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Behaviour of the Mayer cluster sums, b_n, for the Ising lattice-gas

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Abstract. The high-field polynomials $L_n(u)$ (or equivalently the Mayer b_n coefficients) for the spin $S=\frac{1}{2}$ Ising model with nearest-neighbour ferromagnetic interactions (or equivalently the simple lattice-gas) have been studied for a variety of two and three dimensional lattices. We find that (a) the leading zero of $L_n(u)$ on the positive real u axis always corresponds to a temperature T_1 greater than the critical temperature T_c, and approaches T_c as $n\to\infty$ like $1/n^{1/\Delta}$, where Δ is the usual gap exponent. In addition, (b), $L_n(u)$ appears to have exactly $n-1$ zeros in the physical interval $(u_c, 1)$ corresponding to $T_c<T<\infty$.

Result (a) appears to be rather general since it holds for a variety of other Ising systems including those (I) with longer-ranged interactions, (II) with spin $S>\frac{1}{2}$, and (III) on Bethe lattices of coordination numbers $q=2$ (linear chain) and (IV) $q=3$. Result (b), on the other hand, is not generally valid when $S>\frac{1}{2}$ although it does seem to apply for all the other systems studied.

1. Introduction and summary

Mayer and his collaborators (see Mayer and Mayer 1940) showed how the pressure of an imperfect gas can be expanded either in powers of the activity z or the density ρ. The expansions are

$$p/kT=\sum_{n=1}^{\infty} b_n z^n \tag{1.1}$$

and

$$p/kT=\sum_{n=1}^{\infty} B_n \rho^n, \tag{1.2}$$

respectively, where the coefficients b_n and B_n are functions of the temperature T. Over the years, the behaviour of the b_n and B_n coefficients has been the subject of much speculation (for example, see Mayer and Mayer 1940, Katsura 1954, 1958, 1963). Unfortunately, for an interaction potential such as the Lennard-Jones 12–6 potential, only the first five coefficients have been calculated (Barker *et al* 1966). Considerably more progress can be made for the simple Ising lattice-gas, where in two dimensions between 12 and 25 coefficients are available depending on the lattice, and in three dimensions there are between 8 and 17 coefficients. In the hope of throwing some light on the universal features of the behaviour of b_n and B_n coefficients, we have made a detailed study of these coefficients.

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By the Ising/lattice-gas analogy (Lee and Yang 1952), the analogue of the Mayer z-expansion for a simple Ising lattice-gas is

$$\ln \Lambda = \sum_{n=1}^{\infty} L_n(u)\mu^n, \tag{1.3}$$

where $\ln \Lambda$ is the configurational free energy of the simple Ising model with spin $S=\frac{1}{2}$ and nearest-neighbour ferromagnetic interactions (Sykes *et al* 1965), and μ and u are the usual field and temperature variables

$$\mu = \exp(-2mH/kT), \qquad u = \exp(-4J/kT). \tag{1.4}$$

The L_n which are the analogues of the b_n (or more precisely $u^{\frac{1}{2}qn}b_n$, where q is the lattice coordination number) are polynomials in u, called the high-field polynomials. (For the honeycomb lattice which has an odd coordination number $q=3$, the variable $z=u^{1/2}$ is often preferred to u.) The high-field polynomials have been derived to quite high order by the 'code method' using partial generating functions (Sykes *et al* 1965, 1973a,b, 1975). In two dimensions ($d=2$), the numbers of polynomials, N, available are $N=25$, 15 and 12 for the honeycomb (HC), square (SQ) and triangular (T) lattices, respectively, and in three dimensions ($d=3$) $N=17$, 13, 11 and 8 for the diamond (D), simple cubic (SC), body-centred cubic (BCC) and face-centred cubic (FCC) lattices, respectively.

The analogue of the Mayer ρ-expansion (or virial expansion) is not usually studied for the Ising ferromagnet but is readily derived by algebraic manipulation from the b_n (or L_n) in the standard manner (see Domb 1974a, for a recent reference). Unfortunately, we have found that the B_n are lattice dependent and have been unable to discern any simple pattern in their behaviour. On the other hand, the b_n have a rather simple behaviour which we study in detail in the next section. It turns out that for all lattices (a) the leading zero of $L_n(u)$ on the positive real u axis at $u=u_1(n)$ corresponds to a temperature greater than the critical temperature ($u_1>u_c$) and approaches u_c as $n\to\infty$ like $1/n^{1/\Delta}$ where Δ is the usual gap exponent. In addition, (b), $L_n(u)$ appears to have precisely $n-1$ zeros in the physical interval $u_c<u<1$. Both these results are confirmed numerically, and a simple scaling argument is given in support of (a). In § 3 we examine the generality of these results by studying a variety of other Ising systems. It appears that property (a) is rather general since we find the same result for Ising models (I) with further-neighbour interactions, (II) with spin $S>\frac{1}{2}$, and (III) on Bethe lattices of coordination numbers $q=2$ (equivalent to the linear chain) and (IV) $q=3$. Property (b), however, does not hold for all Ising models with $S>\frac{1}{2}$ (although it does seem to apply in cases I, III and IV) and hence is not quite so general.

2. Simple Ising model

We have found that the L_n (or equivalently the b_n) have a rather simple behaviour. Apart from a multiple zero at the origin $u=0$ which is of no interest, all the known L_n have exactly $n-1$ zeros lying in the physical interval $u_c<u<1$ (corresponding to $T_c<T<\infty$) and none in the interval $0<u<u_c$ (corresponding to $0<T<T_c$). The proof of this result for arbitrary n is unknown although the result is probably correct. The second half of the result implies that all the L_n (or b_n) are positive for all

temperatures less than T_c. The remaining zeros lie either on the negative real axis or in the left and right hand halves of the complex u plane. No pattern for the location of the non-physical singularities has been discerned.

As n increases the leading zero on the positive real u axis at $u = u_1(n) > u_c$ appears to approach u_c *monotonically*, while the trailing zero at $u_{n-1}(n)$ gets closer to $u = 1$. Indeed the κth zero (κ fixed) at $u_\kappa(n)$ apparently approaches u_c as n increases. Presumably in the limit of $n \to \infty$ the interval $(u_c, 1)$ becomes dense with zeros.

One of the basic questions is the behaviour of the leading zero $u_1(n)$ as $n \to \infty$. A general scaling *ansatz* is

$$(u_1(n) - u_c)/u_c \sim C_1 n^{-\theta_1} + D_1 n^{-\theta_2} + \dots \tag{2.1}$$

where $C_1 > 0$ and $\theta_2 > \theta_1$. The exponent θ_1 can be predicted from scaling theory as follows. Since $L_n(u)$ is a polynomial, it can be expanded in a Taylor series about u_c,

$$L_n(u) = \sum_{m=0}^{\infty} (1/m!) L_n^{(m)}(u_c)(u - u_c)^m \tag{2.2}$$

where $L_n^{(m)}(u_c)$ is the mth derivative with respect to u of $L_n(u)$ evaluated at $u = u_c$. From standard scaling theory one knows (Gaunt and Domb 1970) that

$$L_n^{(m)}(u_c) \sim A_m n^{-2-(1/\delta)+(m/\Delta)}, \qquad (n \to \infty) \tag{2.3}$$

where A_m is a critical amplitude known to be positive for $m = 0$, 1, 2 and 3, at least for the square and body-centred cubic lattices, δ is the critical exponent describing the shape of the critical isotherm and Δ is the gap exponent. Hence, we may write

$$\begin{aligned} L_n(u) &\sim \sum_{m=0}^{\infty} (A_m/m!) n^{-2-(1/\delta)+(m/\Delta)} (u - u_c)^m \\ &\sim n^{-2-(1/\delta)} \sum_{m=0}^{\infty} (Am/m!)[n^{1/\Delta}(u - u_c)]^m \\ &\sim n^{-2-(1/\delta)} F(x) \end{aligned} \tag{2.4}$$

where

$$x = n^{1/\Delta}(u - u_c). \tag{2.5}$$

Now a zero in $L_n(u)$ for real, positive u is reflected in $F(x)$ by a corresponding zero. In particular, the zero at u_1 corresponds to a zero in $F(x)$ at $x = x_1$, say. From (2.5) this implies $n^{1/\Delta}(u_1 - u_c) = x_1$ or $u_1 - u_c = x_1 n^{-1/\Delta}$ which on comparison with (2.1) yields

$$\theta_1 = 1/\Delta \tag{2.6}$$

and $C_1 = x_1/u_c$. Calculation of the higher-order terms in (2.1) requires a knowledge of the correction-to-scaling terms in (2.3) and these are not known with any certainty even when $m = 0$ (Gaunt and Sykes 1972).

We have seen that the leading zero $u_1(n)$ should approach u_c at an asymptotic rate given by (2.1) with an exponent $\theta_1 = 1/\Delta$. In two dimensions, the best series estimate of Δ (Essam and Hunter 1968) gives

$$\theta_1 = 0{\cdot}535 \pm 0{\cdot}003 \qquad d = 2 \tag{2.7}$$

which corresponds to a scaling value of $\frac{8}{15} = 0{\cdot}5333\dots$ (using $\gamma = 1\frac{3}{4}$, $\beta = \frac{1}{8}$ and

$\Delta=\gamma+\beta$). In three dimensions direct series estimates of Δ (Essam and Hunter 1968) give

$$\theta_1=0{\cdot}640\pm0{\cdot}001 \qquad d=3. \tag{2.8}$$

The conjectures $\gamma=1\frac{1}{4}$ and $\beta=\frac{5}{16}$ (Domb 1974b) give a scaling value of exactly $\theta_1=0{\cdot}64$, while the recent renormalisation group values of $\gamma=1{\cdot}2402\pm0{\cdot}0009$ and $\beta=0{\cdot}325\pm0{\cdot}001$ (Le Guillou and Zinn-Justin 1977) lead to $\theta_1=0{\cdot}6389\pm0{\cdot}0008$.

To test this prediction numerically, we first calculate estimates $\theta_1(n)$ of θ_1, namely

$$\theta_1(n)=\frac{\ln[(u_1(n-1)-u_c)/(u_1(n)-u_c)]}{\ln[n/(n-1)]}, \qquad n=3,4,5,\ldots$$

obtained by substituting successive estimates $u_1(n)$ and $u_1(n-1)$ into (2.1), assuming u_c to be known (see Domb 1974b) and solving for θ_1. These estimates which exhibit strong oscillations of period $p=1$ (T, FCC), $p=2$ (SQ, BCC, SC) and $p=4$ (HC, D), are first smoothed by calculating the averages

$$\bar\theta_1(n,p)=[\theta_1(n)+\theta_1(n-1)+\ldots+\theta_1(n-p+1)]/p$$

before plotting against $1/n$. The plots for two- and three-dimensional lattices are shown in figures 1 and 2, respectively, and are consistent with limiting values of θ_1 equal to $1/\Delta$. The curves seem to be on the verge of attaining their asymptotic approach behaviour which is determined, of course, by the second term on the right hand side of (2.1). Inspection of the curves suggests that $\theta_2-\theta_1\leqslant1$ and $D_1\geqslant0$ are the most likely possibilities.

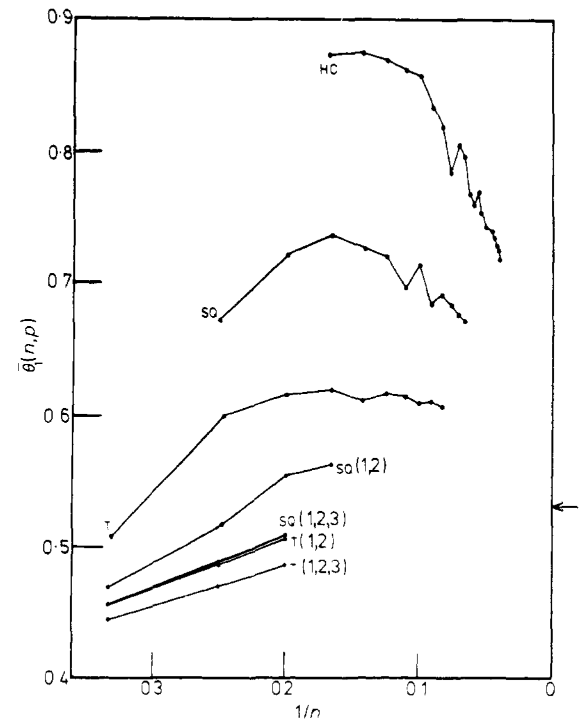

Figure 1. Estimates $\bar\theta_1(n,p)$ of θ_1 plotted against $1/n$ for $d=2$ lattices. The arrow indicates the value $\theta_1=1/\Delta=0{\cdot}5333\ldots$.

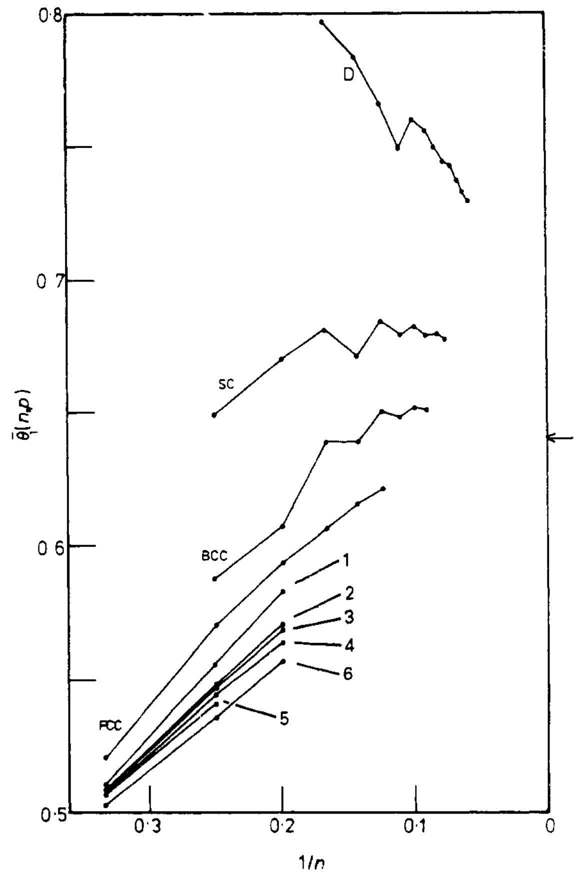

Figure 2. Estimates $\bar{\theta}_1(n, p)$ of θ_1 plotted against $1/n$ for $d=3$ lattices. The arrow indicates the value $\theta_1 = 1/\Delta = 0{\cdot}64$. The curves labelled 1 to 6 are the BCC(1, 2), FCC(1, 2), SC(1, 2), BCC(1, 2, 3), FCC(1, 2, 3) and SC(1, 2, 3) lattices, respectively.

To estimate the amplitude C_1 we have extrapolated successive estimates of

$$C_1(n) = \frac{u_1(n) - u_c}{u_c} n^{\theta_1}$$

using the values $\theta_1 = 0{\cdot}5333\ldots$ $(d=2)$ and $\theta_1 = 0{\cdot}64$ $(d=3)$. We find for the two dimensional lattices:

$$\begin{aligned} C_1 &= 5{\cdot}1 \pm 0{\cdot}1 && (\text{HC}) \\ &= 3{\cdot}25 \pm 0{\cdot}05 && (\text{SQ}) \\ &= 1{\cdot}89 \pm 0{\cdot}02 && (\text{T}) \end{aligned} \tag{2.9}$$

and in three dimensions:

$$\begin{aligned} C_1 &= 2{\cdot}64 \pm 0{\cdot}03 && (\text{D}) \\ &= 1{\cdot}515 \pm 0{\cdot}01 && (\text{SC}) \\ &= 1{\cdot}055 \pm 0{\cdot}005 && (\text{BCC}) \\ &= 0{\cdot}672 \pm 0{\cdot}003 && (\text{FCC}). \end{aligned} \tag{2.10}$$

Since the exponent θ_2 in (2.1) is not known, the estimate $C_1(n)$ were extrapolated against $1/n$ (rather than $1/n^{\theta_2-\theta_1}$) using n-shifts (Gaunt and Guttmann 1974) to allow for any curvature. This should be borne in mind before placing undue weight on the confidence limits quoted in (2.9) and (2.10).

We have also investigated the analogue of (2.1) which uses the temperature T as variable rather than u, namely

$$(T_1(n)-T_c)/T_c \sim C_{T,1}n^{-\theta_1}+\ldots, \tag{2.11}$$

where

$$C_{T,1}=-C_1/\ln u_c. \tag{2.12}$$

It was our hope that the approach to leading asymptotic behaviour would be more rapid using the more 'natural' T variable. In fact, the converse turns out to be the case. Although this is a matter of little consequence in the present instance, it should be remembered when a problem which is less well-understood than the Ising model is being investigated, particularly if the value of $\theta_1 = 1/\Delta$ is not known with any certainty. A second point worth commenting upon is that whereas the amplitudes C_1 appear from (2.9) and (2.10) to be very lattice-dependent, the amplitudes $C_{T,1}$ vary only slowly with either q for fixed d, or d for fixed q. Thus, we find using (2.9), (2.10) and (2.12)

$$C_{T,1}=1{\cdot}94\pm0{\cdot}04\ (\text{HC}),\qquad 1{\cdot}84\pm0{\cdot}03\ (\text{SQ}),\qquad 1{\cdot}72\pm0{\cdot}02\ (\text{T}), \tag{2.13}$$

and

$$\begin{aligned} C_{T,1}&=1{\cdot}78\pm0{\cdot}02\ (\text{D}), && 1{\cdot}71\pm0{\cdot}01\ (\text{SC}),\\ &=1{\cdot}676\pm0{\cdot}008\ (\text{BCC}), && 1{\cdot}646\pm0{\cdot}008\ (\text{FCC}). \end{aligned} \tag{2.14}$$

Some aspects of the preceeding study have been examined previously by Majumdar (1974). However, his work was unsatisfactory in several respects. The main defects were as follows:

(i) Owing to numerical uncertainties associated with his computer program, some of the zeros of $L_n(u)$ lay on the positive real u axis beyond $u=1$. Consequently, the fact that there are exactly $n-1$ zeros in the interval $u_c<u<1$ was not noticed.

(ii) Although the leading zero was assumed to obey a formula of the type (2.1), the exponent θ_1 was not shown to be related to the standard critical exponent Δ.

(iii) The numerical analysis of (2.1) assumed, without justification, higher-order corrections of the form $\theta_2=2\theta_1$, $\theta_3=3\theta_1,\ldots$ and was based upon a least-squares fitting procedure. Such methods are not, in general, appropriate for this type of problem (Gaunt and Guttmann 1974). The estimates of θ_1 so obtained were not dimensionally invariant nor was this restriction placed upon the fitting procedure. Estimates varied between $\theta_1=0{\cdot}652$ and $0{\cdot}934$ for the two dimensional lattices, and between $\theta_1=0{\cdot}356$ and $0{\cdot}648$ in three dimensions.

To conclude this section we return to the scaling arguments and develop them a little further. Firstly, it is clear that not only the leading zero but more generally the κth zero ($\kappa=1,2,3,\ldots$) should scale as in (2.1) with the *same* exponent $\theta_1=1/\Delta$ and amplitude C_κ, corresponding to a zero in $F(x)$ at $x=x_\kappa=C_\kappa u_c$. Secondly, let us consider the max–min points of $L_n(u)$. Since $L_n(0)=L_n(u_1)=0$ and $L_n>0$ in the interval $(0,u_1)$, then $L_n(u)$ must have at least one maximum in this interval. In practice it appears to have only one maximum which occurs in the interval (u_c,u_1). In addition, there will be at least one, and in practice just one, max–min point located between each of the succeeding zeros of L_n. At a max–min point $\dot{L}_n \equiv \mathrm{d}L_n/\mathrm{d}u = 0$, where from (2.4) we have

$$\dot{L}_n \sim n^{-2-(1/\delta)+(1/\Delta)} \dot{F}(x).$$

If $\dot{F}(x) = 0$ (and hence $\dot{L}_n = 0$) at the points $x = t_1$, $x = t_2, \ldots$ then it follows that the value of u at any of the max–min points scales with the exponent $1/\Delta$.

While 'horizontal lengths' of $L_n(u)$, such as the location of its zeros or its max–min points, scale like $1/n^{1/\Delta}$, it is not difficult to show that 'vertical lengths' scale like $1/n^{2+(1/\delta)}$. For example, it follows immediately from (2.3) that

$$L_n(u_c) \sim A_0/n^{2+(1/\delta)}, \qquad n \to \infty. \tag{2.15}$$

In fact, this is essentially the *definition* of the exponent δ since it implies that the magnetisation M along the critical isotherm behaves asymptotically ($H \to 0+$, $\mu \to 1-$) like (Gaunt and Sykes 1972)

$$\begin{aligned} M(u_c, \mu) &= 1 - 2 \sum_{n=1}^{\infty} nL_n(u_c)\mu^n \\ &\sim 1 - 2 \sum_{n=1}^{\infty} A_0 n^{-1-(1/\delta)} \mu^n \sim E(1-\mu)^{1/\delta}. \end{aligned}$$

Series analysis of $M(u_c, \mu)$, or equivalently of $L_n(u_c)$, yields (Gaunt and Sykes 1972)

$$\begin{aligned} \delta &= 15{\cdot}00 \pm 0{\cdot}08 \qquad d = 2 \\ &= \ \ 5{\cdot}00 \pm 0{\cdot}05 \qquad d = 3. \end{aligned} \tag{2.16}$$

The central two-dimensional value has subsequently been proved to be exact by Abraham (1977). In three dimensions, the scaling relation $\delta = 1 + (\gamma/\beta)$ gives $\delta = 5$ on the basic of $\gamma = 1\frac{1}{4}$ and $\beta = \frac{5}{16}$ or $\delta = 4{\cdot}816 \pm 0{\cdot}015$ using the renormalisation group values quoted previously.

Other 'vertical lengths' of interest are the magnitudes of $L_n(u)$ at their max–min points. From (2.4) we see that if there is a max–min point at $x = t_i$, then we should expect

$$L_n \sim F(t_i)/n^{2+(1/\delta)}, \qquad i = 1, 2, 3, \ldots. \tag{2.17}$$

We have tested this relation numerically for the first maximum of $L_n(u)$ and found it to be valid.

3. Other Ising models

We have also investigated several other Ising systems. In all cases, the leading zero on the real, positive u axis at $u = u_1(n)$ lies above u_c ($u_1 > u_c$) and appears to approach u_c (although in one case not monotonically) like $1/n^{1/\Delta}$. The system studied include:

I. The $S = \frac{1}{2}$ Ising model with ferromagnetic interactions extending out to the rth nearest neighbour sites but all interactions being of equal strength. By restricting attention to the so-called 'equivalent neighbour' model, the high-field polynomials L_n are again a function of a single variable rather than r variables. The number of polynomials available are as follows (Dalton and Wood 1969): in two dimensions, $N = 6$ for the SQ(1, 2) and $N = 5$ for the T(1, 2), SQ(1, 2, 3) and T(1, 2, 3), while in three dimensions $N = 5$ for the SC(1, 2), BCC(1, 2), FCC(1, 2), SC(1, 2, 3) and

BCC(1, 2, 3), and $N=4$ for the FCC(1, 2, 3). (The notation indicates over which shells the equal interactions extend.) The results for $\bar{\theta}_1(n, 1)$ are plotted in figures 1 and 2. From universality (Griffiths 1970), we expect to find for lattices of a given dimension the same value of Δ (and hence θ) no matter how far the interaction extends, provided its range is strictly finite. The curves in both figures, although displaced in the direction of increased lattice coordination number, are consistent with such an expectation. Estimates of C_1 obtained by simply extrapolating the last two values of $C_1(n)$ linearly against $1/n$ are:

$$1{\cdot}29\ \text{SQ}(1,2),\qquad 0{\cdot}71\ \text{T}(1,2),\qquad 0{\cdot}70\ \text{SQ}(1,2,3),\qquad 0{\cdot}42\ \text{T}(1,2,3) \tag{3.1}$$

and

$$\begin{aligned} &0{\cdot}57\ \text{BCC}(1,2), &&0{\cdot}41\ \text{SC}(1,2), &&0{\cdot}41\ \text{FCC}(1,2),\\ &0{\cdot}27\ \text{SC}(1,2,3), &&0{\cdot}26\ \text{BCC}(1,2,3), &&0{\cdot}15\ \text{FCC}(1,2,3). \end{aligned} \tag{3.2}$$

These estimates should only be taken as rough guides since the sequences are so short. However, they confirm the trend observed in (2.9) and (2.10) that C_1 decreases with increasing coordination number.

II. The Ising model with nearest-neighbour ferromagnetic interactions only but spin $S>\frac{1}{2}$. Here we have used the data of Fox and Gaunt (1972) which are as follows: $N=12$ (HC, $S=1$), 10 (SQ, $S=1$), 7 (T, $S=1, 1\frac{1}{2}$), 12 (D, $S=1$), 10 (SC, $S=1$), 10 (BCC, $S=1$) and 7 (FCC, $S=1, 1\frac{1}{2}$). In all of these cases, $u_1(n)$ exhibits a marked odd/even oscillation when plotted against $1/n$. The oscillation is so pronounced that the approach to u_c is no longer monotonic at least for small n. Estimates of θ_1 (not shown) are rather erratic and we have been unable to extrapolate them reliably although they are not inconsistent with $\theta_1 = 1/\Delta$ as predicted by universality (Griffiths 1970). For example, using successive averages of

$$\frac{\ln[(u_1(n-2)-u_c)/(u_1(n)-u_c)]}{\ln[n/(n-2)]}$$

as smoothed estimates of θ_1, we find for the $S=1$ simple-cubic lattice 0·649, 0·646, 0·601, 0·640, 0·606 for $n=6$ to 10, respectively. Assuming $\theta_1 = 1/\Delta$, the following estimates of C_1 were obtained:

$$\begin{aligned} C_1 &= 1{\cdot}83 \pm 0{\cdot}12\ (\text{HC}, S=1), && 1{\cdot}15 \pm 0{\cdot}05\ (\text{SQ}, S=1),\\ &\ 0{\cdot}69 \pm 0{\cdot}05\ (\text{T}, S=1), && 0{\cdot}375 \pm 0{\cdot}05\ (\text{T}, S=1\tfrac{1}{2}) \end{aligned} \tag{3.3}$$

and

$$\begin{aligned} C_1 &= 1{\cdot}06 \pm 0{\cdot}03\ (\text{D}, S=1), && 0{\cdot}64 \pm 0{\cdot}02\ (\text{SC}, S=1),\\ &\ 0{\cdot}45 \pm 0{\cdot}02\ (\text{BCC}, S=1), && 0{\cdot}27 \pm 0{\cdot}03\ (\text{FCC}, S=1),\\ &\ 0{\cdot}15 \pm 0{\cdot}05\ (\text{FCC}, S=1\tfrac{1}{2}). \end{aligned} \tag{3.4}$$

It is seen that for $S=1$ as for $S=\frac{1}{2}$, C_1 decreases with increasing coordination number and that for a given lattice, C_1 decreases with increasing S.

III and IV. The $S=\frac{1}{2}$ Ising model with nearest-neighbour ferromagnetic interactions only on Bethe lattices of coordination numbers $q=2$ (III) and $q=3$ (IV). The $q=2$ lattice is equivalent to the Ising linear chain. For both these problems, Joyce (private communication) has proved rigorously that the leading zero approaches the critical point like $1/n^{1/\Delta}$ and has calculated the amplitude C_1 exactly. For the $q=3$ lattice, $\Delta = 1\frac{1}{2}$, the classical or mean field value. The linear chain ($q=2$ case) must be treated rather differently from the other problems we have considered, since the critical temperature is at $T = T_c = 0$ and the exponent Δ cannot be defined in the usual way. Instead one uses the fact that Δ also dictates the rate at which the Yang–Lee zeros (Lee and Yang 1952) on the unit circle $|\mu| = 1$ pinch-down onto the real positive μ axis as $T \to T_c+$. Denoting the critical angle by $\theta_c(T)$ one has in general (Suzuki 1967)

$$\theta_c(T) \sim \Theta(T - T_c)^{\Delta}, \qquad T \to T_c+. \tag{3.5}$$

For the Ising chain it is well known (Lee and Yang 1952) that

$$\theta_c(T) \sim \Theta T^{1/2}, \qquad T \to 0+ \tag{3.6}$$

giving $\Delta = \frac{1}{2}$. For both these problems, Joyce (private communication) has also calculated the high-field polynomials through L_{30}. In figure 3 we have plotted values of $(\bar{\theta}_1(n, 1) - \Delta^{-1})$ against $1/n$. As $n \to \infty$, the curves, which are very smooth, extrapolate accurately to zero from opposite directions; the implications for (2.1) are that $D_1 > 0$ for $q = 3$ and $D_1 < 0$ for $q = 2$. In the $q = 3$ case the curve approaches its limit with an infinite slope implying $\theta_2 - \theta_1 < 1$ in (2.1), which is not unreasonable since $\theta_1 = \frac{2}{3}$. In the $q = 2$ case, however, the curve appears to approach zero with zero slope implying $\theta_2 - \theta_1 > 1$, again a not unreasonable result since $\theta_1 = 2$.

The generality of the $1/n^{1/\Delta}$ result is not too surprising since we would expect the scaling argument presented in § 2 to hold without modification for all the above systems save the linear chain. Our observation for the simple Ising model that L_n has exactly $n - 1$ zeros in the physical interval $(u_c, 1)$ is slightly less general since it does

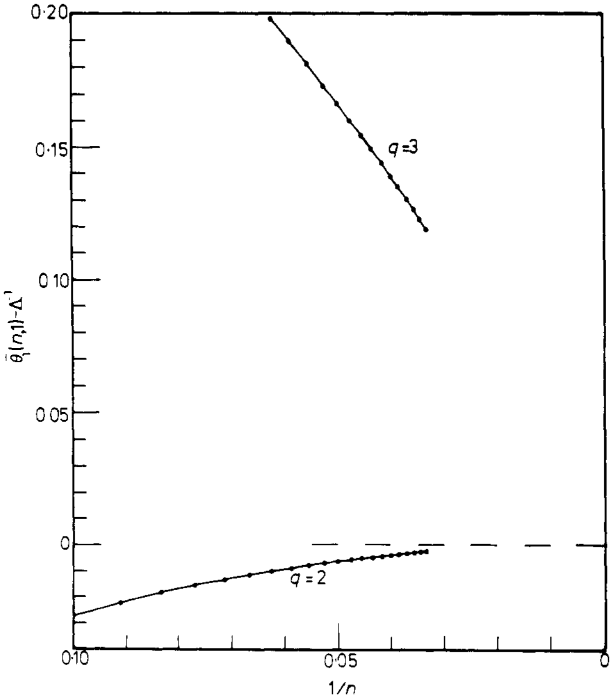

Figure 3. $(\bar{\theta}_1(n, 1) - \Delta^{-1})$ plotted against $1/n$ ($n \leq 30$) for Bethe lattices of coordination numbers $q = 2$ (linear chain) and $q = 3$.

not hold in II above. On the other hand, it does hold for all the other cases considered. Indeed in cases III and IV, L_n has *no* other zeros except the $n-1$ lying in this interval.

Returning to case II, we mention the strong possibility that the $n-1$ rule exists in a slightly modified form. Suppose $S=1$, for example, and one is prepared to classify perturbations from the ordered state ($S_z=+1$, say) according to whether $S_z=0$ or $S_z=-1$. Then, if there are n perturbed spins in all, r of which have $S_z=-1$ and $n-r$ have $S_z=0$, one may write (Fox and Gaunt 1972)

$$\ln \Lambda(u, \mu, \nu) = \sum_{n=1}^{\infty} \sum_{r=0}^{n} l_{n,n-r}(u)\nu^r\mu^{n-r} \tag{3.7}$$

where $\nu=\mu^2$. A pilot study for the $S=1$ body-centred cubic lattice suggests that the polynomials $l_{r,n-r}(u)$ have precisely $n-1$ zeros in the interval $(u_c, 1)$. However, we have not thought it worthwhile to pursue this idea until such a time as the significance of the $n-1$ rule becomes clear.

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