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What we can learn about Lee-Yang zeros from Lattice simulations (in QCD)

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Phase diagrams of some important theories like quantum chromodynamics (QCD), are only accessible through numerical simulations with only finite degrees of freedom. Information about critical phenomena can then only inferred through finite size scaling studies of various moments of the order parameter. Alternatively, one can study the complex zeros of the grand canonical partition function, known as Lee-Yang zeros, which are accessible as poles of the thermodynamic variables. Moreover the temperature and volume scaling of these poles can be used as a probe to understand the nature of phase transitions in many systems. We will discuss here the recent progress that has been made in this direction with respect to the Roberge-Weiss transition, the 2D Ising model and the conjectured QCD critical point. We will further discuss results on the universal location of Lee-Yang edge singularity from continuum extrapolated scaling function for some $O(N)$ models in $3-d$.

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1. Introduction

Our current understanding of the QCD phase diagram is incomplete because the theory is strongly interacting at low energy scales on the one hand and direct lattice simulations are hindered by the numerical sign problem at finite baryon chemical potentials μ_B on the other hand. The only known information about the phase diagram is the nature of the phase transition between the de-confined and the confined phase at vanishing chemical potential. This was shown to be a crossover in [1], by performing direct simulations at zero μ_B. When attempting to deduce the nature of phase transition, which only occur in the limit of infinite degrees of freedom in a system, from finite volume lattice simulations we have to make use of finite size scaling (FSS) analysis. The currently preferred method of doing this is based on studying Binder cumulants [2–4], relying on the remnants of non-analyticities of thermodynamic observables in terms of observing the change in peak heights and positions of susceptibilities.

In this proceedings, our goal is to show the power of an alternative approach, namely the Yang-Lee formalism to infer properties of critical phenomena when only data from finite volume simulations is available. T.D. Lee and C.N. Yang showed in [5, 6] that it is possible to infer the presence and nature of phase transitions in a system by studying the volume and temperature scaling of the complex zeros of the grand canonical partition function of the system. A current open problem is the choice of method used to extract these zeros from lattice data. In the first part of this proceedings, in Sections [2,3,4], we will show how to extract relevant zeros of the partition function using a particular rational function re-summation of the baryon number density in 2+1 QCD and magnetization of the 2D Ising model. In most theories of interest, these zeros called the Lee-Yang zeros lie on well defined curves in the complex plane of the fugacity variable $z = e^{\beta\mu_B}$ in the thermodynamic limit. These curves can be shown to be branch cuts terminating in branch points known as Lee-Yang edge singularities (LYEs) [7] in certain conditions. In the next part of the proceedings, in Section [5] , we will show how the Schofield parametrization [8] of the continuum extrapolated scaling functions in $O(N)$ for $N = \{1, 2, 4\}$ can be used to deduce the location LYEs for the relevant universality classes. We will finally present the summary of these results with some caveats and proposed future activities in Section [6].

2. Rational functions and Lee-Yang zeros

After motivating the advantage of studying Lee-Yang zeros at finite volume, we need to address the question on how to obtain these from lattice data which usually comes with limited precision. As we are aware, currently the only probe into the QCD phase diagram at finite densities is via Taylor expansions at zero chemical potential [9, 10] and direct simulations at imaginary chemical potential [11, 12] where there is no sign problem. Recently a number of re-summation schemes have appeared which aim to combine these Taylor coefficients in one way or another for various purposes. The method that we proposed in [13] can also be seen as a re-summation scheme which aims to combine low order Taylor coefficients measured at various values of imaginary μ_B and zero chemical potential to compute a rational function approximation of a given observable called the “multi-point” Padé approximation. The method of combining many Taylor coefficients of a function into a single point Padé is not new. However, in this one needs precise information of higher Taylor coefficients of the function, which is not accessible cost-wise to lattice simulations. In the multi-point approach on the other hand, one can generate low order Taylor coefficients at many points and obtain a higher order rational functions. The idea to apply this multi-point procedure on lattice data originated from our work on Lefschetz thimble simulations of the 1+1 Thirring model and Heavy-dense QCD in [14]. There we found that the closest pole from such a multi-point Padé captured the true pole of the observables almost perfectly.

For the purposes of our analysis we use two types of Ansätze, the linear solver and the generalised χ^2 approach. The construction of both of these are based on the assumption that we have access to Taylor coefficients of the unknown function at some x_i,

$$R_n^m(x_i) = \frac{P_m(x_i)}{1 + Q_n(x_i)} = \frac{\sum\limits_{k=0}^{m} a_k\, x_i^k}{1 + \sum\limits_{j=1}^{n} b_j\, x_i^j}\,, \tag{1}$$

Assuming that the function to be approximated is $f(x_i)$, the linear solver approach attempts to determine the coefficients of the numerator and denominator of rational approximation by solving the following equations simultaneously. Since this system can become ill-conditioned, we have also solved this system in the fugacity variable, which reduces this ill-conditioning. Incorporating errors on the Taylor coefficient is then a two step process, since we first add noise to the Taylor coefficients and then solve for each such choice of coefficients.

$$\begin{aligned} P_m(x_i) - f(x_i)Q_n(x_i) &= f(x_i) \\ P'_m(x_i) - f'(x_i)Q_n(x_i) - f(x_i)Q'_n(x_i) &= f'(x_i) \\ P''_m(x_i) - f''(x_i)Q_n(x_i) - f(x_i)Q''_n(x_i) - 2f'(x_i)Q'_n(x_i) &= f''(x_i) \\ &\cdots \end{aligned} \tag{2}$$

The other approach we have used to solve for the rational function is based on a generalised fitting procedure, where we minimize the distance of the Taylor coefficients from the rational function ansatz, weighted by the estimated error on the corresponding Taylor coefficient. This method naturally encodes the error on the given Taylor coefficients.

$$\tilde{\chi}^2 = \sum_{j,k} \frac{|\frac{\partial^j R_n^m}{\partial x^j}(x_k) - c_j^{(k)}|^2}{|\Delta c_j^{(k)}|^2}. \tag{3}$$

We find very good agreement on the rational functions obtained from both of these methods. Results from both approaches and their comparison on the same data from our initial studies can be found in [13].

Note on spurious poles : We only consider closest poles to the axis (real or imaginary depending on what system one is studying) that are stable and have non-zero residue.

3. Case study I : Lee-Yang zeros in the vicinity of the Roberge-Weiss transition

As a first test of the method to probe Lee-Yang zeros on lattice theories, we studied 2+1 flavour QCD with physical quark masses at imaginary chemical potentials in [13], at temperatures close to and below the Roberge-Weiss (RW) transition temperature on two lattices namely $24^3 \times 4$ and $36^3 \times 6$. We simulated the system using highly improved staggered quarks (HISQ) [15] for the fermion action and using Symanzik improved Wilson action for the gauge fields. Gauge field configurations were generated using the SIMULATeQCD code from Bielefeld [16]. The RW transition temperature has previously been determined using $24^3 \times 4$ lattice using the above mentioned discretization and found to be around 201 MeV [17]. This provided us with a ballpark temperature to perform our simulations, close to and below $T_{RW} \sim 201$ MeV.

The quantity that we measured on the above lattices were the cumulants of the baryon number density given by,

$$\chi_B^1(T, \hat{\mu}_B) = \frac{n_B(T, \hat{\mu}_B)}{T^3} = \frac{\partial (p(T, \hat{\mu}_B)/T^4)}{\partial \hat{\mu}_B} \propto \frac{\partial \ln Z_{GC}}{\partial \hat{\mu}_B} \tag{4}$$

Given the relation of χ_B^1 with Z_{GC}, we can infer the following : *(i)* Since Z_{GC} is periodic in imaginary μ_B (μ_B^I), χ_B^1 is also periodic, *(ii)* χ_B^1 is odd in imaginary μ_B^I, *(iii)* Zeros of the partition function will show up as poles of χ_B^1. These properties make χ_B^1 a good candidate to choose as our function to be approximated by the multi-point Padé approach. The results of the approximation and the singularity structure can be found in [13, 18–20]. Here we will only show the results for the scaling of the closest poles to the μ_B^I axis in Fig. 1.

The ansatz that we use for the expected trajectory of the Lee-Yang zeros is given by recognizing that in terms of the scaling variable $z = \frac{t}{h^{1/\beta\delta}}$, the location of the edge singularity is a branch point of the singular part of the scaling function and hence it can be used to study the dependence of t and h, which are the relevant scaling fields of the Ising model. In terms of this, after choosing a map from the Ising model fields to the scaling fields of the RW transition, one can write,

$$z = z_c \equiv |z_c| e^{i\pi/(2\beta\delta)} \tag{5}$$

where the phase of the YLE is determined by demanding that for the Ising model, all Lee-Yang zeros lie on the imaginary external magnetic field h axis. Using the following map between the Ising model and RW fields,

$$t = t_0^{-1} \left(\frac{T_{RW} - T}{T_{RW}} \right) , \tag{6}$$

$$h = h_0^{-1} \left(\frac{\hat{\mu}_B - i\pi}{i\pi} \right) , \tag{7}$$

where $\hat{\mu}_B = \mu_B/T$ and t_0, h_0, and T_{RW} are nonuniversal parameters. We now can solve $t/h^{1/\beta\delta} \equiv$

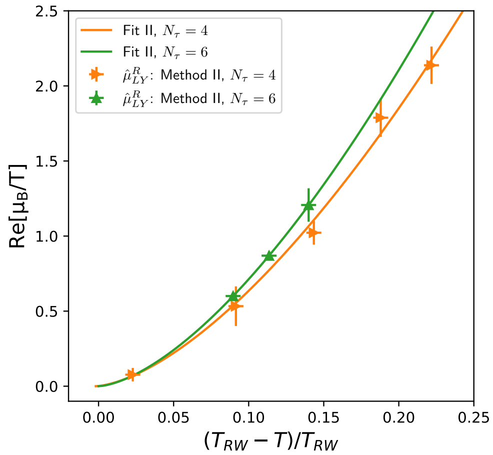

Figure 1: RW scaling (Figure from [19]) : Scaling of the real part of the closest poles to the axis for for $N_\tau = 4$ & 6. Fit : $\mu_B^R = a.\,[(T_C - T)\,/T_C]^{\beta\delta}$

$z_c = |z_c| e^{i\frac{\pi}{2\beta\delta}}$ for $\hat{\mu}_B$ to obtain,

$$\hat{\mu}^R_{LY} = \pm\pi \left(\frac{z_0}{|z_c|}\right)^{\beta\delta} \left(\frac{T_{RW} - T}{T_{RW}}\right)^{\beta\delta}, \tag{8}$$

$$\hat{\mu}^I_{LY} = \pm\pi\,, \tag{9}$$

where the normalization constant z_0 is defined as $z_0 = h_0^{1/\beta\delta}/t_0$. Here Eqs (8) and (9) define the temperature scaling of the Lee-Yang edge singularity, associated with the RW critical point. The scaling is shown in Fig. 1 and the results for the fit are shown in Table 1. The next step is continuum extrapolation of the RW transition temperature for which simulations are underway. For some preliminary finite size scaling results for this analysis see [20]. Some new results for extrapolating to the real μ_B axis have also recently been done by us [21], which also gives us a rough estimate for the critical end point (CEP), conjectured to appear in the QCD phase diagram.

N_τ	a	T_C	χ^2	z_0
4	22.66 (2.18)	206.12 (2.67)	0.61	8.68 (84)
6	26.085 (5)	208.704 (2)	0.000324	8.696 (2)

Table 1: Fit parameters obtained for the expected scaling of the LYEs for the RW transition.

4. Critical exponents of 2D Ising model via Lee-Yang zero analysis

A further test of the method was performed on extracting the critical exponents for the 2D Ising model by us in [22]. This theory is, on the one hand fully solved due to Onsager, and on the other hand rich enough to show a phase transition. Therefore it is a good model for testing new methods aimed at understanding critical phenomena on finite lattice volumes. We can perform a self-consistent study using the complex partition function zeros in the inverse temperature β and

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external magnetic field H planes, to determine the critical temperature, critical exponents ν, and exponent product $\beta\delta$. For this study we have performed two kinds of simulations : *(i)* Setting $H = 0$ and computing the poles of the specific heat in the complex β plane. These are known in the literature as Fisher zeros [7]. The finite size scaling of the closest Fisher zero to the real β axis allows us to determine the critical inverse temperature β_c and the critical exponent ν. *(ii)* Once we determine the critical temperature, one can perform simulations at $T_c = 1/\beta_c$, with the external magnetic field turned on and determine the volume scaling of the closest Lee-Yang zeros. This scaling allows us to determine the gap exponent $\beta\delta$.

For the 2D Ising model simulations performed in [22], we use the cluster spin flip algorithm based on [23], since it is well known that this type of algorithm does not suffer from critical slowing down, allowing us to obtain statistically independent configurations. From the simulations we compute the following quantities : average magnetization $\langle M\rangle$, average energy density $\langle E\rangle$ and the specific heat capacity (at $H = 0$) $C_H = \left(\frac{\partial E}{\partial T}\right)_{H=0}$ for different lattice volumes. We then use the multi-point Padé approximation to approximate C_H and extract the closest stable poles β_0 (Fisher zeros) to the real β axis. These can be shown to have the following finite volume scaling [24],

$$|\beta_0 - \beta_c| \propto L^{-1/\nu} \tag{10}$$

We further approximate $\langle M\rangle$ by the multi-point Padé approximation and extract the stable pole, this time in the complex external magnetic field plane, closest to the real H axis, H_0. We repeat this procedure for different lattice volumes and fit the poles according to the following scaling ansatz [24, 25]

$$|H_0 - H_c| \propto L^{\beta/\nu - d} \tag{11}$$

The results of the fits for the Lee-Yang scaling with volume is shown in Fig. 2 and the results from the fits for the relevant exponents are shown in Table. 2. All calculation details and fits can be found in [22].

Quantity	Fit Results	Exact value	χ^2/dof
ν	1.014(60)	1	1.3
β_c	0.4404(19)	~ 0.4407	1.44
$\beta\delta$	1.881(93)	1.875	1.2

Table 2: Results for the fits for critical inverse temperature β_c, the exponent ν, and the gap exponent $\beta\delta$.

5. Universal location of LYE from continuum extrapolated scaling function in 3d O(N) model

In the thermodynamic limit the Lee-Yang zeros coalesce into branch cuts terminating at Yang-Lee edge singularities (YLE). These YLEs also mark the branch points of the scaling function in the symmetric phase. Although the phase of these branch points can be determined by the underlying

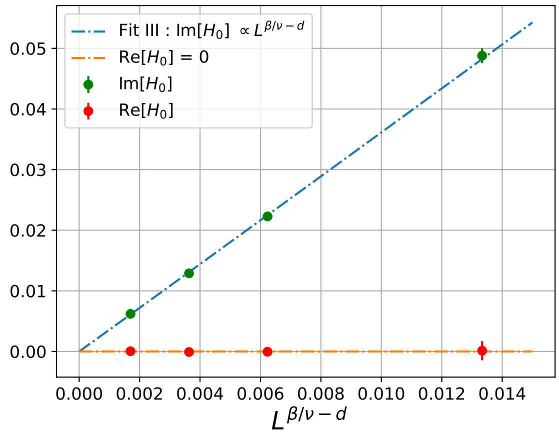

Figure 2: Finite size scaling of $\mathrm{Im}(H_0)$, (Figure from [22]). The value obtained from fits is $\beta/\nu - d = -\beta\delta = -1.881(93)$, as shown in Table 2, which also gives $\beta = 0.119(93)$.

universality class having the Lee-Yang zeros lie entirely on the imaginary external magnetic field axis, there is currently no analytical way to deduce the absolute value of these branch points. Recently, for some $O(N)$ theories, the value has been determined by the Functional Renormalisation Group (FRG) approach [26, 27]. Using continuum extrapolated results from Monte Carlo studies of the scaling functions for $O(N)$ models for $N = \{1, 2, 4\}$ in [28], we have in [29] determined the location of these singularities for the first time from lattice simulated data.

As mentioned, for our analysis we have made use of data on continuum extrapolated infinite volume scaling functions from [28]. Here the authors have performed Monte-Carlo simulations of improved ϕ^4 models in which parameters can be tuned to specify the universality class between $O(1)$, $O(2)$ and $O(4)$. Near criticality, the free energy is dominated by its singular part (denoted below as $f(z)$) which can be expressed as a function of a single variable $z = \frac{t}{h^{1/\beta\delta}}$, called the scaling variable. Here the reduced temperature t and the external magnetic field h are the two relevant scaling fields for the Ising transition. Schofield in [30] introduced a new parametrization in terms of new scaling fields r and θ,

$$M = m_0 r^{\beta}\theta \,, t = r(1-\theta^2) \,, h = h_0 r^{\beta\delta} h(\theta) \,, \tag{12}$$

with M denoting the magnetization, such that the entire scaling-law behaviour is contained in r which can be seen to be a radial coordinate. In the above $h(\theta)$ is a polynomial ansatz. Using this parametrization, we can express the scaling functions and the scaling variable as,

$$f_G(\theta(z)) = -\frac{\partial f}{\partial h} h^{-1/\delta} = \theta \left(\frac{h(\theta)}{h(1)}\right)^{-1/\delta} , \quad z(\theta) = \frac{1-\theta^2}{\theta_0^2 - 1}\theta_0^{1/\beta} \left(\frac{h(\theta)}{h(1)}\right)^{-1/\beta\delta} \tag{13}$$

Further demanding that at the Lee-Yang edge singularity, $\frac{\partial f}{\partial \theta} \to \infty$, we can obtain the location of the edge by solving the following equation,

$$\frac{dz(\theta)}{d\theta} = 0 \quad \Leftrightarrow \quad 0 = 2\beta\delta\theta h(\theta) - \left(\theta^2 - 1\right) h'(\theta) \tag{14}$$

Here we will only list the most important findings of the paper [29] in Table. 3. However, an in-depth analysis has been performed in the paper explicitly showing regions where the map between $z \to \theta$ is invertible and well defined. We also explicitly calculate the jump in the scaling function along the branch cut originating from the LYE which is consistent with theoretical expectations.

Table 3: Comparison of $|z_{LY}|$ values from Lattice data and FRG results for $O(1)$, $O(2)$, and $O(4)$. The value for $O(1)$, $O(2)$ agree within errors whereas the value for $O(4)$ differs by about 15% The FRG results can be found in [26, 27].

Approach	$O(1)$	$O(2)$	$O(4)$
Lattice	2.429(56)	1.95(7)	1.47(3)
FRG	2.43(4)	2.04(8)	1.69(3)

6. Conclusions and Outlook

The goal of this talk and subsequent proceedings was to show how one can extract Lee-Yang zeros and edge singularities from lattice simulations. In the first part, multi-point Padé was shown to be successful in extracting the relevant Yang-Lee zeros associated with the RW transition. From the temperature scaling studies of these zeros, the correct transition temperature was recovered for $N_\tau = 4$, which had been previously determined from independent lattice simulations. Further the transition was shown to be consistent with the $3d - Z_2$ universality class, which has also been seen in earlier studies. The method was then applied to the 2D Ising model and based on the volume scaling of the closest poles of the magnetization and specific heat, the transition temperature β_c and the critical exponents ν and$\beta\delta$ were reproduced with very good precision. For the second part, in another type of study involving continuum extrapolated lattice data available on the infinite volume scaling functions for $O(1)$, $O(2)$ and $O(4)$ universality classes, the universal location of the LYE was computed and shown to be consistent with FRG results (except for the $O(4)$ class, where a difference of about $\sim$ 15% was observed).

The future plans for this work include obtaining continuum extrapolated results for the RW transition by simulating $N_\tau = 8$ lattice volumes. Recently we have used this method also to probe low temperatures and some results have been put forward by us based on obtaining an estimate for the CEP [21]. This is not without caveats for three main reasons : *(i)* Rigorous results on the scope of validity of such multi-point Padé don't yet exist, all information is currently based on numerical experiments performed by our group. *(ii)* Since we can only perform simulations at $\mu_B = 0$ or purely imaginary μ_B, any estimate for the CEP is an extrapolation. It is not yet clear what the effect of a small scaling window will be on these results. *(iii)* On the lattice we have to deal with both finite volume and cut-off effects, while finite volume effects in themselves are not a big problem as we know the finite size scaling laws for these LYEs, the inter-dependence of these limits for any lattice computation can potentially cause problems as not enough research on the cut-off effects for these LY zeros exists. For the latter work on obtaining the universal location of LYE from lattice data, there are not many caveats and the work is mostly self-consistent. However different, non-polynomial Ansätze, for $h(\theta)$ can be considered such that we can deduce information like the critical exponent associated to the LYE, namely the "edge" exponent. With this we hope that we were able to convince the reader to try both the Lee-Yang approach to study phase transitions and the multi-point Padé method to extract them in their research. We further hope that we have provided evidence that continuum lattice studies can give consistent results on critical phenomena when compared to more direct approaches like FRG.

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