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Subdominant Critical Singularities in the bcc Ising Model

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In order to analyze coalescing singularities using series expansion, a modification of the method introduced by Baker and Hunter is proposed. The Padé approximants on the Mellin transform are computed simultaneously for the initial series and its derivatives, allowing unbiased estimates for the critical parameters. The method is applied to the series generated by Nickel for various values of the spin in the bcc Ising model. We show that even with these longer series, the subdominant indices display large variation with the spin, and remain too small compared to the universal renormalization group prediction. However, the method does not detect other singularities in the temperature plane which are responsible for the observed discrepancy. Therefore the discrepancy is not significant.

KEY WORDS: Ising model; critical subdominant singularities; series analysis of critical indices; Pade approximants and mellin transform.

1. INTRODUCTION

The renormalization group approach to critical phenomena initiated by Wilson[1] is generally accepted now, and definite predictions have been given for critical indices starting from field theory models.[2–6] However, there were small but persistent discrepancies with values obtained from series analysis in the spin-1/2 Ising model.[7–9] Additional terms have recently been computed by Nickel[10,11] in the bcc Ising model. Nickel's main observation is related to the dependence of critical indices on the value of the spin: he showed that the critical indices obtained from series analysis depend much more on the value of the spin than expected. Thus uncertainties given by usual ratio or D-log Padé method,[12,13] or Padé Mellin analysis[14] should be enlarged in order to include spin dependence effects. Spin effects were considered before only on fcc lattice,[15,16] but

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shorter series than that now available on bcc lattice. With the new data there seem now to be no serious discrepancies any more for the critical indices γ and ν between field theory and series analysis.[11] New analyses have been performed using Nickel's data,[17,18] which confirm the previous conclusion by Nickel concerning critical indices and hyperscaling. Also deserving mention is a different kind of analysis[19,20,21] using expansion in effective renormalized coupling constant which helps explain the apparent contradiction with previous results.[7,22]

Much less clear is the situation concerning subdominant corrections,[23,19] which appear often much too weak to be in perfect agreement with field theory estimates, although other analyses[17,18] give indirect confirmation of field theory. This paper is devoted to a careful analysis of the bcc series using Nickel's data. The method used is an improvement of the method used by Baker and Hunter,[14] which perform Padé approximation on the Mellin transform of the high-temperature series. In fact the method is sensitive to the value of the critical temperature parameter,[23] an effect also observed in other procedures.[24] We will especially emphasize this question and give an independent determination of the critical temperature parameter, by comparison of the initial series and its derivatives. We also analyze the spin dependence effect. The conclusion is that even the present series are not sufficiently long to detect without any doubt a subdominant universal singularity, and we observe that the subdominant index increases with the spin, an effect which may be related to the increase of the amplitude of the singularity. We show by analysis of test functions that this effect may be attributed to the regular correction to the dominant singularity which cannot be separated, at the available order, from the subdominant one. The presence of other singularities in the temperature plane is in fact responsible of the slowness of convergence. But we need longer series to detect these singularities and remove their effects in an unambiguous way.

2. A BEST CHOICE FOR THE CRITICAL PARAMETERS

We assume that the function $f(K)$, given through its power series, admits a singular behavior near $K = K_c$:

$$f(K) = \sum f_n K^n \sim f_0\left[\left(1 - \frac{K}{K_c}\right)^{-\gamma} + \sum_i A_f^{(i)}\left(1 - \frac{K}{K_c}\right)^{-\gamma_i}\right]$$

The method introduced by Baker and Hunter[14] generates an auxiliary function $S(w)$ which behaves as[23]

$$S(w) = \sum S_n w^n \sim f_0\left(\frac{1}{1+\gamma w} + \sum_i \frac{A_f^{(i)}}{1+\gamma_i w}\right)$$

$S(w)$ will exhibit polar singularities at $w_i = -1/\gamma_i$ related to the singular behavior of f near K_c and also at $w_n = 1/n$ related to the regular part of f near K_c. The series expansion of S can be deduced from the expansion of f.[23] Padé approximants to S will provide estimates for the positions and residues of poles, that is, estimates for weights and indices. However, in principle an exact knowledge of K_c is required to compute the series expansion of S, and uncertainties on K_c will generate instabilities in the results due to an effective strengthening of the regular part. Therefore we will use K_c as an external parameter[23] and examine the variation of estimates $\gamma(K_c)$ and $\gamma_1(K_c)$ with K_c. In the present work we will consider simultaneously $f(K)$ and its derivatives:

$$f^{(n)}(K) = \frac{\partial^n}{\partial K^n} f(K)$$

which admits also a singular behavior of a similar kind. Each series $f^{(n)}(K)$ will provide estimates $\gamma^{(n)}(K_c)$ and $\gamma_1^{(n)}(K_c)$, and the best K_c will be the one for which variation of estimate with the order of derivation is as small as possible. This procedure, which resulted from a discussion with J. Zinn-Justin, seems to be new and gives an independent determination of the best value of the critical parameter K_c. We first consider the susceptibility series. The reader can see how the best K_c can be detected graphically in Fig. 1 for γ and Fig. 2 for γ_1 in the spin-2 case. This particular case has been chosen for illustration, but the method works equally well for the spin 1, 2, and ∞ susceptibility series and also for the corresponding squared correlation length series. Furthermore, the best K_c obtained for γ, γ_1, (2ν), and $(2\nu)_1$ do agree within errors. It is even possible to eliminate K_c by plotting γ against γ_1 as shown in Fig. 3, which shows that a direct determination of the best γ and γ_1 is possible using such a plot.

In the following tables we give the best estimates of the indices γ and $\gamma_1 = \gamma - \Delta_1^{(\gamma)}$ coming from the susceptibility, the indices 2ν and $(2\nu)_1 = 2\nu - \Delta_1^{(\nu)}$ coming from the squared correlation lengths, as well as the weight of the singularities defined as

$$\chi(K) \sim \chi_0 \left[\left(1 - \frac{K}{K_c}\right)^{-\gamma} + A_\chi \left(1 - \frac{K}{K_c}\right)^{-\gamma_1} \right]$$

$$\xi^2(K) \sim \xi_0^2 \left[\left(1 - \frac{K}{K_c}\right)^{-2\nu} + A_{\xi^2} \left(1 - \frac{K}{K_0}\right)^{-(2\nu)_1} \right]$$

These estimates are obtained with the highest-order possible $(n - 1/n)$ Padé approximant, the order n decreasing with the order of derivation. We concentrated our analysis on these particular Padé approximants replacing the analysis of the full Padé table by the analysis of the various derivatives. In addition, use of the derivative will suppress effects of low orders, giving

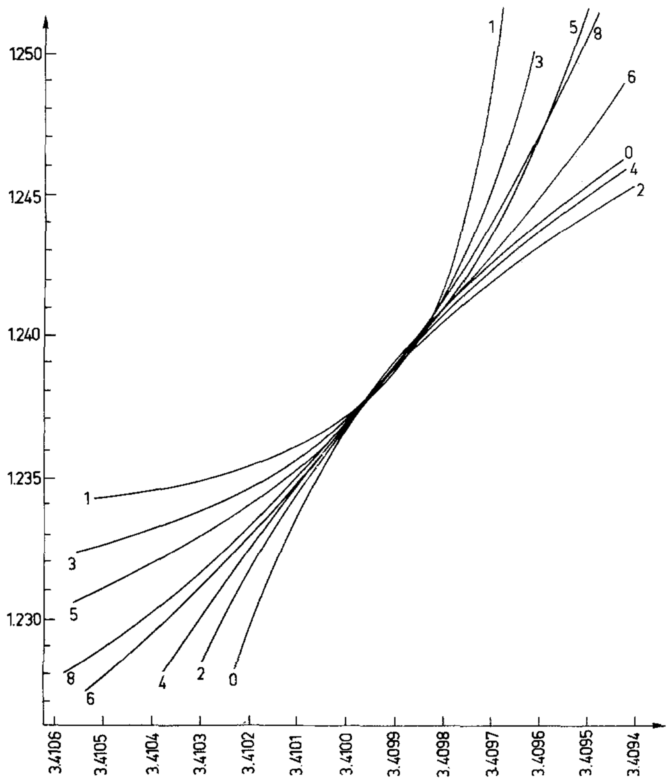

Fig. 1. Estimates for γ versus K_c^{-1} in the spin-2 case, given by various derivatives of the susceptibility series.

more emphasis to higher terms. We want to point out that the rather unexpected stability with order of derivation is our best reason to trust the method. In fact it is known that Padé approximant will give good results when the residues of the dominant pole have the same sign. This property is conserved through derivation, which provides another argument in favor of our procedure.

3. RESULTS

The results obtained in the spin-1/2 case display no stability for the subdominant indices. The values obtained for γ and ν are in agreement with high-temperature series results ($\nu \sim 1.2466$, $\nu = 0.638$); however, the best K_c for γ and ν differ by about 3×10^{-4}, which is about five times more than in the other spin cases. The series expansions at order 22 on power of

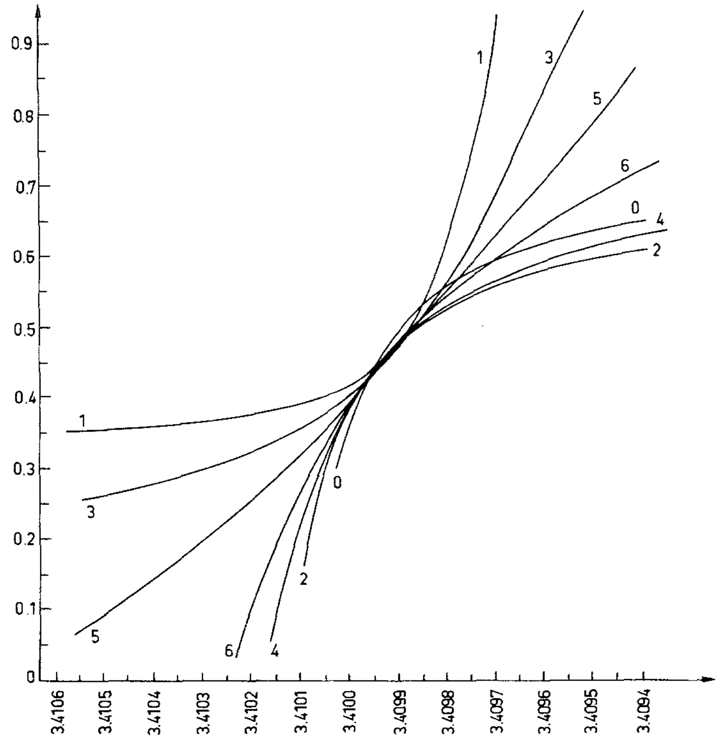

Fig. 2. Estimates for γ_1 versus K_c^{-1} in the spin-2 case given by various derivatives of the susceptibility series.

K show anomalous behavior, and give very unstable subdominant indices, an effect not apparent at order 16 in the expansion on powers of $\tanh K$ considered before by Bessis et al.[23] The smallness of the weight of the subdominant singularities is probably responsible of the present situation, which looks more like the fcc case considered by the same authors.

In the higher spin case, our results for γ and ν agree with results of Nickel[11] and Zinn-Justin.[17] However, renormalization group theory[25,26] predicts that $\gamma - \gamma_1$ and $2\nu - (2\nu)_1$ should also be universal and equal to $\omega\nu = 0.498 \pm 0.020$,[5,6] which gives $\gamma_1 = 0.747 \pm 0.007$ and $(2\nu)_1 = 0.767 \pm 0.008$. Even in the most favorable case, which occurs at infinite spin, we get $\gamma_1 = 0.50 \pm 0.02$ and $(2\nu)_1 = 0.56 \pm 0.02$. Therefore the subdominant singularities obtained through the present analysis remain too weak. However, we observe that our estimates of the subdominant singularity depend very much on the spin, an effect reminiscent of the variation of γ and ν already observed by Nickel. Results are displayed in Tables I and II.

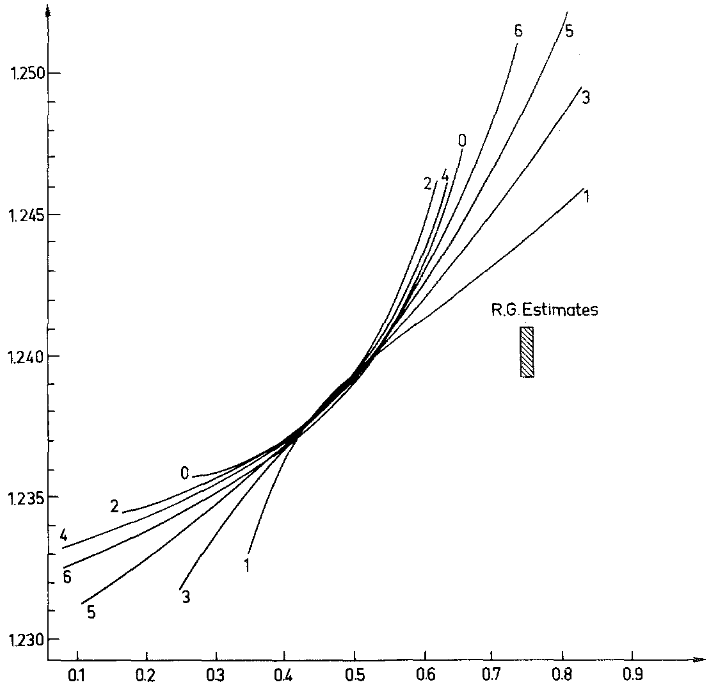

Fig. 3. Estimates for γ versus γ_1 in the spin-2 case given by various derivatives of the susceptibility series, compared to renormalization group estimates.

We want to mention that the uncertainties we quoted take into account not only the variation of indices with order of derivation, but also the values we can determine by comparison of amplitudes of the various derivatives. We have checked that the amplitudes of the singularities do vary with the order of derivation in a way consistent with our estimates of indices.

We have also obtained values for $R = A_\xi / A_\chi = \frac{1}{2} A_{(\xi^2)} / A_\chi$. We get 1 ± 0.5 for spin $1/2$, 0.80 ± 0.06 for spin 1, 0.73 ± 0.04 for spin 2, 0.67 ± 0.04 for spin 2. These number (except for spin $1/2$ as mentioned above) give estimates for R which are close to the universal predicted values $R = 0.65 \pm 0.05$.[27–29] However, our result still display a variation with the spin.

So at least we can conclude that the present series do not yield a universal isolated singularity at K_c. Universality might be restored by taking into account other singularities in the K plane. There is some indication[17] that this could occur. In fact, other singularities will generate through the Mellin transform regular contribution $\sum a_n (K_c - K)^n$, that is, additional poles corresponding to positive indices in the Padé Mellin approximant. We shall see in the next section that the available orders are not sufficiently high to separate all the present singularities; in particular we should also see contribution at $\gamma, \gamma - \omega\nu, \gamma - 1, \gamma - 2\omega\nu, \ldots$. Our result could fit in the scheme of renormalization theory if we assume that our subdominant singularity represents in fact a combination of two singularities at $\gamma - \omega\nu \simeq \gamma - 0.5$ and $\gamma - 1$. But a direct check of universal properties of γ_1 is still lacking.

4. COMPARISON WITH TEST FUNCTIONS

In order to verify the last statements of the previous section, we have considered test functions of the following form:

$$f(K) = \left(1 - \frac{K}{K_c}\right)^{-\gamma} + \sum_{i=1}^{3} t_i \left(1 - \frac{K}{K_c}\right)^{-\gamma_i} + t_a \left(1 + \frac{K}{K_c}\right)^{1-\alpha}$$

We have used $\gamma = 1.24$, $\gamma_1 = \gamma - 1/2$, $\gamma_2 = \gamma - 1$, $\gamma_3 = \gamma - 2$, and $\alpha = 0.1$, in order to simulate a realistic susceptibility series; with an antiferromagnetic singularity at $K = -K_c$. We have observed that using 22 terms, our diagrams (Figs. 1.2, 3) are well reproduced with values $t_1 = t_2 = t_a = 0.1$, t_3 small. However, this is not intended to be a fit, but only an example given in order to understand why the value we get for γ_1 are too small. In fact we get only two poles corresponding to positive indices γ and γ_1 close to 1.24 and 0.5, respectively. The values obtained for γ_1 stay in between 0.24 and 0.74. We have also observed the following features of the subdominant poles.

(i) Stability is lost if t_1 or t_2 are negative.

(ii) The subdominant index decreases toward 0.24 when we reduce t_1 and increases toward the right value 0.74 when we reduce t_2.

(iii) For the best K_c, we observe $\Delta K_c / K_c \sim 2 \times 10^{-5}$ with 22 terms and 10^{-6} with 34 terms.

(iv) We get the right number of positive indices (three in our case) when we use 34 terms, but only in a small range around the exact K_c. We

Table I. Analysis of the Susceptibility Series

Spin	Best K_c^{-1}	γ	$\gamma_1 = \gamma - \Delta_1$	χ_0	A_χ
1/2	6.35320 ± 8.10^{-5}	1.2466 ± 0.0002	—	0.998 ± 0.001	$2.10^{-2} \pm 0.5\ 10^{-2}$
1	4.45120 ± 5.10^{-5}	1.2394 ± 0.0005	0.30 ± 0.03	0.614 ± 0.002	0.122 ± 0.007
2	3.40995 ± 4.10^{-5}	1.2375 ± 0.0004	0.41 ± 0.03	0.437 ± 0.004	0.210 ± 0.006
∞	2.29838 ± 4.10^{-5}	1.2372 ± 0.0002	0.50 ± 0.02	0.280 ± 0.002	0.268 ± 0.008

Table II. Analysis of the Squared Correlation Length Series

Spin	Best K_c^{-1}	2ν	$(2\nu)_1 = 2\nu - \Delta_1$	ξ_0^2	A_{ξ^2}
1/2	6.35290 ± 7.10^{-5}	1.2766 ± 0.0003	—	7.72 ± 0.01	$4.10^{-2} \pm 1.10^{-2}$
1	4.45110 ± 4.10^{-5}	1.2641 ± 0.0004	0.32 ± 0.03	4.70 ± 0.02	0.196 ± 0.006
2	3.40993 ± 3.10^{-5}	1.2612 ± 0.0006	0.48 ± 0.02	3.33 ± 0.02	0.309 ± 0.009
∞	2.29836 ± 4.10^{-5}	1.2608 ± 0.0006	0.56 ± 0.02	2.14 ± 0.02	0.359 ± 0.011

get $\gamma = 1.2396$, $\gamma_1 \simeq 0.67$, $\gamma_2 = 0.10$; however, one has to be careful in analyzing the variation of γ and γ_1: the interesting range is reduced when the order increases.

(v) The results are not considerably better when the amplitude t_a of the singularity at $(-K_c)$ is reduced even by a factor of 10. We still have only two positive indices. However, if we consider a new function with singularity at $(-2K_c)$ instead of $(-K_c)$, we get with 22 terms somewhat improved results: A third positive pole appears in the vicinity of the exact K_c, and γ_1 increases. But results are not very stable.

5. CONCLUSION

The comparison with test functions shows that, as long as we do not get the right number of poles corresponding to positive indices, we will not get accurate values for subdominant indices. The number of expansion terms required in order to get the right answer seems to be prohibitive. Nevertheless, our analysis shows that the discrepancy with renormalization group result is not significant. In other words, our results can be interpreted indirectly in the renormalization group frame. A direct verification is still lacking. Our work provides also a warning: it is possible to reproduce rather well the series expansion with a somewhat inappropriate function (here two instead of three positive indices). Therefore we can have fake stability, an effect already observed by Nickel.[11] This warning will still be valid for future methods devised in order to include antiferromagnetic effects, which may be perturbed by other unknown singularities. A mystery remains in the spin-1/2 case. Why are stability values for K_c obtained from susceptibility and square correlation length so different?

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