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LETTER TO THE EDITOR

Ising model phase boundary†

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Abstract. We compute, on the basis of available power series expansions, a large number of derivatives, with respect to the magnetic field, of the free energy for the two-dimensional spin-$\frac{1}{2}$ Ising model along the phase boundary $H=0$, $T<T_c$. We find this series to be divergent, and so the phase boundary is a line of analytic singularities. The same analysis in three dimensions leads to the same conclusion, with lower precision.

The nature of the possible singularity of the spin-$\frac{1}{2}$ Ising model free energy along the first-order phase transition line $H=0$, $T<T_c$ has been of considerable theoretical interest. In mean-field-type approximations, and in the exact solution for the Bethe lattice, the free energy of one phase, say $H>0$, can be analytically continued through the $H=0$ line to the 'spinodal' point, conceivably representing the metastable state. Gaunt and Baker (1970), on the basis of an examination of the series expansion then available, found no numerical evidence against this picture. On the other hand, Fisher (1967) suggested, based on the droplet model, that the $H=0$ line might be a line of branch-point singularities. Recently Enting and Baxter (1979) obtained long activity series at two temperatures below the critical temperature for the square lattice and concluded that the behaviour of their coefficients is consistent with the existence of a line of essential singularities, as suggested by the renormalisation group approach of Klein *et al* (1976). Another possibility was proposed by Domb (1976), who modified the droplet approach and argued that the first singularity in the activity series is located beyond the $H=0$ line and that the first singularity is one type of branch-point for low temperatures and a different type for temperatures closer to T_c. Finally, recent rigorous results for the percolation problem (Kunz and Souillard 1978a, b) strongly suggest (Deylon 1979) that the $H=0$ line is a line of singularities for $T<T_c$.

The purpose of this Letter is to show that the expansions of the free energy, or equivalently the magnetisation $M(T, H)$, around $H=0$ give rise to divergent series for all $T<T_c$. This result implies that there is a line of singularities exactly at $H=0$, $0<T<T_c$. We further show that the large-order behaviour of the expansion is consistent with the idea that, when $M(T, H)$ for $H>0$ is continued into the complex H plane, there is a cut along the negative real axis across which the imaginary part of M has a finite discontinuity.

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We take $\bar{M}(u, \mu) = (1 - M(T, H))/2$, $H > 0$ as the basic quantity, where $u = \exp(-4\beta J)$ and $\mu = \exp(-2\beta H)$, and consider the expansion

$$\bar{M} = \sum_{n=1}^{\infty} b_n(u)\mu^n \tag{1}$$

$$= \sum_{n=0}^{\infty} a_n(u)(-2h)^n, \tag{2}$$

where $h = \beta H$. The coefficients $a_n = (n!)^{-1} \Sigma_{l=0}^{\infty} l^n b_l$ exist for all n when $u \neq u_c$ (Lebowitz 1972). The approach taken by Enting and Baxter (1979) was to try to determine whether the radius of convergence of series (1) is exactly unity. Our approach is to investigate whether series (2) has a finite radius of convergence or not. If the magnetisation can be continued from $h > 0$ to $h < 0$, it is necessary that equation (2) have a finite radius of convergence. We have determined the coefficients numerically using the available low-temperature series expansion data (Baxter and Enting 1979, Sykes *et al* 1973, 1975). The best currently available series are for the square lattice. For each field derivative we have constructed various first-order integral approximants (Hunter and Baker 1979) to the series in u, and we have evaluated them at several temperatures. Some typical series, so obtained, for the square lattice are given in table 1. They have been cross-checked where possible against the series summation results of the high-field series of Enting and Baxter (1979). We plot in figure 1 the ratios of successive coefficients $r_n = a_n/a_{n-1}$ as a function of n. The asymptotic behaviour of the r_n is apparently linear, and we conclude that

$$r_n \sim A(n + n_0) \qquad \text{as } n \to \infty, \tag{3}$$

where $A = 0{\cdot}096 \pm 0{\cdot}001$ and $24{\cdot}5 \pm 0{\cdot}5$ for $u/u_c = 0{\cdot}1$ and $0{\cdot}9$ respectively. We found this behaviour for the whole range $0 < u < u_c$. The parameter A of equation (3) is strongly temperature-dependent and increases steadily as $u \to u_c$. In fact, if we assume the scaling behaviour near the critical point,

$$a_n(u) \sim \Gamma_n(1 - T/T_c)^{-n\Delta+\beta}, \tag{4}$$

where $\beta = \frac{1}{8}$ and $\Delta = \frac{15}{8}$, then we can determine the first several critical amplitudes (see also Essam and Hunter 1968). We have tabulated our estimates for the square lattice in table 1. From these estimates we may also estimate

$$A(u) \sim (0{\cdot}124 \pm 0{\cdot}01)(1 - T/T_c)^{-\Delta} \qquad \text{as } T \to T_c. \tag{5}$$

The parameter n_0 seems to be relatively insensitive to u, and we estimate $n_0 = 0{\cdot}1 \pm 0{\cdot}2$ for all $u < u_c$. The behaviour of the r_n for the triangular lattice is found to be similar to that for the square lattice. Here we estimate $A(u) \sim (0{\cdot}125 \pm 0{\cdot}015)(1 - T/T_c)^{-\Delta}$ and $n_0 = 0 \pm 0{\cdot}5$.

We have also considered the series for the three-dimensional lattices. Due to the relative shortness of the available series, our results are not as good as in two dimensions. However, we do find at least that the a_n for the BCC and FCC lattices in the range $0{\cdot}1 \leq u \leq 0{\cdot}4$ are consistent with equation (2) being a divergent series.

If we assume that the series, equation (2), is Borel-summable (Hardy 1949) and let $B(h)$ be the Borel transform of $M(h)$,

$$B(h) = \sum_{n=0}^{\infty} \frac{a_n}{n!}(-2h)^n, \tag{6}$$

Table 1. The estimated values of a_n (equation (2)) for $u = 0{\cdot}1u_c$ and $0{\cdot}9u_c$ ($u_c = 3-\sqrt{8}$) and Γ_n (equation (4)) for the square lattice. The uncertainties are at most ± 1 in the last digit shown unless otherwise indicated.

n	$a_n(u=0{\cdot}1u_c)$	n	$a_n(u=0{\cdot}9u_c)$
1	$0{\cdot}340676\times10^{-3}$	1	$0{\cdot}857637$
2	$0{\cdot}198419\times10^{-3}$	2	$0{\cdot}303338\times10^{2}$
3	$0{\cdot}895862\times10^{-4}$	3	$0{\cdot}206224\times10^{4}$
4	$0{\cdot}392154\times10^{-4}$	4	$0{\cdot}200902\times10^{6}$
5	$0{\cdot}194603\times10^{-4}$	5	$0{\cdot}250383\times10^{8}$
6	$0{\cdot}115696\times10^{-4}$	6	$0{\cdot}37716\times10^{10}$
7	$0{\cdot}807868\times10^{-5}$	7	$(0{\cdot}66386\pm0{\cdot}000035)\times10^{12}$
8	$0{\cdot}641871\times10^{-5}$	8	$(0{\cdot}133496\pm0{\cdot}000004)\times10^{15}$
9	$0{\cdot}569247\times10^{-5}$	9	$(0{\cdot}30173\pm0{\cdot}000015)\times10^{17}$
10	$0{\cdot}557617\times10^{-5}$	10	$(0{\cdot}7570\pm0{\cdot}0006)\times10^{19}$
11	$0{\cdot}598638\times10^{-5}$	11	$(0{\cdot}2086\pm0{\cdot}0003)\times10^{22}$
12	$0{\cdot}699371\times10^{-5}$	12	$(0{\cdot}626\pm0{\cdot}001)\times10^{24}$

n	$a_n(u=0{\cdot}1u_c)$	n	Γ_n
13	$0{\cdot}883482\times10^{-5}$	1	$0{\cdot}638424\times10^{-2\dagger}$
14	$0{\cdot}120013\times10^{-4}$	2	$0{\cdot}110134\times10^{-2}$
15	$0{\cdot}174467\times10^{-4}$	3	$0{\cdot}37419\times10^{-3}$
16	$0{\cdot}27029\times10^{-4}$	4	$0{\cdot}18226\times10^{-3}$
17	$0{\cdot}44458\times10^{-4}$	5	$0{\cdot}11357\times10^{-3}$
18	$(0{\cdot}77381\pm0{\cdot}00002)\times10^{-4}$	6	$(0{\cdot}85542\pm0{\cdot}00002)\times10^{-4}$
19	$(0{\cdot}14209\pm0{\cdot}00002)\times10^{-3}$	7	$0{\cdot}7529\times10^{-4}$
20	$(0{\cdot}27454\pm0{\cdot}00005)\times10^{-3}$	8	$0{\cdot}7570\times10^{-4}$
21	$(0{\cdot}5568\pm0{\cdot}0002)\times10^{-3}$	9	$(0{\cdot}8555\pm0{\cdot}00015)\times10^{-4}$
22	$(0{\cdot}11829\pm0{\cdot}00004)\times10^{-2}$	10	$0{\cdot}1073\times10^{-3}$
23	$(0{\cdot}2627\pm0{\cdot}0004)\times10^{-2}$	11	$(0{\cdot}1478\pm0{\cdot}0002)\times10^{-3}$
24	$0{\cdot}609\pm0{\cdot}002)\times10^{-2}$	12	$(0{\cdot}2214\pm0{\cdot}0005)\times10^{-3}$

† Exact value

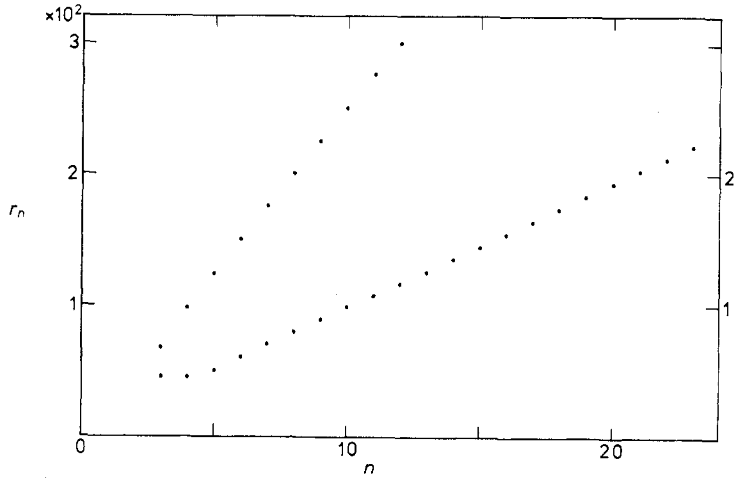

Figure 1. $r_n = a_n/a_{n-1}$ versus n for the two temperatures $u/u_c = 0{\cdot}1$ and $0{\cdot}9$ for the square lattice. The lower (upper) set of data are for $u/u_c = 0{\cdot}1$ $(0{\cdot}9)$ with the RHS (LHS) scale.

then the large-order behaviour implied by equation (3) gives us $B(h) \sim (1+2Ah)^{-(1+n_0)}$ as $h \to (2A)^{-1}$. This leading singularity in B adds to $\bar{M}$ a term proportional to ${}_2F_0(1, 1+n_0; -2Ah)$, where ${}_2F_0$ is a confluent hypergeometric function (Abramowitz and Stegun 1964). The function ${}_2F_0\,(1, \alpha; -z)$ has a cut on the negative real axis, and the imaginary part has the discontinuity $-2\pi^{1/2}(\Gamma(\alpha))^{-1}g^{-\alpha}\exp(-g^{-1})$ across the cut at $z=-g<0$. Therefore, when we continue $\bar{M}(h)$ for $h>0$ into the complex h plane, we expect to find a discontinuity across the negative real axis proportional to $\mathrm{i}(-2Ah)^{-(1+n_0)}\exp[(2Ah)^{-1}]$ as $h \to 0^-$.

If one were to assume, following Enting and Baxter (1979), that the b_n of equation (1) are of the form

$$b_n \sim n^{-g}a^{n^\sigma}, \tag{7}$$

then one can easily compute that

$$r_n \sim (-\ln a)^{-1/\sigma}n^{-1}\Gamma\left(\frac{n-g+1}{\sigma}\right)\Big/\Gamma\left(\frac{n-g}{\sigma}\right) \qquad \text{as } n \to \infty, \tag{8}$$

If we compare equation (3) and (8), we may immediately conclude that $\sigma = \frac{1}{2}$, $a = \exp(-2/\sqrt{A})$ and $g = \frac{1}{4} - \frac{1}{2}n_0$. Thus the simple assumption that $g = 1 + 1/\delta = \frac{16}{15}$ in two dimensions for $T < T_c$ does not accord with our results. We remark that a direct investigation of series (1) by Padé methods indicates that the unit circle in the complex μ plane is likely to be free of singularities except perhaps near $\mu = \pm 1$.

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