Universal location of the Yang-Lee edge singularity in $O(N)$ theories

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(Dated: June 24, 2020)

We determine a previously unknown universal quantity, the location of the Yang-Lee edge singularity for the $O(N)$ theories in a wide range of $N$ and various dimensions. At large $N$, we reproduce the $N \to \infty$ analytical result on the location of the singularity and, additionally, we obtain the mean-field result for the location in $d = 4$ dimensions. In order to capture the nonperturbative physics for arbitrary $N$, $d$ and complex-valued external fields, we use the functional renormalization group approach.

I. INTRODUCTION

From the work of Yang and Lee [1, 2], it is known that the proper domain of the partition function is the complex plane of the thermodynamic parameters. Yang and Lee established that the infinite volume partition function has zeroes and their distribution determines the phase diagram of the system in the infinite volume limit. Specifically, the Lee-Yang theorem states that the zeroes lay at purely imaginary values of symmetry-breaking external field $h$ for Ising-like systems such as $O(N)$ symmetric $\phi^4$ theory. In the case of the spontaneously broken regime with temperatures $T < T_c$, the distribution of zeroes crosses the real $h$ axis, resulting in a first-order phase transition as one varies the field $h$ across the $h = 0$ line. In the symmetric region with $T > T_c$, there is no phase transition for any real value of $h$; in the complex plane of $h$, this is manifested by the formation of a gap in the distribution of zeroes with edges located at $h_c = \pm ih_c(T)$. In the infinite volume limit, the zeroes coalesce forming branch-point singularities at $h_c$, also known as Yang-Lee edge singularities. These singularities can be treated as ordinary critical points. In their vicinity, independent of the number of field components $N$, the system is described by a one-component $\phi^4$ theory (with purely imaginary coupling) [3] and thus has upper critical dimension $d = 6$. It was established that near $h_c$, the magnetization behaves as $M \sim M_c + (h^2 - h_c^2)^{\sigma_{YL}}$, where $\sigma_{YL}$ is the so-called edge critical exponent. Its value was computed with good precision $\sigma_{YL} = 0.085(1)$ [3, 4] (see also functional renormalization group analyses with compilations of different approaches in Ref. [5, 6]).

Near the critical point, due to the absence of a relevant length scale, the free energy is a homogeneous function of the relevant thermodynamic parameters, the reduced temperature, $t \propto (T - T_c)$, and the external field, $h$. This homogeneity allows one to quantify critical properties of the system by a function of one variable: the so-called magnetic equation of state $M = h^{1/\Delta} f_G(z)$, where $z$ is the scaling variable $z = th^{-1/\Delta}$, where $\Delta = \beta \delta$, $\beta$ and $\delta$ are universal critical exponents, and $f_G(z)$ is the universal scaling function characterizing all systems within the same universality class.

The scaling function naturally incorporates the edge singularities. As we alluded to above, the Lee-Yang theorem states that they are located at purely imaginary values of the external field. This uniquely fixes the argument of the scaling variable at the edge singularity $z_c = \exp(\pm i \pi / \Delta)$. The critical exponents $\beta$, $\delta$, and $\sigma_{YL}$, have been well studied and determined to high precision, while the location itself, i.e. the absolute value $|z_c|$, has never been found for $1 < d < 4$ outside of the mean-field approximation or the large $N$ limit! The importance of finding the location is difficult to overstate, as being the closest to the real axis, this branch point determines the behaviour of the magnetization for real values of the temperature and the external field. The high-order coefficients of a Taylor expansion of the free energy around any finite value of $z$ are defined by $z_c$ and $\sigma_{YL}$. This is of particular interest, e.g., for the determination of the QCD equation of state at finite density on the lattice, where a sign problem hinders direct simulations. A common strategy is to use extrapolations based on the expansion of the free energy about vanishing chemical potential [7, 8]. The edge singularity determines the radius of convergence of this expansion [9–11].

We want to note that the often-applied $\epsilon$-expansion to $\phi^4$ theories near four dimensions is not suitable for determining the location of the edge singularity. This is due to the aforementioned fact that in the vicinity of the edge the critical dimension of the system is six, rather than four as for the original $\phi^4$ theory. This manifests itself in the appearance of non-perturbative terms [12] when one attempts to extract the location of the edge singularity. Lattice simulations, a powerful non-perturbative method often applied to determine the universal properties, are hindered by a sign problem as in order to extract the location of the singularity one has to perform them at imaginary values of $h$ or complex values of the temperature.

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In this letter, for the first time, we determine the previously unknown location of the Yang-Lee edge singularity for \( O(N) \) symmetric \( \phi^4 \) theories for a wide range of \( N \) in three dimensions demonstrating the known analytic result in the large \( N \) limit and, by varying the number of dimensions, reproducing the mean-field approximation. To do so, the nonperturbative functional renormalization group is implemented using approximations that enable us to determine the location \( z_c \).

II. FRG APPROACH TO SCALING FOR COMPLEX EXTERNAL FIELDS

To capture the inherently nonperturbative physics in the vicinity of a second order phase transition, we use the functional renormalization group (FRG) [13–15]. It describes the RG flow of the scale-dependent effective action, \( \Gamma_k \), as a function of a momentum scale parameter, \( k \),

\[
\partial_t \Gamma_k[\phi] = -\frac{1}{2} \text{Tr} \left\{ \partial_k R_k \left( \delta^2 \Gamma_k[\phi] \over \delta \phi \delta \phi^j \right) + R_k \right\},
\]  

(1)

where \( R_k \) is the infrared regulator function which determines how the low momentum modes are screened at scale \( k \). The flow equation (1) prescribes the behaviour of \( \Gamma_k \) between the classical action at an initial scale \( k = \Lambda \) in the ultraviolet, \( \Gamma_k = S \), and the desired full quantum action at \( k = 0 \), \( \Gamma_k = \Gamma \). The FRG provides a versatile realization of the Wilsonian RG and is as such well-suited to study critical physics. Both the scaling function and the critical exponents have been computed in great detail for \( O(N) \) theories for real external fields with the FRG, see, e.g., [16–30].

In this letter, we use the first order derivative expansion [18, 31] of the scale-dependent effective action in Euclidean space,

\[
\Gamma_k = \int d^{d+1}x \left\{ \frac{1}{2} Z_k(\rho)(\partial_{\rho}\phi)^2 + U_k(\rho) - h\sigma \right\},
\]  

(2)

where \( d \) is the number of spatial dimensions, the field \( \rho \) is defined as \( \rho = \frac{1}{2} \phi^2 = \frac{1}{2}(\sigma^2 + \pi^2) \), \( U_k(\rho) \) is the scale dependent potential, and \( h \) is the external field explicitly breaking the \( O(N) \) symmetry. \( \sigma \) denotes the radial excitation, and \( \pi \) the Goldstone modes. The extension to finite temperature is done by using the standard Matsubara formalism \( \int \frac{d\rho}{2\pi} \rightarrow T \sum_n \) and \( p_0 \rightarrow 2n\pi T \). Accordingly, we use the optimized regulator function \( R_k \) for the spatial momentum modes, 

\[
R_k(\tilde{\rho}) = Z_k(k^2 - \tilde{\rho}^2)\Theta(k^2 - \tilde{\rho}^2),
\]

put forward in [32, 33] and refer to [34–36] for detailed discussions regarding the regularization scheme. Here we comment that the commonly applied local potential approximation (LPA) which neglects the scale-dependence of the wavefunction renormalization, \( Z_\phi,k(\rho) = 1 \), giving zero anomalous dimension \( \eta \), is not appropriate to study the location of the edge singularity since \( \eta \) is expected to be of order one in its vicinity. This necessitates the inclusion of scale-dependent wavefunction renormalization, which we assume to be field-independent, \( Z_k(\rho) = Z_k \). This approximation is referred to as LPA'. The anomalous dimension is related to the wavefunction renormalization via \( \partial_t Z_k = -\eta_k Z_k \), where we introduced the RG time \( t = \ln(k/\Lambda) \).

To describe critical phenomena, it is helpful to look at the renormalization flow of dimensionless observables rather than the dimensionful counterparts as their magnitudes can vary wildly. The flow for the dimensionless effective potential, \( \bar{U}_k(\rho) = k^{-d-1}U_k(\rho) \) where \( \rho = Z_k k^{d-1}\bar{\rho} \) is the dimensionless renormalized field, can be obtained by evaluating (1) on uniform field configurations at fixed \( \bar{\rho} \) which yields

\[
\partial_t \bar{U}_k(\rho) = -(d + 1)\bar{U}_k + (d - 1 + \eta_k)\bar{\rho}\bar{U}_k' + \frac{v_d}{2(2\pi)^d} \left\{ \frac{N - 1}{\sqrt{1 + m^2}} \left( 1 + 2n_\pi \right) \sqrt{1 - \frac{\rho}{\bar{\rho}}} \right\},
\]  

(3)

where \( v_d = S_{d-1}/d \) with \( S_{d-1} = 2\pi^{d/2}/\Gamma(d/2) \), \( n_{\sigma,\pi} = n_{\sigma,\pi}(T, k) \) are the standard Bose-Einstein distribution functions, and the primes denote derivatives with respect to \( \rho \). The dimensionless renormalized masses, \( m_{\sigma,\pi} \), are given by \( \bar{m}^2 = \bar{U}' \) and\( \bar{m}^2 = \bar{U}' + 2\bar{\rho}\bar{U}'' \).

In order to numerically solve (3) we consider a third order Taylor expansion of the dimensionless effective potential about the scale dependent minimum \( \bar{\rho}_{0,k} \): \( \bar{U}_k = \sum_{i=0}^3 \frac{a_{i,k}}{(\rho - \bar{\rho}_{0,k})^i} \) for the sake of simplicity. It is important to note that for a non-zero external field \( h \), one must have \( \partial_h \bar{U}_k = \bar{h} \), or \( a_{1,k} = \bar{h} \), where \( \bar{h} \) is the dimensionless renormalized counterpart of \( h \), \( \bar{h} = k^{-(d+3)/2}\pi^{-1/2}h \). This ensures that the expansion is about the physical minimum. If \( h = 0 \), we see that we have either \( a_{1,k} = 0 \) and \( \bar{h} \neq 0 \) (spontaneously broken regime) or \( a_{1,k} \neq 0 \) and \( \bar{h} = 0 \) (symmetric regime).

To extract the anomalous dimension, one uses the projection

\[
\eta_{\phi,k} = -\frac{1}{2Z_k} \frac{\partial}{\partial p_0} \left[ \frac{\delta^2}{\delta \pi_k(\rho)(-\pi_k)} \right],
\]  

(4)

where the choice of \( i \) is arbitrary. The result is

\[
\eta_{\phi,k} = \frac{4v_d}{(2\pi)^d} \bar{U}_k(\bar{\rho}_0)^2 \times \frac{1}{k} \sum_{n = -\infty}^{\infty} \frac{1}{\left( \frac{\bar{m}^2}{k^2} + \bar{m}^2 + 1 \right)^{2}}.
\]  

(5)

The above sum is evaluated to a closed form in practice, though its form is not insightful [37].

The flow equations above, along with a set of initial conditions at the scale \( \Lambda \), describe a system which begins
in the spontaneously broken regime at $T = 0$ and experiences symmetry restoration at an intermediate scale below $\Lambda$ for temperatures above the critical temperature $T_c$. We choose the following initial conditions for the FRG flow. For each $N$ and $d$, we set $\Lambda = 800, a_{2,\Lambda} = 10^{-2}\Lambda^{d-3}, a_{3,\Lambda} = 0$, and tune $\rho_{0,\Lambda}$ such that the critical temperature is somewhere in the range $0.01 < T_c/\Lambda < 0.4$. We omitted the units on $\Lambda$ since the choice is arbitrary.

Note that the parameter $\rho_0$ is non-perturbative and cannot be found using the $\epsilon$-expansion. The dash-dotted line shows a fit motivated by the parametrization of the equation of state for O(1) $|z_c| = |z_c^{\text{MF}}| \{1 + (4 - d)^2[p_1 \ln(4 - d) + p_2]\}$, see Ref. [12]. Note that the parameter $p_2$ is non-perturbative and cannot be found using the $\epsilon$-expansion. The dash-dotted line shows a fit motivated by the parametrization of the equation of state for O(1) $|z_c| = |z_c^{\text{MF}}| \{1 + (4 - d)^2[p_1 \ln(4 - d) + p_2]\}$, see Ref. [12].

and its failure to capture first-order phase transitions. Furthermore, the edge occurs at purely imaginary values of the external field, another case for which the FRG equations become numerically challenging. To circumvent this issue, we note that the edge can be treated as an ordinary second-order phase transition, and we can determine its location by studying the peak of the magnetic susceptibility, $\chi_\sigma \propto 1/m_0^2$, at a complex external field with just a small real part. Given that near the edge the order parameter $\sigma$ behaves as $\sigma - \sigma_c \sim (h^2 - h_0^2)^{\gamma YL}$ [3], the susceptibility for the sigma field behaves as $\chi_\sigma \sim 2h^2 \sigma_Y h^2 (h^2 - h_0^2)^{\gamma YL-1}$. From this form, we see that for any sufficiently small $\text{Re}(h)$, $|\chi_\sigma|$ will have a peak at some $\text{Im}(h) = h_{\text{peak}}$. Moreover, $h_{\text{peak}}$ is a quadratic function of $\text{Re}(h)$ for sufficiently small values of $\text{Re}(h)$. Thus, we can scan the complex $h$-plane at fixed reduced temperature $t$ along the first quadrant parallel to the imaginary axis. Then $h_c$ can be determined by incrementally decreasing $\text{Re}(h)$, determining $h_{\text{peak}}$ for each increment, performing a quadratic fit to the data, and extrapolating to purely imaginary external fields. From this, we find the location of the edge as $z_c = th_{\epsilon^{-1/\Delta}}$.

There are several sources of error in this work, presumably the largest being the systematic error which results from working in LPA' with a low-order Taylor expansion of the effective potential. One manifestation of the systematic error can be the violation of the hyperscaling relation between the exponents: $2 - \eta = d(\delta - 1)/(\delta + 1)$. For our work, we find this violation to be at the sub-permille level. Regarding the critical exponents themselves, e.g. for $d = 3$ and $N = 1(2)$, the disagreement with well-known results from Ref. [39] for the edge critical exponent $\Delta$ is about $6\%$ ($8.5\%$), for $\eta$ about $0.6\%$ ($8\%$). We note that a

FIG. 1. The magnitude of the location of the Yang-Lee edge singularity $|z_c|$ as a function of $N$ in three dimensions. The large $N$ result is indicated by the solid line. There is a non-monotonous behaviour in the approach to large $N$ limit.

FIG. 2. The magnitude of the location of the Yang-Lee edge singularity $|z_c|$ for $N = 1, 2, 4, 100$ as a function of the number of dimensions $d$. The solid line demonstrates the mean-field value. The dashed lines display a fit motivated by the parametrization of the equation of state for O(1) $|z_c| = |z_c^{\text{MF}}| \{1 + (4 - d)^2[p_1 \ln(4 - d) + p_2]\}$, see Ref. [12].
TABLE I. The location of the Yang-Lee edge singularity for different values of $N$ in three dimensions. In addition, the analytical result of Eq. (8) for $N \to \infty$ is $|z_c| \approx 1.6494$. The errors are from the numerical determination of $|z_c|$.

| $N$ | 1 | 2 | 3 | 4 |
|-----|---|---|---|---|
| $|z_c|$ | $2.171^{+0.004}_{-0.009}$ | $2.004^{+0.007}_{-0.005}$ | $1.833^{+0.010}_{-0.001}$ | $1.730^{+0.004}_{-0.009}$ |

| $N$ | 5 | 6 | 7 | 10 |
|-----|---|---|---|---|
| $|z_c|$ | $1.623^{+0.010}_{-0.001}$ | $1.583^{+0.004}_{-0.005}$ | $1.562^{+0.009}_{-0.001}$ | $1.548^{+0.009}_{-0.001}$ |

| $N$ | 20 | 100 | 200 | 500 |
|-----|-----|-----|-----|-----|
| $|z_c|$ | $1.572^{+0.001}_{-0.009}$ | $1.627^{+0.001}_{-0.007}$ | $1.637^{+0.003}_{-0.005}$ | $1.644^{+0.008}_{-0.001}$ |

Other error sources are from the implementation of a finite infrared scale $k_0$ at which the RG flows are terminated, and from the fits to obtain the exponents and the value of $h_c$. In the region with spontaneously restored symmetry, both the radial and the Goldstone modes have a finite mass which cuts-off the RG flow at scales below these mass scales. The same is true for the system with non-zero $h$, as the explicit symmetry breaking renders the Goldstone modes massive even in the broken phase. However, in the broken phase at vanishing $h$, for all $N > 1$ the massless Goldstone bosons prohibit the flows from ever terminating. One can still choose a $k_0$ such that the continued running of the flows below this value contributes negligibly to the error. The case of $N = 1$ is saved from this as there are no Goldstone bosons, and the sigma mass stops the flows. For this work, we chose a common $k_0$ for all $N$ and $d$ such that the error is negligibly small.

The fits for the exponents also yield error, although they are at or below the percent level and we do not report them here. The sole contributor to the error bars seen in Figures 1 and 2 and Table I is the extrapolation to pure imaginary values of the field $h$ described above. Instead of using the errors from the quadratic fit and the use of splines, we prescribe a surely larger error around the determination of $h_c$ by its distance to the nearest data point. Consequently, the error bars are all of very similar size.

### III. RESULTS AND DISCUSSIONS

Our results for the location of the Yang-Lee edge singularity, $z_c$, are shown in Figure 1 for $d = 3$ and numerous $N$, and in Figure 2 for $N = 2, 4, 100$ and various $d$. Analytically, $z_c$ is only known in two limiting cases: large $N$ limit, i.e. for $N \to \infty$, and in the mean-field approximation. For both, the magnetic equation of state can be written in the following form (see e.g. [42–44])

$$ f_G(z) \left[ z + f_G^2(z) \right]^{\gamma} = 1, \tag{7} $$

where $\gamma = 1 \left( \gamma = \frac{2}{d-2} \right)$ for mean-field (large $N$ in $d < 4$ dimensions). Due to its nature as a branch point, the location of the Yang-Lee edge singularity can be found from the condition that the derivative of the inverse function is zero, $z'(f_G) = 0$. This leads to

$$ |z_c| = (2\gamma + 1)((2\gamma)^{\frac{2}{2\gamma+1}}), \quad \text{Arg} \ z_c = \frac{\pi}{2\gamma+1}. \tag{8} $$

Thus in mean-field approximation (in the large $N$ limit, $d = 3$) one gets $|z_c^\text{MF}| \approx 1.8899 \ (|z_c^\infty| \approx 1.6494)$.

The fact that our numerical calculations reproduce the analytical results for $|z_c|$ is highly non-trivial in that it provides a direct test of our FRG approach and the method of extracting the location of the singularity. Figure 1 demonstrates the converge of $|z_c|$ to the large $N$ value. The results are tabulated in Table I to highlight the precision. We note that $|z_c|$ displays some non-monotonous behavior as it dips below its large $N$ value before approaching the limit from below. For the convergence of $|z_c|$ to its mean field result, see Figure 2. We also see here non-monotonous behavior as the dimension is varied. Our numerical calculations for $N = 100$ faithfully reproduce infinite $N$ result in arbitrary number of dimensions $3 < d < 4$.

To give an explicit example for importance of the edge singularity, we determine the asymptotic form of the coefficients of the Taylor expansion of $f_G(z)$. This can be done solely based on its analytic structure in the complex plane. For the sake of simplicity, we consider the expansion near the origin. In this case, the theorem of Darboux states (see e.g. Ref. [45]) that the $n$-th expansion coefficient for sufficiently large $n$ is

$$ f_G^{(n)} \sim 2B_0 |z_c|^{-n} n^n \frac{n^{\sigma_{\text{YL}}-1}}{\Gamma(\sigma_{\text{YL}})} \cos \left( \beta_0 - \frac{\pi n}{2\Delta} \right), \tag{9} $$

where $B_0$ and $\beta_0$ are defined as the value of the analytic part of the magnetization at the singularity $B_0 \exp(i\beta_0) = \lim_{z \to z_c}(1 - z/z_c)^{-\sigma_{\text{YL}}} (f_G(z) - f_G^*(z_c))$. This explicitly demonstrates that the expansion coefficients are uniquely defined by $|z_c|$, $\Delta$ and $\sigma_{\text{YL}}$.

### IV. CONCLUSIONS

In this letter we have provided the first results on a previously unknown universal quantity for $O(N)$-like theories. We determined the location of the Yang-Lee edge singularity for the $O(N)$ universality class for a wide range of $N$ and dimensions $d$. Our numerical calculations reproduce known analytical results for $z_c$ in the infinite $N$ limit and in the mean-field approximation ($d = 4$).
ACKNOWLEDGMENTS

We thank B. Friman, A. Kemper, J. M. Pawlowski, R. Pisarski, K. Redlich, T. Schaefer, M. Stephanov, M. Unsal, and N. Wink for illuminating discussions. V.S. is thankful to S. Mukherjee for encouragement and discussions which eventually led to this work. V.S. acknowledges support by the DOE Office of Nuclear Physics through Grant No. DE-SC0020081. F.R. is supported by the U.S. Department of Energy under contract DE-SC0012704. V.S. thanks the ExtreMe Matter Institute EMMI (GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany) for partial support and hospitality.

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We checked that our numerical calculations reproduce the O(4) magnetic equation of state of Ref. [46] for real values of the argument.

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