NONANALYTICITY OF THE BETA-FUNCTION AND SYSTEMATIC ERRORS IN FIELD-THEORETIC CALCULATIONS OF CRITICAL QUANTITIES

M. CASELLE

Dip. di Fisica dell'Università di Torino and INFN, Sez. Torino, I-10125 Torino, Italy
E-mail: caselle@to.infn.it

A. PELISSETTO

Dip. di Fisica dell'Università di Roma "La Sapienza" and INFN, Sez. Roma 1, I-00185 Roma, Italy
E-mail: andrea.pelissetto@roma1.infn.it

E. VICARI

Dip. di Fisica dell'Università di Pisa and INFN, Sez. Pisa, I-56100 Pisa, Italy
E-mail: vicari@df.unipi.it

By considering the fixed-dimension perturbative expansion, we discuss the nonanalyticity of the renormalization group functions at the fixed point and its consequences for the numerical determination of critical quantities.

1 Introduction

In the last thirty years there has been a significant progress in the understanding of critical phenomena. It has been realized that the behavior in the neighborhood of a critical phase transition, i.e. a transition characterized by long-range correlations, is determined by very few properties: the space dimensionality, the range of the interactions, the number of components of the order parameter, and the symmetry of the Hamiltonian. This means

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that physically different systems may have the same critical behavior. For instance, a simple fluid at the liquid-vapor transition and a uniaxial magnet at the Curie point behave identically: critical exponents, dimensionless amplitude ratios, and scaling functions are numerically equal. This phenomenon, which is referred to as universality, has been understood within the Wilson's renormalization group (RG) approach. The conceptual setting is thus quite well established, and the theory of critical phenomena has reached the maturity of well-verified theories like, for instance, QED or the standard model of weak interactions. Nonetheless, it is important to improve experiments and theoretical calculations in order to understand the limits of validity of these theories. In order to test QED and the standard model several experiments have provided accurate estimates that can be directly compared with the theoretical predictions. The most classical ones are the experiments on the g-factor of electrons and muons, and on the Lamb shift in hydrogen. In the theory of critical phenomena, the superfluid transition in ^{4}He plays a very special role, since it is essentially the only case in which one can determine a critical exponent with an accuracy of 10^{-4}. This is due to a combination of extremely favorable conditions: the singularity in the compressibility of the fluid is particularly weak; it is possible to prepare very pure samples; experiments may be performed in a microgravity environment (for instance on the Space Shuttle), thereby reducing the gravity-induced broadening of the transition. A recent experiment [1,2] obtained an extremely accurate estimate[a] of the critical exponent of the specific heat, $\alpha = -0.01056(38)$. This result should be compared with the most precise theoretical estimates: the analysis of high-temperature (HT) expansions gives [3,4] $-0.0146(8)$, $-0.0150(17)$; Monte Carlo (MC) simulations give [3,5] $-0.0148(15)$, $-0.0169(33)$; the analysis of the $d = 3$ perturbative expansion gives $-0.0112(21)$ (variational perturbation theory [6–8]) and $-0.011(4)$ (Borel resummation [9]). There is a clear discrepancy between the most accurate theoretical estimates and the experimental result. However, in order to understand whether the difference is truly significant, we must ask the question: Are the quoted errors reliable? Our experience, looking backward in time, is that there is a natural tendency to be overconfident in one's own results, and thus to systematically underestimate the errors: As Hagen Kleinert [8] put it, each one has a tendency to

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[a]The original result reported in Ref. [1] was incorrect. The new estimate is reported in Ref. [2]. The error which is reported in the text is a private communication of J. Lipa to the authors of Ref. [3].

apply the "principle of maximal optimism". Clearly, further theoretical and experimental investigation is needed to settle the problem.

In order to set correct error bars, it is necessary, although clearly not sufficient, to have a good understanding of the possible sources of systematic error. In MC and HT works, most of the systematic error is due to the nonanalytic corrections to scaling. Indeed, in N-vector systems, there are corrections t^Δ (t is the reduced temperature) to the leading scaling behavior, with $\Delta \approx 0.5$–0.6 in the physically relevant cases $0 \leq N \leq 4$. In the analysis of the MC data and of the HT series, these slowly decaying corrections require careful extrapolations, in the absence of which precise but incorrect results are obtained. To give an example, we report here some recent results for the four-point renormalized coupling g^* in the three-dimensional Ising model (see the discussion in Sec. 5 of Ref. [10] and Fig. 1 reported there):

MC, no nonanalytic corrections [11]: $g^* = 25.0(5)$;
MC, with nonanalytic corrections [10]: $g^* = 23.7(2)$;
HT, no nonanalytic corrections [12]: $g^* = 24.5(2)$;
HT, with nonanalytic corrections [13,10]: $g^* = 23.69(10), 23.55(15)$.

For comparison, perturbative field theory gives $g^* = 23.64(7)$ [9], while a recent analysis of improved HT expansions gives $g^* = 23.49(4)$ [14]. Clearly, neglecting the corrections to scaling introduces a large systematic error. And, even worse, there is no way to evaluate it, unless one assumes that nonanalytic corrections are really there.

A solution to these problems is represented by the improved models [3–5,14–18] which are such that the leading scaling correction (approximately) vanishes. The systematic errors are now sensibly reduced and one obtains more reliable estimates.

MC and HT analyses, although different in practice, are very similar in spirit, and indeed they are affected by the same type of systematic errors. In order to assess the reliability of the results, it is thus important to have a different approach to compare with. Field theory provides it and indeed independent estimates can be obtained by using a variety of different methods: the ϵ-expansion pioneered by Wilson and Fisher, the fixed-dimension expansion proposed by Parisi, the perturbative expansion in the minimal-subtraction scheme without ϵ-expansion proposed by Dohm, and the so-called exact RG (there are many different versions, see, e.g. Ref. [19]), which essentially consists in *approximately* solving nonperturbatively the RG equations.

Here we will focus on the fixed-dimension expansion method, which is the one providing the most precise estimates, and, together with the ϵ-expansion, has been most widely used. We consider the standard ϕ^4-theory with N-vector fields and discuss the role of the singularities of the RG functions at the critical point in the numerical determination of critical quantities.

2 Singularities of the RG Functions

An important controversial issue [20–24] in the field-theoretic (FT) approach in fixed dimension is the presence of nonanalyticities at the fixed point g^*, which is defined as the zero of the β-function. The question was clarified long ago by Nickel [21] who gave a simple argument to show that nonanalytic terms should in principle be present in the β-function. The same argument applies also to other series, like those defining the critical exponents: any RG function is expected to be singular at the fixed point.

To understand the problem, let us consider the four-point renormalized coupling g as a function of the temperature T. For $T \to T_c$ we can write down an expansion of the form

$$g = g^* \left[1 + a_1 t + a_2 t^2 + \ldots + b_1 t^\Delta + b_2 t^{2\Delta} + \ldots \right.$$
$$\left. + c_1 t^{\Delta+1} + \ldots + d_1 t^{\Delta_2} + \ldots + e_1 t^\gamma + \ldots \right], \tag{1}$$

where Δ, Δ_2, ... are subleading exponents and t is the reduced temperature $t \equiv (T - T_c)/T_c$. The corrections proportional to t^γ are due to the presence of an analytic background in the free energy. On general grounds, we expect that $a_1 = a_2 = a_3 = \ldots = 0$. Indeed, these analytic corrections arise from the nonlinearity of the scaling fields, and their effect can be eliminated in the Green's functions by an appropriate change of variables [25]. For dimensionless RG-invariant quantities such as g, the leading term is universal and therefore independent of the scaling fields, so that no analytic term can be generated. Analytic correction factors to the singular correction terms are generally present, and therefore the constants c_i in Eq. (1) are expected to be nonzero.

Starting from Eq. (1) it is easy to compute the β-function. Since the mass gap m scales analogously, we obtain for $\Delta < \gamma$ (this condition is usually, but

not always, satisfied[b]) the following expansion:

$$\beta(g) = m\frac{\partial g}{\partial m} = \alpha_1 \Delta g + \alpha_2 (\Delta g)^2 + \ldots + \beta_1 (\Delta g)^{\frac{1}{\Delta}} + \beta_2 (\Delta g)^{\frac{2}{\Delta}} + \ldots +$$
$$\gamma_1 (\Delta g)^{1+\frac{1}{\Delta}} + \ldots + \delta_1 (\Delta g)^{\frac{\Delta_2}{\Delta}} + \ldots + \zeta_1 (\Delta g)^{\frac{\gamma}{\Delta}} + \ldots, \quad (2)$$

where $\Delta g = g^* - g$. It is easy to verify the well-known fact that $\alpha_1 = -\Delta/\nu \equiv -\omega$ and that, if $a_1 = a_2 = \ldots = 0$ in Eq. (1), then $\beta_1 = \beta_2 = \ldots = 0$. Equation (2) clearly shows the presence of several nonanalytic terms with exponents depending on $1/\Delta$, Δ_i/Δ, and γ/Δ.

As pointed out by Alan Sokal [22,23], the nonanalyticity of the RG functions can also be understood within Wilson's RG approach. We repeat here his argument. Consider the Gaussian fixed point which, for $3 \leq d < 4$, has a two-dimensional unstable manifold $\mathcal{M}_u$: the two unstable directions correspond to the interactions ϕ^2 and ϕ^4. Notice that continuum field theories are in a one-to-one correspondence with Hamiltonians on $\mathcal{M}_u$ and that the FT RG is nothing but Wilson's RG restricted to $\mathcal{M}_u$. But now $\mathcal{M}_u$ has no special status at the nontrivial fixed point. In particular, there is no reason why it should approach it exactly along the leading irrelevant direction. Barring miracles, the approach should be along a generic direction, which is tangent to the leading irrelevant one, but which has nonzero components along any of the irrelevant directions. If this happens, nonanalytic terms are present in any RG function.

In order to clarify the issue, Ref. [10] determined the asymptotic behavior of $\beta(g)$ for $g \to g^*$ in the continuum field theory for $N \to \infty$ and $2 < d < 4$, and showed that Eq. (2) holds and that the expected nonanalytic terms are indeed present. In Ref. [26] the computation was extended to two dimensions, finding again nonanalytic terms.

The presence of nonanalyticities gives rise to systematic deviations in FT estimates, as it did in MC and HT studies. In the next section we will present a test-case and we will discuss the type of deviations one should expect.

3 A Simple Example

In order to understand the role of the nonanalytic terms in the analyses of the FT perturbative expansions we consider a simple zero-dimensional example.

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[b]In some models, for instance in the 2D Ising model, $\Delta > \gamma$. In this case, Eq. (2) is still correct [26] if γ and Δ are interchanged and $\alpha_1 = -\gamma/\nu$.
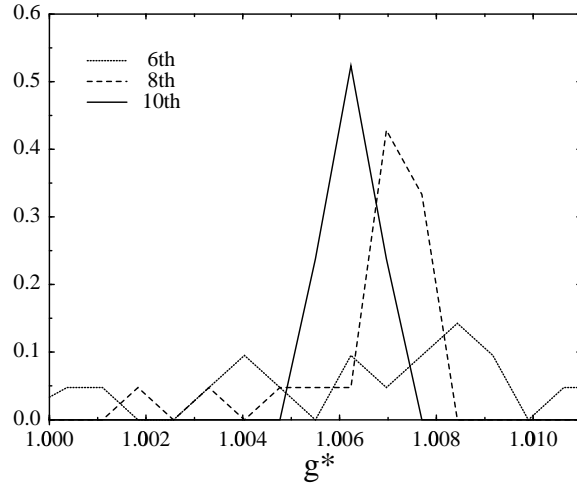
Figure 1.   Distribution of the results for the resummations of g^* for $p = 1/10$, $c = -Z_1/5$.

Define

$$f(g; c, p) = c(1 - g)^{1+p} + \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} \, x^4 \, \exp\left[-\frac{x^2}{2} - \frac{gx^4}{24} \right]. \qquad (3)$$

For $c \neq 0$ and p not integer, this function has a branch point for $g = 1$ and thus it should mimic the behavior we expect for FT expansions. For $g \to 1$, we have

$$f(g; c, p) \approx Z_0 - Z_1(1 - g) + c(1 - g)^{1+p} + O((1 - g)^2), \qquad (4)$$

where $Z_0 = 1.37556014$, $Z_1 = -0.679325$. We wish to repeat here the same steps performed in the calculation of g^* and ω. Therefore, we determine g^* and Z_1, by solving the equations:

$$f(g^*; c, p) = Z_0, \qquad\qquad Z_1 = f'(g^*; c, p). \qquad (5)$$

Of course, $f(g; c, p)$ is replaced with an appropriate resummation of its perturbative expansion. We use here the resummation scheme proposed in Ref. [27] that makes explicit use of the location of the Borel-transform singularity, but similar results are obtained extending the Borel transform by means of Padé approximants (note that one could also use the perturbative series in the *bare*
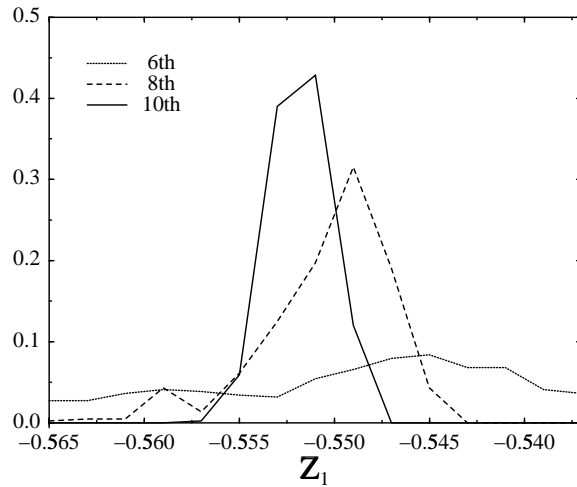
Figure 2.   Distribution of the results for the resummations of Z_1 for $p = 1/10$, $c = -Z_1/5$.

coupling [28]). The mean values and errors are determined by using the procedure of Ref. [29]. In the absence of the nonanalytic term, i.e. for $c = 0$, using the nth-order expansion, we obtain

$$
\begin{aligned}
n = 6: &\quad g^* = 1.00025(131) &\quad Z_1 = -0.6791(178), \\
n = 8: &\quad g^* = 0.99997(10) &\quad Z_1 = -0.6800(18), \\
n = 10: &\quad g^* = 1.00000(1) &\quad Z_1 = -0.6791(2).
\end{aligned}
$$

There is good agreement, the precision increases by a factor of 10 every two orders, and the error bars are correct.

The next step is to consider the role of the nonanalytic corrections, by adding a term that is small compared to the analytic one. We choose $c = -Z_1/5$.

Now, for $p = 1/10$ we obtain

$$
\begin{aligned}
n = 6: &\quad g^* = 1.0043(62) &\quad Z_1 = -0.550(20), \\
n = 8: &\quad g^* = 1.0066(15) &\quad Z_1 = -0.550(3), \\
n = 10: &\quad g^* = 1.0062(5) &\quad Z_1 = -0.552(2).
\end{aligned}
$$

In this case the agreement is poor, especially for Z_1, and, even worse, the errors are completely incorrect. This can be understood from Figs. 1 and 2

where we show the distribution of the approximants that are used. These distributions are nicely peaked, but unfortunately at an incorrect value of g^* and Z_1. Thus, in the presence of these (strong) nonanalyticities, the fact that the approximants have a narrow distribution is not a good indication that the results are reliable. Also, the stability of the results with the number of terms of the series is completely misleading. As we shall discuss below, this is what we believe is happening in two dimensions.

If we consider instead a weak nonanalyticity, i.e. $p \approx 1$, the discrepancies we have found for $p = 1/10$ are much smaller, although still present. For instance, for $p = 9/10$ we have

$$
\begin{aligned}
n = 6: &\quad g^* = 1.013(45) \quad Z_1 = -0.755(270), \\
n = 8: &\quad g^* = 1.014(7) \quad\ Z_1 = -0.655(23), \\
n = 10: &\quad g^* = 1.006(4) \quad\ Z_1 = -0.668(2).
\end{aligned}
$$

In this case the results are consistent with the exact values, although the errors are still slightly underestimated. As expected, the largest discrepancies are observed for Z_1.

4 Conclusions

We have shown that nonanalytic terms may give rise to systematic deviations and a systematic underestimate of the error bars. Now, what should we expect in the interesting two- and three-dimensional cases?

In three dimensions $\Delta \approx 0.5$ and Δ_2/Δ is approximately 2 [30]. Thus, the leading nonanalytic term has the exponent Δ_2/Δ and is not very different from an analytic one. As a consequence, we expect small corrections and indeed the FT results are in substantial agreement with the estimates obtained in MC and HT studies. However, small differences are observed for γ and ω for $N = 0$ and $N = 1$:

$$
\begin{aligned}
N = 0 &\quad \gamma_{\mathrm{FT}} = 1.1596(20) \quad \text{Ref. [9]}, &\quad \gamma_{\mathrm{MC}} = 1.1575(6) \quad \text{Ref. [31]}, \\
N = 0 &\quad \Delta_{\mathrm{FT}} = 0.478(10) \quad \text{Ref. [9]}, &\quad \Delta_{\mathrm{MC}} = 0.517(7)^{+10}_{-0} \quad \text{Ref. [32]}, \\
N = 1 &\quad \gamma_{\mathrm{FT}} = 1.2396(13) \quad \text{Ref. [9]}, &\quad \gamma_{\mathrm{HT}} = 1.2371(4) \quad \text{Ref. [14]}, \\
N = 1 &\quad \Delta_{\mathrm{FT}} = 0.504(8) \quad \text{Ref. [9]}, &\quad \Delta_{\mathrm{MC}} = 0.533(6) \quad \text{Ref. [33]}.
\end{aligned}
$$

There are slight differences, especially for ω, but still at the level of a few error bars. Note that, as discussed in Ref. [10], part of the error may be due to a slightly incorrect estimate of g^*. Using the estimate of g^* obtained from the analysis of the HT expansions, the FT estimates change towards the HT and MC values.

Larger discrepancies are observed in two dimensions. For $N \geq 3$ it is easy to predict the behavior of the RG functions at the critical point. Indeed, the theory is massive for all temperatures. The critical behavior is controlled by the zero-temperature Gaussian point and can be studied in perturbation theory in the corresponding N-vector model. One finds only logarithmic corrections to the purely Gaussian behavior. It follows that the operators have dimensions that coincide with their naive (engineering) dimensions, apart from logarithmic multiplicative corrections related to the so-called anomalous dimensions. The leading irrelevant operator has dimension two [34,35] and thus, for $m \to 0$, we expect

$$g(m) = g^* \left\{ 1 + c\, m^2 \left(-\ln m^2 \right)^\zeta \left[1 + O \left(\frac{\ln(-\ln m^2)}{\ln m^2} \right) \right] \right\}, \qquad (6)$$

where ζ is an exponent related to the anomalous dimension of the leading irrelevant operator, and c is a constant. Therefore,

$$\beta(g) = m \frac{\partial g}{\partial m} = -2\Delta g \left(1 + \frac{\zeta}{\ln \Delta g} + \cdots \right), \qquad (7)$$

with $\Delta g \equiv g^* - g$. Clearly there are logarithmic corrections in this case and therefore, we expect large deviations in the determinations of ω, which should be 2. These deviations are indeed observed: for $N = 3$ the analysis of the five-loop series [36] yields the estimate $\beta'(g^*) = 1.33(2)$, which is very different from the expected result $\beta'(g^*) = 2$.

For $N = 1$, we can repeat Nickel's analysis, using the fact that, from conformal field theory, we can compute the RG dimensions of all relevant and irrelevant operators. Using these results we predict that[c]

$$\beta(g) = -\frac{7}{4}\Delta g \left(1 + b_1 |\Delta g|^{1/7} + b_2 |\Delta g|^{2/7} + b_3 |\Delta g|^{3/7} + \cdots \right), \qquad (8)$$

where $\Delta g \equiv g^* - g$. Such an expansion is confirmed by an analysis of the lattice Ising model. Again we find strong nonanalyticities, and correspondingly we expect large deviations. And, indeed such large deviations are observed: the analysis of the five-loop series gives $g^* = 15.39(25)$ [36] and $\beta'(g^*) = 1.31(3)$, to be compared with the exact prediction $\beta'(g^*) = 7/4$ and the estimates $g^* = 14.69735(3)$ in Ref. [37] and $g^* = 14.6975(1)$ in Ref. [38].

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[c]Sometimes it has been claimed that the leading irrelevant operator in the Ising universality class has $\omega = 4/3$, so that $\beta'(g^*) = 4/3$. This claim is incorrect. Indeed, such an operator can only appear in nonunitary extensions of the Ising model, but not in the standard (unitary) ϕ^4-field theory. For a detailed discussion, see Appendix A of Ref. [26].

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