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Fisher zeros in the Kallen–Lehmann approach to 3D Ising model

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ABSTRACT

The distribution of the Fisher zeros in the Kallen–Lehmann approach to three-dimensional Ising model is studied. It is argued that the presence of a non-trivial angle (a cusp) in the distribution of zeros in the complex temperatures plane near the physical singularity is realized through a strong breaking of the 2D Ising self-duality. Remarkably, the realization of the cusp in the Fisher distribution ultimately leads to an improvement of the results of the Kallen–Lehmann ansatz. In fact, excellent agreement with Monte Carlo predictions both at high and at low temperatures is observed. Besides, agreement between both approaches is found for the predictions of the critical exponent α and of the universal amplitude ratio $\Delta = A_+/A_-$, within the 3.5% and 7% of the Monte Carlo predictions, respectively.

0. Introduction

A proper understanding of non-perturbative phenomena in field theory and statistical mechanics is a major challenge in theoretical physics. Among the most important examples of such phenomena it counts the problem of color confinement in QCD, which, despite tireless attempts along the years, is still begging for a theoretical description. Another renowned unsolved problem is that of the Ising model in three dimensions. Actually, both problems are known to be connected, as the Svetitsky–Yaffe conjecture [2] states that the three-dimensional Ising model is closely related to the problem of color confinement and that it likely captures its main non-perturbative features near the transition. More generally, three-dimensional Ising model is closely related to a large class of physical systems near the critical point. Consequently, a deeper understanding of the non-perturbative dynamics of the three-dimensional Ising model would be of great importance in several areas of theoretical physics [1]. In turn, trying to find new semi-analytical methods, non-perturbative in nature, to shed new light on this problem represents a very interesting program.

In a recent work [3], it has been proposed to address the problem of three-dimensional Ising model by using a method originally inspired in the spirit of Regge's theory of scattering [4,5]. Regge theory is a fully non-perturbative approach which allows the description of many experimental data in terms of an ansatz with few parameters, these to be determined in comparison with observations and/or by using theoretical arguments. The idea in [3] was to propose an ansatz, also with few parameters, to describe the free energy of the three-dimensional Ising model. The ansatz is heuristically motivated by mimicking the relation existing between the expression for the free energy in one and two dimensions. Then, tuning the parameters of the model for it to describe the high temperature regime, one ends up with an expression that also reproduces the results at low temperature with remarkable accuracy.

This idea was first discussed in [6] and it was partially confirmed by the results of [7], where, even in its most simplified formulation (in which a *minimal duality breaking* was assumed), such a method was shown to give results in a surprising agreement with observations and Monte Carlo data. In order to investigate the model in more detail (and with modest computational resources) it is necessary to find a theoretical tool able to fix (or at least to

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find some bounds on) the *Regge parameters* appearing in the model of [6]. Here, we report a remarkable progress in this direction.

A suitable tool to theoretically constraint the ansatz of [6] is the analysis of the Fisher zeros, which is a powerful technique developed by M. Fisher in the 1960's. Following the ideas of Yang and Lee [9], Fisher suggested to think of the inverse temperature β as a complex variable [8]. This technique permits to get relevant physical information about the statistical system by looking at the analytic properties of the (extended) thermodynamical functions. For instance, the distribution of zeros of the partition function in the complex β plane (Fisher zeros) near the critical point permits to determine the universal amplitude ratio $\Delta = A_+/A_-$ of the specific heat; see the classical papers [10,11]. It has been also stressed that Fisher zeros technique turns out to be useful in analyzing the strength of the phase transitions (see for instance [12,13] and references therein).

In this Letter, we will be concerned with the analysis of Fisher zeros within the framework of [6,7]. As it will be explained in more details in the next sections, the ansatz proposed in [6] appears to be well suited for this kind of analysis since it is, in a sense, already in a *Fisher zeros form*. This method suggests a simple way to realize a *strong breaking of duality*, leading to an improvement of the semi-analytical results in comparison with the numerical data.

The Letter is organized as follows. In Section 1, a short introduction to Fisher zeros is given. In Section 2, the relations between Fisher zeros and duality breaking in Ising model is discussed. In Section 3, the nice interplay between Fisher zeros and the Kallen–Lehmann representation (KL) is analyzed in detail. In Section 4, we introduce what we call the *strong duality breaking* in the KL free energy for the three-dimensional Ising model. In Section 5, it is shown how the strong duality breaking improves the comparison with Monte Carlo results, both at high and at low temperatures. In Section 6, the behavior of the critical exponent at the critical point is described, together with the behavior of the universal amplitude ratio of the specific heat Δ. Besides, some feasible further improvements are pointed out. We conclude with a discussion in Section 7.

1. Fisher zeros: A short introduction

As it has been argued originally by Fisher [8], a very powerful method to analyze the thermodynamics of a generic spin system is to complexify its temperature and to study the distribution of zeros of the partition function in the complex β plane. Let $Z(\beta)$ and $F(\beta)$ be the partition function and the free energy of the system under analysis, respectively, and let $g(r)$ be the distribution of zeros of $Z(\beta)$ in the complex β-plane, such that $g(r)\,dr$ is the number of zeros of $Z(\beta)$ between r and $r+dr$, where near the critical point β_c one has $\beta_{\mathbb{C}} = \beta_c + r\exp(i\phi)$ (the meaning of the parameter ϕ is clarified below). Then, one can show that, near the critical point β_c, the non-analytic part of the internal energy (that is, the singular part of the derivative of the free energy) and of the free energy itself, responsible for the phase transition, have the following form

$$E(\beta) \approx \partial_\beta F \approx \int_0^R \frac{g(r)\,dr}{\beta_c - \beta + r\exp(i\phi)} + \text{c.c.},$$

$$F \approx \int_0^R g(r)\log\bigl(\beta_c - \beta + r\exp(i\phi)\bigr)\,dr, \tag{1}$$

where "c.c." means the complex conjugate and R is a suitable cutoff. The angle ϕ is the angle formed by the tangent to the curve of zeros of $Z(\beta)$ and the real axis at the critical point β_c. From the formulas above, one can derive an expression for the singular part of the specific heat[1]

$$C = -\beta_c^2\left(\int_0^R \frac{g(r)\,dr}{(\beta_c - \beta + r\exp(i\phi))^2} + \text{c.c.}\right).$$

Then, let us consider a system undergoing a second order phase transition, so that the singular part of the specific heat reads

$$\begin{aligned}
C &= A_+|\beta-\beta_c|^{-\alpha}, \quad \beta<\beta_c,\ \alpha>0,\\
C &= A_-|\beta-\beta_c|^{-\alpha}, \quad \beta>\beta_c,\\
C &= A_+\log|\beta-\beta_c|, \quad \beta<\beta_c,\ \alpha=0,\\
C &= A_-\log|\beta-\beta_c|, \quad \beta>\beta_c,
\end{aligned}$$

where α is the critical exponent and, in general, $A_+ \neq A_-$. It is worth mentioning that the ratio $\Delta = A_+/A_-$ is a universal quantity, so that its computation is a relevant (and challenging) question. The ratio Δ can be measured in many interesting physical systems. It can be shown (see, for instance, [10,11]) that both $g(r)$ near the critical point and the value of Δ are related to ϕ in such a way that, for $\alpha \neq 0$, the relations read

$$\Delta = \frac{\cos[(2-\alpha)\phi]}{\cos[(2-\alpha)\phi + \alpha\pi]}, \qquad g(r) \approx g_0 r^{1-\alpha},$$

so that the amplitude ratio is trivial (namely $\Delta = 1$) when the intersection between the zeros and the real axis is vertical (corresponding to $\phi = \pi/2$). In the exact solution of the Ising model in two dimensions [15] $\Delta = 1$, but it is not the case in three dimensions, where it is known that

$$\Delta_{3D} \approx 0.55, \qquad \phi_{3D} \neq \pi/2$$

(see, for an updated review, [1]).

The aim of the present Letter is to discuss the relation between the existence of a cusp in the Fisher curve (i.e. the fact that $\Delta \neq 1$) and a breaking of the 2D Ising self-duality. Such a duality symmetry is absent in the 3D Ising model; consequently, any suitable attempt to dimensionally extend analytic methods from two to three dimensions would require to specify a precise mechanism of self-duality breaking. In [7] self-duality was broken in the softest possible way. Here we will show that a stronger breaking is favoured by the comparison with observations.

2. Fisher zeros and duality breaking

Let us shortly describe the case of the two-dimensional ferromagnetic Ising model. The free energy is given by

$$F_{2D}(\beta) = \log 2\cosh 2\beta + \frac{1}{2\pi}\int_0^\pi dt\,\log\left\{\frac{1}{2}\left[1+\sqrt{1-k_{2D}(\beta)^2\sin^2 t}\right]\right\}, \tag{2}$$

$$\bigl(k_{2D}(\beta)\bigr)^2 = \left(\frac{2}{\cosh 2\beta\coth 2\beta}\right)^2 = \left(4\frac{\exp(2\beta)-\exp(-2\beta)}{(\exp(2\beta)+\exp(-2\beta))^2}\right)^2,$$
$$0 \leqslant \bigl(k_{2D}(\beta)\bigr)^2 \leqslant 1. \tag{3}$$

The critical point of the two-dimensional Ising model is located at the maximum of $k_{2D}(\beta)$, namely

$$\bigl(k_{2D}(\beta_c)\bigr)^2 = 1$$

and, *being* k_{2D} a smooth function, it is also true that

[1] Here we will only consider the case of second order phase transitions.

$\partial_\beta k_{2D}|_{\beta=\beta_c} = 0$.

The function k_{2D} (a sort of effective coupling constant) encodes the duality properties of the model: if one writes k_{2D} in terms of $\tau = \tanh\beta$ (the high temperatures variable) or in terms of $u = \exp(-2\beta)$ (the variable at low temperatures) it turns out that k_{2D} looks the same, and this is a convenient way to express the self-duality of the 2D Ising model (the self-duality of the 2D Ising model was discovered in [14], before the discovery of its exact solution in 1944). From the exact solution (1)–(2) one can determine the Fisher zeros of the 2D Ising model, which lay on a circle in the complex $u = \exp(-2\beta)$ plane. The equation determining the curve on which the Fisher zeros lay is:

$$\left|\left(k_{2D}(\beta)\right)^2\right| = 1,$$

where β is now a complex variable; while in the complex u-plane Fisher zeros have the following form:

$$u = 1 - \sqrt{2}\exp(i\theta).$$

Being the Fisher zeros located on a circle whose center is on the real axis, the intersection of the Fisher zeros with the real axis is vertical and thus the angle ϕ is $\pi/2$, implying $\Delta = 1$. In the two-dimensional Ising model, the reason why the intersection at the critical point is vertical is simple: the physical singularity of the two-dimensional Ising model is the real positive solution (in β) of the equation

$$1 - \left(k_{2D}(\beta)\right)^2 (\sin t)^2 = 0, \tag{4}$$

which cannot be fulfilled unless

$$(\sin t)^2 = \left(k_{2D}(\beta)\right)^2 = 1.$$

Then, let us call the complex zeros near the critical point $\beta^* = \beta_c + x + iy$ (near the critical point x and y are both small). Thus, x is implicitly defined in terms of y by the equation

$$H_{2D}(x, y) = 1 - \left|k_{2D}(\beta_c + x + iy)^2\right| = 0. \tag{5}$$

Near the critical point, when the intersection is not vertical, one can think of x as a monotonic function of y (or *vice versa*). Therefore, in order for x to be defined implicitly in terms of y by the equation above near $x = y = 0$, the derivative of $H_{2D}(x, y)$ with respect to y should be different from zero. On the other hand, in order to have only one physical singularity, one has to demand the existence of only one solution of Eq. (4) on the real positive β-axis and such a solution necessarily occurs at the maximum of k_{2D}^2.

As long as $k_{2D}^2(\beta)$ is a smooth function that admits an analytic extension near β_c, the derivative of $H_{2D}(x, y)$ (defined as in Eq. (5)) with respect to y vanishes at $x = y = 0$, and this represents an obstruction to think of x as implicitly defined in terms of y through (5) at that point. So, no cusp in the Fisher curve could exist since the curve of distributions of zeros intersects the x-axis vertically.

On the other hand, in physics one is often interested in systems with non-trivial ratio $\Delta \neq 1$, where the cusp manifests itself. For instance, this is what happens in the Ising model in three dimensions, in what we are interested here. In order to analyze the possibility of achieving a realization yielding $\Delta \neq 1$, first we have to make some comments on the general form of the partition function: let us assume for a moment that for a systems with only one phase transition, near the critical point, the equation that determines the singularities can be written in the form

$$1 - \left(k_{\mathrm{eff}}(\beta)\right)^2 (\sin t)^2 = 0 \tag{6}$$

for some real function $k_{\mathrm{eff}}(\beta)$ whose only positive maximum occurs at the critical point β_c, being t some dummy integration variable as in (1). In such a case, there is only one positive real solution occurring when both $(k_{\mathrm{eff}}(\beta))^2$ and $(\sin t)^2$ are at their maxima (equal to one).

Thus, Fisher zeros can be described by an equation which is formally analogous to the one of the two-dimensional Ising model; namely

$$1 = \left|\left(k_{\mathrm{eff}}(\beta)\right)^2\right|. \tag{7}$$

This is part of the proposal in [6]. Actually one may introduce at least implicitly a suitable k_{eff} for many statistical system (with standard Fisher zeros) in such a way that (7) represents precisely the Fisher zeros of the system of interest.

Eqs. (6) and (7) simply encode the fact that there is only one physical singularity. Function $k_{\mathrm{eff}}(\beta)$ indicates how far from being self-dual a system is. Therefore, according the discussion above, having a value $\Delta \neq 1$ would imply $k_{\mathrm{eff}}(\beta)$ in (6) to be non-differentiable at the critical point, where it takes its maximum value. Actually, in order to achieve a cusp in the distribution of the Fisher zeros, it is enough to require a non-analiticity of $k_{\mathrm{eff}}(\beta)$ at the critical point. As a matter of fact, our results indicate that the first derivative of $k_{\mathrm{eff}}(\beta)$ is continuous while the second derivative is discontinuous. This is one of the hints for constructing our ansatz, as we are reminded of the fact that in three dimensions $\Delta_{3D} < 1$.

In [7], for the sake of simplicity (and because of the computational resources) a minimal duality breaking was assumed, according to what $k_{\mathrm{eff}}(\beta)$ still was smooth at the critical point. As a result, the agreement with Monte Carlo data and observations was found to be very good. Nevertheless, as it will be explained in the next sections, when the cusp ($\Delta \neq 1$) in the Fisher curve is implemented, the comparison with Monte Carlo data turns out to be even better, showing a new and more efficient way of exploring the space of parameters of the model.

3. Fisher zeros in the Kallen–Lehmann representation

A powerful non-perturbative technique in field theory is the Kallen–Lehmann representation. Such a tool allows to encode in a very natural way many analytical properties of the spectral functions. It is interesting to adapt this method (often exclusively associated to Quantum Field Theory) to the analysis of the 3D Ising model. This representation [6] gives rise to an ansatz for the free energy of the three-dimensional Ising model of the following form[2]

$$F_{3D}^{(\zeta_i,\lambda)}(\beta) = F_{2D}(\beta) + \frac{\lambda}{(2\pi)^2}\int_0^\pi dz \int_0^\pi dy \times \log\left\{\frac{1}{2}\left[1 + \left(1 - \left[2\frac{(\Delta(z)-1)^{\zeta_1}}{\Delta(z)}\right]^{\zeta_2} \sin^2 y\right)^{\zeta_3}\right]\right\}, \tag{8}$$

where

$$\Delta(z) = \left(1 + \left(1 - k_{\mathrm{eff}}(\beta)^2 \sin^2 z\right)^{\zeta_0}\right)^2, \qquad \zeta_0, \zeta_1, \zeta_2, \zeta_3 > 0, \tag{9}$$

$$0 \leqslant \left(k_{\mathrm{eff}}(\beta)\right)^2 \leqslant 1, \qquad 1 \leqslant \Delta(z) \leqslant 4, \tag{10}$$

and where the values of the parameters $\zeta_0, \zeta_1, \zeta_2, \zeta_3$ (henceforth *Regge parameters*) in the case of the two-dimensional Ising model would correspond to $\lambda = 1$, $\zeta_i = 1/2$ for $i = 0, \ldots, 3$.

[2] The "Regge parameters" appearing in these formulas are related with those appearing in [6] by the following identities $\zeta_1 = \nu$, $\zeta_3 = 1/2 = \zeta_2$, $\zeta_0 = \alpha$.

Expression (8) will be referred as Kallen–Lehmann free energy. The heuristic argument that suggests to write down (8) goes as follows: think of an operator $\mathbf{O}_{1\to 2}$ which "dresses" the trivial one-dimensional solution of the Ising model giving rise to the Onsager solution. Then, the Kallen–Lehmann ansatz for the free-energy for the three-dimensional Ising model is obtained by modifying $\mathbf{O}_{1\to 2}$ in such a way that the parameters[3] $\lambda = 1$ and $\zeta_i = 1/2$ now become free parameters, and then applying such a modified dressing operator $\mathbf{O}_{2\to 3}$ to the Onsager solution. The result is Eq. (8).

A nice feature of this dimensional-recursive method is that it permits to distinguish between the problem of fixing five external Regge parameters[4] λ and ζ_i $(i = 0, \ldots, 3)$, and the problem of determining the function $k_{\mathrm{eff}}(\beta)$. The function $k_{\mathrm{eff}}(\beta)$ plays the same role that $k_{2\mathrm{D}}(\beta)$ plays in (3). Namely, it encodes the information about how different the degrees of freedom are in the low and the high temperature regimes. Thus, at least in principle, one could fix $k_{\mathrm{eff}}(\beta)$ by analyzing how the duality is broken in the three-dimensional Ising model. Then, Regge parameters can be found by looking, for instance, at the high temperatures behavior.

An important piece of information is given by knowing which are the more relevant parameters in writing down the ansatz (8), as well as understanding their physical interpretation. In particular, as it will be discussed in the next sections, one learns that tuning appropriately just three Regge parameters is sufficient to get an excellent agreement, both at high and at low temperatures. Besides, a very good description near the critical point is also observed. Our results suggest that the agreement with observations and Monte Carlo data improves its performance by resorting to a careful analysis of duality breaking, instead of trying to select the Regge parameters *ad hoc*. From our analysis herein we achieve a substantial improvement of the method of [6].

Nevertheless, it is worth mentioning that our analysis is still far from being an exhaustive exploration of the whole space of parameters of the model. In fact, this is what makes the results more surprising, as the agreement with Monte Carlo data is excellent despite only a small piece of the moduli space was analyzed.

Let us now compute the internal energy in the Kallen–Lehmann representation. A simple computation yields

$$E_{3\mathrm{D}}^{(\zeta_i,\lambda)}(\beta) \approx \partial_\beta F_{3\mathrm{D}}^{(\zeta_i,\lambda)}(\beta) = E_{2\mathrm{D}}(\beta) + \frac{\lambda}{(2\pi)^2}\int_0^\pi dz \int_0^\pi dy \left\{ \left(-\frac{\zeta_3\zeta_2 \sin^2 y}{N} \right) \times D^{\zeta_3 - 1} R^{\zeta_2 - 1} (\partial_\Delta R) \frac{\partial \Delta}{\partial (k_{\mathrm{eff}}(\beta)^2)} \frac{\partial (k_{\mathrm{eff}}(\beta)^2)}{\partial \beta} \right\}, \tag{11}$$

where

$$N = 1 + \left(1 - \left[2\frac{(\Delta(z) - 1)^{\zeta_1}}{\Delta(z)} \right]^{\zeta_2} \sin^2 y \right)^{\zeta_3}, \qquad N \geqslant 1,$$

$$D = 1 - R^{\zeta_2} \sin^2 y, \quad R = 2\frac{(\Delta(z) - 1)^{\zeta_1}}{\Delta(z)}, \tag{12}$$

and

$$\frac{\partial \Delta}{\partial (k_{\mathrm{eff}}(\beta)^2)} = -2\bigl(1 + \bigl(1 - k_{\mathrm{eff}}(\beta)^2 \sin^2 z\bigr)^{\zeta_0}\bigr) \times \bigl(\zeta_0 \sin^2 z\bigr)\bigl(1 - k_{\mathrm{eff}}(\beta)^2 \sin^2 z\bigr)^{\zeta_0 - 1},$$

$$\bigl(\Delta(z) - 1\bigr)^{\zeta_1} = \bigl\{\bigl[2 + \bigl(1 - k_{\mathrm{eff}}(\beta)^2 \sin^2 z\bigr)^{\zeta_0}\bigr] \times \bigl[\bigl(1 - k_{\mathrm{eff}}(\beta)^2 \sin^2 z\bigr)^{\zeta_0}\bigr]\bigr\}^{\zeta_1},$$

$$\partial_\Delta R = 2\frac{(\Delta(z) - 1)^{\zeta_1 - 1}}{(\Delta(z))^2}\bigl[1 + (\zeta_1 - 1)\Delta(z)\bigr].$$

It is worth noticing that, from the point of view of Fisher zeros distribution, there is a special value for ζ_1. In order to have a "singularity equation" similar to the one arising in the two-dimensional Ising model, it is necessary to ask that all the singular terms of the internal energy have their origin in factors like

$$\bigl(1 - k_{\mathrm{eff}}(\beta)^2 \sin^2 z\bigr)^{e_i}, \tag{13}$$

where the exponents e_i depend on the Regge parameters ζ_i. A potentially disturbing term in (11), which is not of the form (13), is $D^{\zeta_3 - 1}$, since $D = 1 - R^{\zeta_2} \sin^2 y$ could be negative and $\zeta_3 - 1$ could be negative.[5] Then, to avoid undesired divergences in the internal energy, one may ask whether a special of ζ_1 exists such that the maximum[6] m_0 of R

$$m_0 = \max_\Delta R = \max_\Delta \left\{ \left[2\frac{(\Delta - 1)^{\varsigma_1}}{\Delta} \right] \right\},$$

is less than or equal to one, and such that m_0 does not depend on z and β:

$$0 \leqslant \left[2\frac{(\Delta - 1)^{\varsigma_1}}{\Delta} \right] \leqslant m_0 = 1.$$

Interestingly enough, such a special value of ς_1 does exist and it is precisely $1/2$, the value of the two-dimensional Ising model. Thus, with $\varsigma_1 = 1/2$, when function R in (12) attains its maximum m_0 (this happens for $\Delta = 2$), it is always multiplied by its derivative $\partial_\Delta R$ (see Eq. (13)), which vanishes. In this way, all the potential singular terms in Eq. (11) are of the *Fisher form* in Eq. (13) so that they can be analyzed with the method described in the previous sections. The condition $\varsigma_1 = 1/2$ (which in [7] was imposed for simplicity) is obtained here as being the appropriately value from the point of view of the Fisher zeros. Thus, the Kallen–Lehmann free energy is a smooth function everywhere apart from the critical point singled out by Eq. (7).

4. Duality breaking and $k_{\mathrm{eff}}(\beta)$

The previous analysis, relating Fisher zeros to duality breaking, suggests how to break duality taking into account the non-triviality of the amplitude ratio $\Delta \neq 1$ in three dimensions. A second important ingredient in the discussion is the Marchesini–Shrock symmetry [16], which states that the partition function of Ising model on regular hypercubic lattices is invariant under

$$\beta \to \beta + in\frac{\pi}{2}, \quad n \in \mathbb{Z}.$$

The simplest possible choice of $k_{\mathrm{eff}}(\beta)$ which satisfies this constraint is

$$k_{\mathrm{eff}}(\beta) = 4\frac{d_3 \exp(2\beta) - d_2 \exp(-2\beta)}{(d_1 \exp(2\beta) + d_0 \exp(-2\beta))^2}.$$

In [7], two of the parameters d_i $(i = 0, \ldots, 3)$ have been fixed by asking the expected transition to occur at

$$k_{\mathrm{eff}}(\beta_c) = 1, \quad \beta_c = 0.22165, \tag{14}$$

[3] Namely, in the two-dimensional Ising model, the parameters which appear in $\mathbf{O}_{1\to 2}$ are $\lambda = 1$, $\zeta_i = 1/2$. In order to change the critical exponents one needs to change (at least) λ and ζ_i.

[4] In [7], for sake of simplicity, the parameters ζ_1 and ζ_3 were fixed to $1/2$; that is, to the values they take in the two-dimensional problem. Thus, already by using only three parameters, very good results in comparisons with Monte Carlo data were obtained.

[5] This term is also disturbing since it could give rise to complex numbers in the case D is negative and $\zeta_3 - 1$ is negative.

[6] Where one "maximizes" C over the Δ fulfilling Eq. (10).

and by requiring the vanishing of the derivative of $k_{\text{eff}}(\beta)$ in β_c, namely

$$\beta^* \big|\partial_\beta k_{\text{eff}}(\beta)\big|_{\beta=\beta^*} = 0. \tag{15}$$

On the other hand, the other two parameters d_i were chosen to be equal to those values they take in the two-dimensional model. However, from the previous discussion, we learn that condition (15) should not be kept in the cases of systems exhibiting non-trivial amplitude ratio Δ. Thus, we will assume that β_c is a maximum of k_{eff} but with a left-derivative different from the right-derivative at β_c.

Indeed, there are an infinite number of possible choices of parameters that leads to strong duality breaking such that $k_{\text{eff}}(\beta)$ has a cusp at the critical point. As in [7], we will follow a simplicity criterion: we will assume that both for $\beta < \beta_c$ and for $\beta > \beta_c$ the function $k_{\text{eff}}(\beta)$ has a form similar to that of $k_{2\text{D}}(\beta)$ in two dimensions (the numerical results indicate that the discontinuity appears in the second derivative, while the first derivative at the critical point is continuous). In addition, we will consider two constraints on the parameters: the first is that, for $\beta < \beta_c$, $k_{\text{eff}}(\beta)$ is decreasing, while for $\beta < \beta_c$ it is increasing; the second is the continuity of $k_{\text{eff}}(\beta)$ together with Eq. (14). Summarizing, we have

$$k_{\text{eff}}(\beta) = k_{\text{eff}}^{(+)}(\beta) = 4\frac{d_3^{(+)}\exp(2\beta) - d_2^{(+)}\exp(-2\beta)}{[(d_1^{(+)}\exp(2\beta) + d_0^{(+)}\exp(-2\beta)]^2}, \quad \beta < \beta_c, \tag{16}$$

$$k_{\text{eff}}(\beta) = k_{\text{eff}}^{(-)}(\beta) = 4\frac{d_3^{(-)}\exp(2\beta) - d_2^{(-)}\exp(-2\beta)}{[d_1^{(-)}\exp(2\beta) + d_0^{(-)}\exp(-2\beta)]^2}, \quad \beta > \beta_c, \tag{17}$$

obeying

$$k_{\text{eff}}^{(+)}(\beta_c) = k_{\text{eff}}^{(-)}(\beta_c) = 1, \tag{18}$$

and

$$\partial_\beta k_{\text{eff}}(\beta) > 0, \quad \beta < \beta_c, \tag{19}$$

$$\partial_\beta k_{\text{eff}}(\beta) < 0, \quad \beta > \beta_c. \tag{20}$$

Eq. (18) fixes one of the $d_i^{(+)}$ (as well as one of the $d_i^{(-)}$) in terms of the others and the critical temperature, while Eqs. (19) and (20) ensure that β_c is actually a maximum. In principle, the relevant "duality breaking" parameter (to be found by comparing the theory with the available data) is the discontinuity $\Delta k'$ of the first derivative of $k_{\text{eff}}(\beta)$, namely

$$\Delta k' = \big(\partial_\beta k_{\text{eff}}^{(+)}(\beta) - \partial_\beta k_{\text{eff}}^{(-)}(\beta)\big)\big|_{\beta=\beta_c}. \tag{21}$$

However, from the practical point of view, it is much easier to work with the parameterization (16)–(17), where a non-vanishing $\Delta k'$ is seen to be given by a non-vanishing $\Delta_{d_i} = d_i^{(+)} - d_i^{(-)} \neq 0$, $i = 0, \ldots, 3$, which implies $\Delta k' \neq 0$.

Thus, some of the parameters $d_i^{(+)}$ and $d_j^{(-)}$ can be appropriately chosen in order to improve the agreement with the *experiments*.

The parameterization (16) and (17) is actually the simplest one being compatible with the *strong duality breaking*, inspired by the exact solution of the two-dimensional model. So, in principle, the results obtained by this method could be improved if it were possible to explore the whole space of parameters more exhaustively.

Because of limitations in computational resources, we are able to explore only in a very restrictive region of the space of parameters of [7]. Even in this case, the results are remarkably good if we make use of some hints. We will proceed as follows: first, we will chose some of the parameters to be equal to the best values found in [7]. Then, the novelty here will be to introduce a parameter that controls the *strong duality breaking*. In principle, one would expect the optimal set of parameters to be far from the set found in [7], where quite simplifying hypothesis of minimal duality breaking were assumed. However, as a very encouraging signal, one finds that a very good agreement with observations is found by studying this region of the moduli space. Thus, from now on, we will fix

$$\zeta_0 = \zeta_0^* = 1.9389, \qquad \zeta_1 = \zeta_1^* = \frac{1}{2}, \qquad \zeta_2 = \zeta_2^* = 1.9205,$$

and we will test the strong duality breaking in a small neighborhood varying λ, ζ_2 and $\Delta k'$.

Afterwards it will be useful to express $k_{\text{eff}}^{(-)}$ in terms of the low temperatures variable u as follows

$$k_{\text{eff}}^{(-)}(u) = 4\frac{u(d_3^{(-)} - d_2^{(-)}u^2)}{(d_1^{(-)} + d_0^{(-)}u^2)^2}. \tag{22}$$

Now, let us move on and study the high and low temperature regimes.

5. High and low temperatures

The idea of this section is to find the optimal set of parameters $(\zeta_3^*, \lambda^*, \Delta k'^*)$ in Eqs. (9) and (21) that reproduce as close as possible the available Monte Carlo data at high temperature (see [17]). A hyper-cubic lattice has been chosen in the parameters space (every point in the lattice representing a possible set of high temperature parameters), then the free energy (8) will be evaluated at every point of the lattice. The optimal choice of parameters will be the one minimizes the following deviation function which, to some extent, represents the deviation between the ansatz and the Monte Carlo data,

$$\chi(\zeta, \nu, \lambda) = \sum_i^{50} \big|F_{3\text{D}}^{(\zeta,\nu,\lambda)}(\beta_i) + I_0 - F_{\text{HT}}^{\text{MC}}(\beta_i)\big|^2,$$

where

$$\beta_i - \beta_{i-1} = \frac{0.03}{50}, \qquad \beta_{50} = \beta_{\max} = 0.03, \qquad I_0 = 2.4819,$$

$$F_{\text{HT}}^{\text{MC}}(\beta) = 3\cosh\beta + \big(3(\tanh\beta)^4 + 22(\tanh\beta)^6 + 187.5(\tanh\beta)^8 + +1980(\tanh\beta)^{10} + 24\,044(\tanh\beta)^{12} + 319\,170(\tanh\beta)^{14} + \cdots\big).$$

Here, we keep the terms up to the 15th order of [17] since our algorithm is not sensitive to higher order terms. $F_{\text{HT}}^{\text{MC}}$ is the high temperature Monte Carlo free energy, β_m can be assumed to be of order[7] 0.03, and I_0 is a constant introduced for numerical convenience.

In order to compare the Regge coefficients with the high temperature coefficients in [17], we need to change variable from β to $t = \tanh\beta$.

Candidates to be the best parameters are

$$\zeta_3^* = 0.3273, \qquad \frac{\lambda^*}{(2\pi)^2} = 0.1095, \tag{23}$$

while the discontinuity at the critical point is given by $\Delta k' = 0.75 \times 10^{-4}$ (which according to our precision is compatible with

[7] Above $\beta \approx 0.05$ is not in the high temperature regime as the critical temperature is at $\beta^* \approx 0.22$ which is only a factor of four larger. Indeed, $\beta \approx 0.03$ appears to be not small enough. Nevertheless, we will see that the agreement of our semi-analytical free energy with Monte Carlo data is excellent up to $\beta \approx 0.03$.

zero). As expected, the discontinuity of second derivative $\Delta k''$ is of order one. This can be achieved, for instance, by the following choice of $d_i^{(\pm)}$:

$$d_0^{(+)} = 1, \quad d_1^{(+)} = 1, \quad d_2^{(+)} = -0.1575, \quad d_3^{(+)} = 0.7116,$$
$$d_0^{(-)} = 0.27, \quad d_1^{(-)} = 1, \quad d_2^{(-)} = 0.3498, \quad d_3^{(-)} = 0.6251.$$

The agreement appears to be excellent: the deviation at high temperatures turns out to be $\sigma_{\mathrm{HT}}(\zeta^*, \nu^*, \lambda^*) \approx \sqrt{\chi(\zeta^*, \nu^*, \lambda^*)/50} \approx 3 \times 10^{-6}$, which is certainly compatible with Monte Carlo results (see for instance [1] and references therein).

Once the optimal set of parameters have been found at high temperature, it is observed that such set also leads to a good agreement at low temperatures. The internal energy at low temperature is ($k_{\mathrm{eff}}^{(-)}(\beta)$ has to be expressed in terms of u as in Eq. (22))

$$\left\langle \frac{E}{N} \right\rangle^{\mathrm{KL}}(u) + 2I_1 = 2u \frac{\partial}{\partial u} F_{3\mathrm{D}}^{(\zeta_3, \lambda, \Delta k')}(u). \tag{24}$$

This is the average energy per spin[8] to be compared with $\langle \frac{E}{N} \rangle^{\mathrm{MC}}$, the polynomial form in u which represents the Monte Carlo average energy for spin for small u found in [18].

We learned in [7] that it is not convenient to use the expression on the right-hand side of (24). Instead, the polynomial expression of [18] can be used to obtain the Monte Carlo estimation for the free energy at low temperatures; namely

$$\left\langle \frac{E}{N} \right\rangle^{\mathrm{KL}}(u) + 2I_1 = 2u \frac{\partial}{\partial u} F_{\mathrm{LT}}^{\mathrm{MC}}(u) = \sum_{i=6}^{14} a_i^{(L)} u^i,$$

where

$$F_{\mathrm{LT}}^{\mathrm{MC}}(u) = \frac{1}{2} \left(\sum_{i=6}^{14} \left(\frac{a_i^{(L)}}{i} \right) u^i - 2I_1 \log u \right).$$

Low temperature test function reads

$$\chi_{\mathrm{LT}}(\zeta^*, \nu^*, \lambda^*) = \sum_{i=1}^{50} \left| F_{3\mathrm{D}}^{(\zeta^*, \nu^*, \lambda^*)}(u_i) + I_2 - F_{\mathrm{LT}}^{\mathrm{MC}}(u_i) \right|^2,$$

$$u_i - u_{i-1} = \frac{0.03}{50}, \qquad u_1 = u_{\min}, \qquad u_{50} = u_{\max} = 0.03,$$

$$F_{\mathrm{LT}}^{\mathrm{MC}}(u) = \left[\frac{1}{2} \left(\frac{12}{6}(u)^6 + \frac{60}{10}(u)^{10} - \frac{84}{12}(u)^{12} + \frac{420}{14}(u)^{14} + \cdots \right) + I_1 \log u \right],$$

where $I_1 = -1$ and $I_2 = 0.0954$. Our algorithm is sensitive up to the 15th order of the polynomial expression of [18], so we keep all these terms. $u_{\max}$ has to be much smaller than $u_{\mathrm{crit}} = \exp(-2\beta_{\mathrm{crit}}) \approx 0.6$, so it can be reasonably assumed to be of order 0.03.

The deviation at low temperature between the Kallen–Lehmann and the Monte Carlo free energies *evaluated for the same optimal parameters* in (23), which have been found by asking the optimal agreement at high temperature, is $\sigma_{\mathrm{LT}}(\zeta^*, \nu^*, \lambda^*) \approx \sqrt{\chi_{\mathrm{LT}}(\zeta^*, \nu^*, \lambda^*)/50} \approx 7 \times 10^{-6}$.

Remarkably, one finds the agreement at low temperature to be an order of magnitude better than that in the case of minimal duality breaking studied in [7].

Moreover, in the next section we will show that, besides improving the agreement with Monte Carlo results at low and high temperature, the implementation of the strong duality breaking also permits to describe features at the critical point.

[8] To be more precise, both expressions can differ by a I_1.

6. The critical point

Once the parameters have been fixed as in (23) one may verify that the behavior at the critical point is correctly reproduced as well. To do this one can fit near the critical point the non-analytic[9] part of the free energy in Eq. (8) with the optimal parameters with a function of the form

$$F_{\mathrm{crit}} \approx A_+ |\beta - \beta^*|^{2-\alpha} + c, \quad \beta < \beta_c,$$
$$F_{\mathrm{crit}} \approx A_- |\beta - \beta^*|^{2-\alpha} + c, \quad \beta > \beta_c$$

and find the optimal values of the constants c, A_+, A_- and α, so that α will be our prediction for the critical exponent and A_+/A_- will be our estimate for the universal amplitude ratio. This form of the free energy's critical part is expected both from Conformal Field Theory and from experiments. The results of the fit done[10] with *Mathematica* by fitting the (non-analytic part of the) Kallen–Lehmann free energy with the optimal parameters in Eq. (23) with the above functions (25) from $\beta_{\min} = 0.22104$ to $\beta_{\max} = 0.22208$ yield

$$A_- = 4.18, \qquad A_+ = 2.27, \qquad c = -0.19, \qquad \alpha = 0.11, \tag{25}$$

the agreement appears to be very good when compared with recent estimations in [19], where the value $\alpha_{\mathrm{obs}} \approx 0.114(6)$ was found. In turn, we find

$$\Delta\alpha \approx \frac{\alpha_{\mathrm{obs}} - \alpha}{\alpha_{\mathrm{obs}}} \approx 0.035,$$

$$\Delta(A_+/A_-) \approx \frac{(A_+/A_-)_{\mathrm{obs}} - (A_+/A_-)}{(A_+/A_-)_{\mathrm{obs}}} \approx 0.07.$$

Both theoretical and experimental determinations of α can be found in [1]. The deviation $\Delta\alpha$ of our prediction (25) from observations appears to be less than 4% in all the more recent values, improving the minimal duality breaking results [7]. Fig. 1 shows the matching between the (non-analytic part of the) Kallen–Lehmann free energy and the F_{crit}, and it confirms that in the parts of the graph of F_{crit} in which the dependence on α is important the agreement is satisfactory.

We expect that more general strong duality breaking can improve the very good agreement with observations and numerical data we found at high, low temperatures as well as at the critical point. For sake of simplicity (and because of our computational resources) we considered the simplest form of strong duality breaking in which (inspired by the Onsager solution in two dimensions) the functional form of k_{eff} at high and at low temperature is the same (see Eqs. (16) and (17)). In turn, in our approach the cusp in the Fisher curve was implemented by the difference Δ_{d_i} between the coefficients $d_i^{(+)}$ at high temperatures and the corresponding coefficients $d_i^{(-)}$ at low temperature. However, one could argue that it is likely the case the functional form of k_{eff} at low temperature in Eq. (17) to be substantially different from the one at high temperature in Eq. (16). In fact, there are infinite possible terms compatible with the Marchesini–Shrock symmetry that one can add to (17) (still satisfying conditions (18) and (20)) so that, in a sense, the very good agreement we found here is unexpected. It would be very interesting to explore theoretical arguments to further constrain k_{eff}. As a matter of fact, one may also try to add terms to k_{eff} compatible with the above physical requirements and

[9] That is, one has to exclude the term $\log 2\cosh\beta$ which does not contribute to the critical behavior.

[10] A regular sampling is chosen with step $\Delta\beta = 2 \times 10^{-5}$, thus the points of the sampling of Kallen–Lehmann are of the form $\beta_{\min} + n\Delta\beta$ and $\beta_{\max} - m\Delta\beta$ up to the critical point.

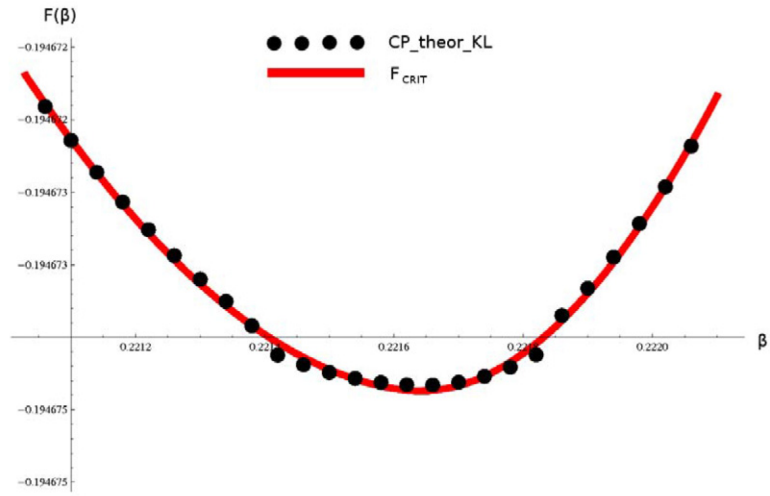

Fig. 1. Bold points in the graph represent a sampling of Kallen–Lehmann free energy $F_{3D}^{(\zeta_i^*,\lambda^*)}(\beta)$, while the continuous line corresponds to the critical part of the expected free energy F_{crit} versus β. One can observe the different leanings in the left and right sides of the critical point, which is ultimately related to a non-trivial Δ.

see what happens. However, without a theoretical guide, the time required for an exhaustive exploration of the moduli space would be out of range. The lack of sophisticated computational resources restricted us to explore a little region of the space of parameters. In particular, some parameters (ζ_0, ζ_2, λ) were here kept fixed to take the same values found in [7] just as a working hypothesis, and it is likely the case the optimal values to be slightly different from those of the ansatz in [7]. Nevertheless, the implementation of the strong duality breaking led us to a quality leap, bringing our predictions at low temperature closer to Monte Carlo simulations. Remarkably, at the same time our model permits to reproduce the universal amplitude ratio Δ and to predict the critical exponent α.

7. Conclusions

In this Letter we studied the distribution of Fisher zeros in the Kallen–Lehmann approach to the three-dimensional Ising model. It was shown that non-trivial amplitude ratios $\Delta = A_+/A_-$ are compatible with the ansatz proposed in [3]. We proposed a mechanism (which we called *strong duality breaking*) by generating a cusp in the curve of the zeros of the free energy $F(\beta)$ in the complex β-plane, being the cusp located at the critical point.

This mechanism not only permitted us to reproduce the Monte Carlo prediction for the value of Δ, but also led us to improve the results of [7] bringing the predictions of the Kallen–Lehmann ansatz at low temperature closer to Monte Carlo simulations. The agreement turns out to be remarkable. In particular, the matching between our results and Monte Carlo estimations for the critical exponent α and for the amplitude ratio Δ exhibit a relative deviation of 3.5% and 7%, respectively.

We interpret our result as a motivation to continue the investigation of phenomenological semi-analytic methods of this kind as a promising approach to solve interesting problems in statistical physics.

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