\frac{1}{2}+\gamma\right)-\frac{\gamma}{\pi}\phi-T\int\frac{dk}{2\pi}\prod_{\eta=\pm1}\log\left[\left(1+e^{-(\sqrt{k^2+\phi^2}+\eta\mu)/T}\right)\right]. \quad (4)$$

which determines the fermion mass at a given temperature and chemical potential. The pressure, from which other thermodynamic functions can be derived, is given as $p(T,\mu)=-\min_\phi \Omega(\phi,T,\mu)$. Finally, the LY edge singularities occur at

$$\frac{\partial\Omega(\phi,T,\mu)}{\partial\phi}=\frac{\partial^2\Omega(\phi,T,\mu)}{\partial\phi^2}=0, \quad (5)$$

where for a given $T>T_c$ is satisfied for a complex pair $\mu=|\mu_{LY}|e^{\pm i\theta}$ whose form is given in Eq. (2).

4. Resummations

Suppose we only have access to a Taylor series expansion of the equation of state as in the case for many strongly interacting many-body systems:

$$p(T,\mu)\approx\sum_{n=0}^{N}p_n(T)\mu^{2n}\,. \quad (6)$$

The natural expansion parameter is μ^2 due to the charge conjugation symmetry. Extracting information regarding the critical point from a such a truncated expansion is challenging since in this form it has no singularities. In principle this Taylor expansion has a radius of convergence given by $|\mu_{LY}|$ as the LY singularity is the closest singularity. However it is numerically difficult to extract it from a ratio test as the singularities are complex and the ratios has an oscillating envelope. Alternatively Padé resummation, $\mathrm{P}_{\mathrm{N}/2}[p](\mu^2):=p(\mu^2)/q(\mu^2)$ where p and q are $N/2^{th}$ order polynomials, approximates a branch point singularity, like the LY singularity in the thermodynamic limit, as accumulation point of a sequence of poles and zeros. In essence Padé resummation transforms the information contained in N terms in the original Taylor expansion into locations of $N/2$ poles and zeros which approximate the underlying branch cuts. At the same time, Padé resummation typically generates spurious poles, especially when the number of Taylor coefficients is small. Padé resummation can be significantly improved by supplementing it by a suitably chosen conformal map. The idea is to map the original domain of the function conformally into a region in the complex plane, such as the unit disk (i.e. $\mu^2:=\phi(z)$) and do the Padé resummation in the new variable z. I will refer this method simply as "conformal Padé". For a wide class of functions conformal Padé provides the optimal approximation to the original function with a finite set of Taylor coefficients [28]. In this work I used two different conformal maps, $\phi_1(z)=4\mu_{LY}^2 z/(1+z)^2$, and $\phi_2(z)=4|\mu_{LY}|^2\left[\theta/(1-z)^2\right]^\theta\left[1-\theta/(1+z)^2\right]^{1-\theta}$. They respectively map one-cut and two-cut complex plane into the unit disk. I used the former to extract the LY trajectory, Eq. (2), for a set of temperatures and the latter to approximate various thermodynamic functions such as susceptibilities. The results are presented in the next section.

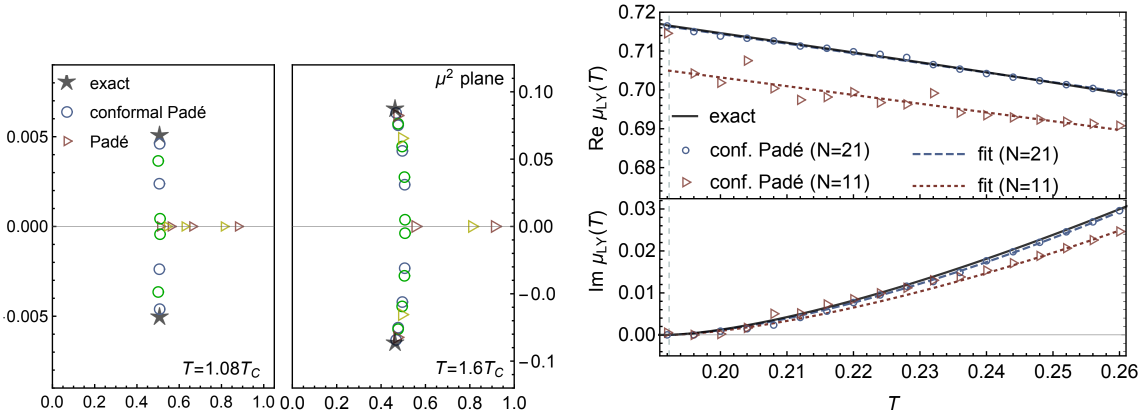

Figure 2: Left: The poles and zeroes of the Right: The Lee-Yang singularity trajectory, $\mu_{LY}(T)$, reconstructed from conformal Padé with 20 and 10 terms. The vertical line denotes T_c.

5. Results

The starting point is Taylor series expansion of the equation of state, Eq. (6), obtained by first solving $\partial_\phi \Omega(\phi) = 0$ order-by-order in μ^2 and for a range of $T \gtrsim T_c$, then plugging this solution into Eq. (4), and finally expanding in μ^2. A non-zero bare quark mass is used by fixing $\gamma = 0.1$. The Lee-Yang singularities are then extracted by applying conformal Padé resummation with the conformal map $\phi_1(z)$ defined above. The results are shown in Fig. 2. The left figure shows the locations of poles and zeros of Padé (red, yellow triangles) and conformal Padé (blue, green circles) resummations for two different temperatures close to and further away from T_c. The alternating set of poles and zeros accumulate towards the LY singularity (and its complex conjugate pair). Especially close to T_c, Padé cannot resolve the small imaginary part whereas conformal Padé does. The right figure shows the reconstructed LY trajectory, Eq. (2), namely the real and imaginary parts of the singularities extracted from conformal Padé for a range of temperatures. From this trajectory I then computed the location of the critical point and the combination if mapping parameters given in Eq. (2). The results are shown in the table below.

	T_c	μ_c	c_1	c_2
exact	0.192	0.717	0.249	4.684
conf. Padé (N=21)	0.195	0.716	0.248	4.323
conf. Padé (N=11)	0.185	0.707	0.225	3.666

Table 1: The location of the critical point and the Ising model mapping parameters extracted from conformal Padé.

Let me now discuss the susceptibilities $\chi_n(T,\mu) = \partial^n p(T\mu)/\partial\mu^n$ for $n = 2, 3, 4$. Especially the higher order susceptibilities play an important role in the search for the QCD critical point as their magnitude grows near the critical point which make them ideal observables. The results are shown in Fig. 3. Notice that due to the spurious poles, Padé resummation breaks down at around $\mu = \mathrm{Re}\mu_{LY}$, whereas conformal Padé agrees with the exact result for much higher values of μ.

Furthermore conformal Padé successfully captures the double and triple peak behaviors of χ_3 and χ_4, even with 10 terms. With 20 terms it is almost indistinguishable from the exact result.

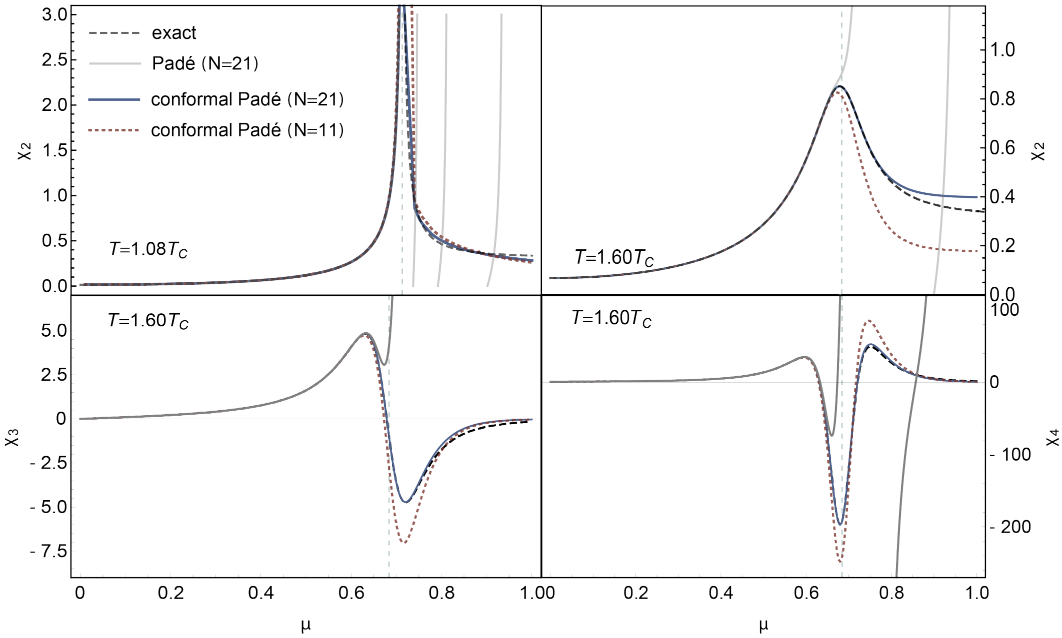

Figure 3: The susceptibilities computed via Padé and conformal Padé with 10 and 20 Taylor coefficients.

6. Conclusions

In this work I tackled a fairly general problem regarding static critical phenomena. Only having access to a finite number of coefficients of the Taylor expansion of the equation of state, how much information one can extract regarding the critical point and critical contribution to the equation of state? Through the Gross-Neveu model, I illustrated that by using a combination of Padé resummation and conformal mapping one can obtain significantly more information regarding the location of the critical point and the equation of state around it compared to the truncated Taylor expansion. Furthermore, this technique does not require any additional information. The ultimate goal is to use these ideas to refine the theoretical estimations of the critical point signatures for QCD and have a more accurate implementation of the equation of state in hydrodynamic simulations. Of course for QCD, we do not have the luxury of having as many terms in the Taylor series as in these examples. It is therefore important to pair these ideas with various other resummation methods such as [29–31] to gather as much information as possible in the search for the critical point.

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