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High temperature series for the susceptibility of the Ising model I. Two dimensional lattices

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Abstract. Extended series expansions for the high temperature zero-field susceptibility of the Ising model are given in powers of the usual high temperature counting variable $v = \tanh K$; for the triangular lattice to v^{16}, for the square lattice to v^{21} and for the honeycomb lattice to v^{32}, inclusive. The asymptotic behaviour of the ferromagnetic and antiferromagnetic susceptibility is studied. It is concluded that the ferromagnetic singularity is not exactly factorizible. The antiferromagnetic susceptibility of the square and honeycomb lattices has a singularity of the same type as the energy at the antiferromagnetic critical temperature. The amplitudes are probably symmetric and close to those given by the energetic approximation. For the triangular lattice the antiferromagnetic susceptibility is probably singular at absolute zero although the form of the singularity remains unknown.

1. Introduction

No exact solution has so far been given for the zero-field susceptibility of the two dimensional Ising model. Knowledge of the critical behaviour of the susceptibility is largely based on a study of exact series expansions (Domb and Sykes 1961, Baker 1961, Sykes and Fisher 1962). We have extended high temperature series expansions for the susceptibility and this paper presents the new data and a numerical analysis. We assume a general familiarity with the problem; introductions are given by Domb (1960) and Fisher (1967). We first indicate briefly the method of derivation of the series coefficients and summarize the salient conclusions that have been drawn from earlier analyses.

We study high temperature expansions in a form first derived by Oguchi (1951). We define the reduced susceptibility χ as $kT\chi_0/m^2$ where χ_0 is the zero-field susceptibility per spin, k Boltzmann's constant, m the moment of a single spin and T the absolute temperature; we denote the energy between parallel spins by J, the quantity J/kT by K and $\tanh K$ by v. The variable v, often called the high temperature counting variable, plays a fundamental role in the theory of high temperature expansions for the spin $\frac{1}{2}$ Ising model. Oguchi showed that if the reduced susceptibility is expanded in the form

$$\chi(v) = \sum_{r=0}^{\infty} a_r v^r \qquad a_0 = 1 \tag{1.1}$$

the coefficients a_r can be related to the number of weak embeddings (Sykes *et al* 1966) in the lattice of a restricted class of linear graphs (magnetic graphs). A detailed study of the

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configurational problem (Sykes 1961) leads to the conclusion that the susceptibility can be written in the form

$$\chi(v) = (1-\sigma v)^{-2}\{1-(\sigma-1)v+v^2-2vU(v)+G(v)\} \tag{1.2}$$

where $\sigma+1$ is the coordination number, $U(v)$ the reduced configurational energy and $G(v)$ a new function, which we call the residual correlation function. This new function can be expanded in the form

$$G(v) = \sum_{r=5}^{\infty} d_r v^r \tag{1.3}$$

and the coefficients d_r can be related to the number of weak embeddings of a more restricted class of linear graphs (no-field and closed magnetic graphs). We shall not describe the method in detail; it presents complex configurational problems and the technique is not directly relevant to our present objectives. By means of it we have extended the series expansions for the susceptibility of the triangular lattice by four coefficients to v^{16}, of the square lattice by five to v^{21}, and of the honeycomb lattice by six to v^{32}, inclusive.

In the critical region for a ferromagnet the reduced susceptibility is found to behave asymptotically as

$$\chi \sim A_{\pm}(1-v/v_{\mathrm{f}})^{-1\cdot75} \qquad v \to v_{\mathrm{f}}\mp \tag{1.4}$$

where $v_{\mathrm{f}} = \tanh J/kT_{\mathrm{C}}$, and the amplitudes A_+ and A_- above and below the critical (Curie) temperature T_{C} respectively, are constants. The critical index of 1·75 was first proposed on the basis of numerical extrapolations (Domb and Sykes 1957, Essam and Fisher 1963); subsequent theoretical studies (Fisher 1959a, Kadanoff *et al* 1967, Wu 1966, Cheng and Wu 1967) suggest strongly that the result is exact. An extensive bibliography is given by Fisher (1963, 1967). There is a pronounced asymmetry in the amplitudes, A_+/A_- being of the order of 37 (Essam and Fisher 1963).

We investigate higher order terms in the asymptotic expansion (1.4) above T_{C}. A precise knowledge of the asymptotic behaviour in the critical region for a two dimensional lattice has an important application in the provision of guidelines for a study of three dimensional lattices. Since the critical temperature is known exactly in two dimensions, conclusions on the general pattern of asymptotic behaviour should be firmly based; it can then be investigated whether the same general pattern can be recognized in three dimensions. We do this in a subsequent paper; we anticipate our conclusions and state that we believe they can.

For a loose-packed lattice a negative interaction energy gives rise to a second critical region, that of the antiferromagnet. In two dimensions the reduced susceptibility is there found to behave asymptotically as

$$\chi \sim \chi_{\mathrm{a}} - a_{\pm}(1-v/v_{\mathrm{a}})\ln|1-v/v_{\mathrm{a}}| \qquad v \to v_{\mathrm{a}}\pm \tag{1.5}$$

where χ_{a} denotes the now finite value of the susceptibility at $v_{\mathrm{a}} = -v_{\mathrm{f}}$ (which corresponds to the antiferromagnetic critical or Néel temperature). For equal absolute values of J the critical temperature of the ferromagnet (T_C) and the antiferromagnet (T_N) are the same.

The functional form of (1.5) was first proposed on the basis of (1.2) (Sykes and Fisher 1958, Sykes 1961). The residual correlation function is found to make the most important contribution to the susceptibility of a ferromagnet; for an antiferromagnet on the other hand the dominant contribution appears to come from the energy (Sykes and Fisher 1962). By setting $G(v)$ equal to zero we obtain an approximation, the energetic approximation χ^E, which can be calculated exactly for two dimensional lattices. In particular, the susceptibility and energy have singularities of the same functional form; explicitly

$$\chi^E \sim \chi_a^E - a_\pm^E(1+v/v_f)\ln|1+v/v_f| \qquad v \to v_a\pm \tag{1.6}$$

where for the square lattice

$$\chi_a^E \simeq 0{\cdot}1647 \qquad a_+^E = a_-^E \simeq 0{\cdot}2097$$

and for the honeycomb lattice

$$\chi_a^E \simeq 0{\cdot}1244 \qquad a_+^E = a_-^E \simeq 0{\cdot}2375.$$

Although rigorous theoretical justification is a matter of some difficulty the functional form (1.5) is probably exact (Fisher 1959a, 1962). It follows from these theoretical studies that, as predicted by the energetic approximation, the antiferromagnetic susceptibility is expected to behave asymptotically in the same way as the energy; one therefore expects the amplitudes a_+ and a_- to be equal, since the energy is symmetric in this sense. The extrapolations of Sykes and Fisher (1962) were inconclusive, but favoured the view that $a_+ > a_-$. We re-examine this problem and make the tentative hypothesis that $a_+ = a_-$.

Estimates for the antiferromagnetic amplitude below T_N, a_-, have to be based on low temperature expansions. The expansions studied by Sykes and Fisher (1962) have been extended by Sykes *et al* (1965) and further extended by Sykes *et al* (1973). Since the evidence is relevant to the question of symmetry we have repeated the investigation with the new data; a full treatment of low temperature expansions is outside the scope of the present paper.

For a close-packed lattice a negative interaction energy does not necessarily give rise to a second critical region; when it does, the critical temperature is not necessarily the same as that of the ferromagnet with the same absolute value of J. There is some evidence that the three dimensional face-centred cubic lattice has an antiferromagnetic singularity for which $|v_a| \neq v_f$ (Danielian 1961, 1964). For the Kagomé lattice it can be proved that the susceptibility is not singular in the whole antiferromagnetic temperature range $-1 \leqslant v \leqslant 0$ (Sykes and Zucker 1961). For the triangular lattice it follows from the magnetic moment transformation of Fisher (1959b) that the susceptibility is not singular in the range $-1 < v \leqslant 0$. Sykes and Zucker concluded that the susceptibility was probably not singular at $v = -1$; we shall re-examine this question and write, tentatively, $v_a = -1$ without implying that the function is necessarily singular there. In fact we shall find this question unresolved.

2. Ferromagnetic susceptibility of triangular lattice above T_C

We have derived the expansion of the reduced susceptibility of the plane triangular lattice through v^{16}. We find

$$\begin{aligned}\chi(v) = {} & 1+6v+30v^2+138v^3+606v^4+2586v^5+10818v^6+44574v^7 \\ & +181542v^8+732678v^9+2935218v^{10}+11687202v^{11} \\ & +46296210v^{12}+182588850v^{13}+717395262v^{14} \\ & +2809372302v^{15}+10969820358v^{16}+\ldots . \end{aligned} \tag{2.1}$$

We begin our analysis by investigating the effect of dividing out the usually assumed dominant singularity $(1-v/v_{\mathrm{f}})^{-1\cdot75}$ which is conveniently done by using the critical polynomial and writing

$$\chi(v) = (1-4v+v^2)^{-1\cdot75}Q(v) \tag{2.2}$$

$$\begin{aligned}Q(v) = {} & 1-v+0\cdot25v^2-0\cdot25v^3-0\cdot59375v^4+0\cdot59375v^5+3\cdot9296875v^6 \\ & -3\cdot9296875v^7-11\cdot11572v^8-4\cdot88428v^9-1\cdot40540v^{10} \\ & -34\cdot5946v^{11}-140\cdot211v^{12}-410\cdot289v^{13}-1167\cdot012v^{14} \\ & -3478\cdot863v^{15}-10869\cdot172v^{16}-\ldots . \end{aligned} \tag{2.3}$$

This procedure is that suggested by Park (1956) and used subsequently by Sykes and Zucker (1961) and Sykes and Fisher (1962); the critical polynomial is introduced because it is expected, by analogy with the known form both of the zero-field partition function and the spontaneous magnetization, that the critical point $v_{\mathrm{f}} = 2-\sqrt{3}$ will be associated with the conjugate root $v = 2+\sqrt{3}$; in general this second root will have an asymptotically negligible effect on the quotient $Q(v)$.

The form of the quotient shows very clearly that the usually assumed dominant behaviour really does dominate; in fact it is only after about a dozen terms that any definite trend in the coefficients becomes established. Ultimately they all seem of one sign but are difficult to extrapolate with precision. It seems most likely that $Q(v)$ is singular at v_{f}. From the behaviour of the higher terms in the quotient we conclude that a second order asymptotic behaviour is becoming established and that the assumption that the dominant singularity can be removed by division is a questionable one.

To study the second order asymptotic behaviour we start afresh and make the more general assumption that

$$\chi(v) \sim (1-v/v_{\mathrm{f}})^{-\gamma}\Phi(v)+\Psi(v) \tag{2.4}$$

where $\Psi(v_{\mathrm{f}}) \neq 0$. We investigate the simplest possibility, that Φ and Ψ are regular in the disc $|v| \leqslant v_{\mathrm{f}}$, by expanding $\Phi(v)$ in a Taylor series about $v = v_{\mathrm{f}}$. Writing $v/v_{\mathrm{f}} = t$, we obtain

$$\begin{aligned}\chi(v) \sim {} & (1-t)^{-\gamma}\Phi(v_{\mathrm{f}})-(1-t)^{-\gamma+1}v_{\mathrm{f}}\Phi'(v_{\mathrm{f}})+\tfrac{1}{2}(1-t)^{-\gamma+2}v_{\mathrm{f}}^2\Phi''(v_{\mathrm{f}}) \\ & -\ldots+\Psi(v). \end{aligned} \tag{2.5}$$

According to a theorem by Darboux (Darboux 1878, Ninham 1963), the additive function $\Psi(v)$ has an asymptotically negligible effect on the coefficients of $\chi(v)$. Thus we assume $\gamma = 1{\cdot}75$ and attempt to represent the singular part of the susceptibility by successive approximations

$$\chi_1 = A_1(1-t)^{-1\cdot75}$$
$$\chi_2 = A_2(1-t)^{-1\cdot75}+B_2(1-t)^{-0\cdot75}$$
$$\chi_3 = A_3(1-t)^{-1\cdot75}+B_3(1-t)^{-0\cdot75}+C_3(1-t)^{0\cdot25}$$
$$\ldots \qquad (2.6)$$

where $A_r, B_r, C_r, \ldots$ are determined from the last r available coefficients of $\chi(v)$. The departure of the remaining coefficients is allowed for by a correction polynomial, $\Psi_r(t)$. Thus, we write

$$\chi(v) \simeq \chi_r(t)+\Psi_r(t) \qquad (2.7)$$

where in the limit of $r \to \infty$, $\Psi_r(t) \to \Psi(t)$, and the coefficients of Ψ_r are chosen to obtain complete agreement with the available coefficients of $\chi(v)$. If $\chi(v)$ is known through v^m, then the correction polynomial will be of degree $(m-r)$.

The order to which the approximation may be carried with advantage depends on the number of coefficients available and the quality of their convergence. The behaviour of the quotient already examined indicates that some smoothness has been established, at least to second order. A numerical study for fixed $r(= 1, 2, 3 \ldots)$ is made by applying the procedure to the expansion with successive increments in the number of coefficients up to the maximum available. We quote the values found for the second and third approximations from $m = 12$ to $m = 16$ in table 1. The second approximation yields a

Table 1. Successive approximations for triangular lattice

m	A_2	B_2	A_3	B_3	C_3
12	0·847132	0·1742	0·847066	0·1763	0·0442
13	0·847122	0·1743	0·847070	0·1762	0·0417
14	0·847116	0·1745	0·847082	0·1758	0·0322
15	0·847112	0·1746	0·847086	0·1756	0·0280
16	0·847109	0·1747	0·847086	0·1756	0·0287

smooth sequence of estimates for A and B. The third approximation also yields smooth sequences for A and B, but the sequence for C is less smooth. It is to be noted however that the values of A and B are not very much modified as we change the order of the approximation; we conclude that the data are consistent with our assumptions. We have found that, with the available coefficients, higher order approximations lead to no further improvement. We therefore adopt the third approximation at $m = 16$ as our final representation to obtain

$$\chi(v) \simeq 0{\cdot}847086(1-t)^{-1\cdot75}+0{\cdot}1756(1-t)^{-0\cdot75}+0{\cdot}0287(1-t)^{0\cdot25} + \Psi_3(t) \qquad (2.8)$$

where we calculate the correction polynomial in accordance with (2.7) as (correct to 4 decimal places)

$$\Psi_3(t) = -0{\cdot}0514+0{\cdot}0008t+0{\cdot}0031t^2+0{\cdot}0029t^3+0{\cdot}0002t^4 -0{\cdot}0009t^5-0{\cdot}0002t^6+0{\cdot}0001t^7. \qquad (2.9)$$

The correction polynomial is nonsingular; asymptotically it effectively has a constant value $\Psi_3(1) = -0{\cdot}0272$. This very small value accords with the observation that the dominant singularity very nearly factors. The equations (2.8) and (2.9) should provide a good numerical representation over the range $0 \leqslant v \leqslant v_f$. Finally, from table 1 we estimate the ferromagnetic amplitude

$$A_+ = 0{\cdot}84709 \pm 0{\cdot}00002 \tag{2.10}$$

in good agreement with the earlier estimate from 12 coefficients (Sykes and Fisher 1962) of 0·8473.

The representation (2.8) is also valid in the range $-v_f \leqslant v \leqslant 0$. The triangular antiferromagnet does not order at $v = -v_f$; it remains to determine the behaviour in the range $-1 \leqslant v < -v_f$. This we investigate in § 4.

3. Ferromagnetic and antiferromagnetic susceptibility of square lattice above T_C

We have derived the expansion of the reduced susceptibility of the plane square lattice through v^{21}. We find

$$\begin{aligned}\chi(v) = {} & 1+4v+12v^2+36v^3+100v^4+276v^5+740v^6+1972v^7+5172v^8 \\ & +13492v^9+34876v^{10}+89764v^{11}+229628v^{12}+585508v^{13} \\ & +1486308v^{14}+3763460v^{15}+9497380v^{16}+23918708v^{17} \\ & +60080156v^{18}+150660388v^{19}+377009300v^{20} \\ & +942105604v^{21}+\dots\end{aligned} \tag{3.1}$$

As in the previous section, we begin by dividing out the critical polynomial and write

$$\chi(v) = (1-2v-v^2)^{-1{\cdot}75}Q(v) \tag{3.2}$$

$$\begin{aligned}Q(v) = {} & 1+0{\cdot}5v-1{\cdot}125v^2+0{\cdot}5625v^3-1{\cdot}6641v^4+1{\cdot}7148v^5-3{\cdot}3877v^6 \\ & +7{\cdot}5591v^7-11{\cdot}7523v^8+18{\cdot}8268v^9-34{\cdot}3695v^{10}+66{\cdot}8638v^{11} \\ & -140{\cdot}9139v^{12}+297{\cdot}008v^{13}-636{\cdot}817v^{14}+1330{\cdot}752v^{15} \\ & -2844{\cdot}056v^{16}+5972{\cdot}24v^{17}-12946{\cdot}48v^{18}+27685{\cdot}2v^{19} \\ & -61114{\cdot}2v^{20}+132027{\cdot}8v^{21}-\dots\end{aligned} \tag{3.3}$$

The quotient for the square lattice is in marked contrast to that for the triangular lattice. The signs alternate right from the start and the behaviour of the coefficients is clearly dominated by the presence of the antiferromagnetic singularity at $v_a = -v_f$; this dominance is sufficient to mask any second order ferromagnetic effects of the kind seen in the previous section. The behaviour is quantitatively in accord with the presence of a singularity of the type

$$-a^*(1+v/v_f)\ln|1+v/v_f|. \tag{3.4}$$

If successive coefficients in (3.3) are multiplied by $n(n-1)v_f^n(-1)^{n+1}$, where n is the power of v, we obtain estimates for a^*. The antiferromagnetic amplitude a_+ of (1.5) is simply related through (3.2) by $a_+ = (4v_f)^{-1\cdot75}a^*$ and we calculate the sequence

n	a_+	n	a_+	
14	0·20963	18	0·21094	
15	0·20938	19	0·20882	(3.5)
16	0·21183	20	0·21216	
17	0·20882	21	0·20983.	

All these estimates are remarkably close to the amplitude corresponding to the energetic approximation of

$$a_+^{\mathrm{E}} = \frac{20\sqrt{2}+4}{49\pi} = 0{\cdot}20972\ldots. \tag{3.6}$$

This is not in good agreement with Sykes and Fisher (1962) who concluded that a_+ was some 50% higher than (3.6). This rather large discrepancy appears to be due to the fact that the original extrapolation, based on five fewer coefficients, was made using $\ln Q(v)$. We have found by numerical study of numerous algebraic functions with singularities of the type (1.4) and (1.5) combined in various ways that in general the convergence of $\ln Q$ is extremely slow (Roberts 1971).

As before, since the assumption that the dominant singularity occurs as a factor is a questionable one, we start afresh and seek to represent the susceptibility by a function that behaves like $(1-v/v_f)^{-1\cdot75}$ near $v = v_f$ and like $(1+v/v_f)\ln|1+v/v_f|$ near $v = v_a = -v_f$. The question at once arises of whether we should adopt a sum of two functions, one with the ferromagnetic and the other with the antiferromagnetic singularity, or a product, or more generally, a combination of both. This dilemma can be avoided because of a second theorem (Darboux 1878, Szëgo 1959) which we illustrate by an example. Suppose f_1 and f_2 are two functions with singularities on the same radius of convergence, say explicitly

$$\begin{aligned} f_1 &= (1+x)^{-\alpha} \\ f_2 &= (1-x)^{-\beta}. \end{aligned} \tag{3.7}$$

Then the product

$$F = (1+x)^{-\alpha}(1-x)^{-\beta} \tag{3.8}$$

may be represented asymptotically by $2^{-\alpha}(1-x)^{-\beta}$ near $x = 1$ and by $2^{-\beta}(1+x)^{-\alpha}$ near $x = -1$. The theorem states that the expansion coefficients of the product F behave asymptotically like those of the sum $2^{-\alpha}f_2 + 2^{-\beta}f_1$. Thus effectively the product can be represented asymptotically by a sum. Since the ferromagnetic and antiferromagnetic singularities have the same radius of convergence we can exploit this result and omit the product term. The appropriate generalization of (2.4), with $\gamma = 1{\cdot}75$, is now

$$\chi(v) \sim (1-v/v_f)^{-1\cdot75}\Phi_f(v) - (1+v/v_f)\ln|1+v/v_f|\Phi_a(v) + \Psi(v) \tag{3.9}$$

where we now suppose Φ_f, Φ_a and Ψ are regular in the disc $|v| \leqslant v_f$. Following the method of § 2 we expand the second term as a Taylor series about $v = v_a = -v_f$ and attempt to represent the antiferromagnetic component by a sequence of approximations

$$
\begin{aligned}
&-a_1(1+t)\ln|1+t| \\
&-a_2(1+t)\ln|1+t|-b_2(1+t)^2\ln|1+t| \\
&-a_3(1+t)\ln|1+t|-b_3(1+t)^2\ln|1+t|-c_3(1+t)^3\ln|1+t| \\
&\ldots
\end{aligned}
\tag{3.10}
$$

(where no confusion will arise between the amplitudes a_n and the coefficients defined in (1.1)).

We have found by numerical experiment that for the 21 coefficients available only three parameters can be fitted with advantage. We therefore adopt the asymptotic approximation

$$\chi_{2,1}(v) = A_2(1-t)^{-1\cdot75}+B_2(1-t)^{-0\cdot75}-a_1(1+t)\ln|1+t| \tag{3.11}$$

which corresponds to a second order approximation to the ferromagnetic singularity and a first order approximation to the antiferromagnetic singularity. As before the constants A_2, B_2 and a_1 are determined from the last three coefficients. We quote the values found from $m = 17$ to $m = 21$ in table 2.We consider the data in table 2 consistent

Table 2. Successive approximations for square lattice

m	A_2	B_2	a_1
17	0·771740	0·3473	0·1971
18	0·771734	0·3474	0·1974
19	0·771745	0·3471	0·1983
20	0·771732	0·3475	0·1994
21	0·771742	0·3472	0·2003

with our assumptions. The ferromagnetic amplitude is well defined; the estimates for the antiferromagnetic amplitude are increasing slowly and are close to the value found for the energetic approximation (3.6). We adopt the last entry for our final representation to obtain

$$
\begin{aligned}
\chi(v) \simeq\; & 0\cdot771742(1-t)^{-1\cdot75}+0\cdot3472(1-t)^{-0\cdot75} \\
& -0\cdot2003(1+t)\ln|1+t|+\Psi_{2,1}(t)
\end{aligned}
\tag{3.12}
$$

where the correction polynomial $\Psi_{2,1}$ is chosen to obtain complete agreement with the coefficients available. We calculate (correct to 4 decimal places)

$$
\begin{aligned}
\Psi_{2,1}(t) = & -0\cdot1189+0\cdot2462t+0\cdot0742t^2-0\cdot0051t^3+0\cdot0081t^4 \\
& -0\cdot0006t^5-0\cdot0003t^6+0\cdot0005t^7+0\cdot0004t^8 \\
& -0\cdot0002t^9+0\cdot0004t^{10}-0\cdot0002t^{11}+0\cdot0002t^{12}.
\end{aligned}
\tag{3.13}
$$

We estimate the ferromagnetic amplitude from table 2 as

$$A_+ = 0\cdot77174\pm0\cdot00002 \tag{3.14}$$

and near the ferromagnetic critical temperature

$$\chi \sim 0{\cdot}77174(1-t)^{-1{\cdot}75}+0{\cdot}3472(1-t)^{-0{\cdot}75}-0{\cdot}073 \qquad t \to +1 \tag{3.15}$$

which accords with the observation that the dominant singularity very nearly factors. Near the antiferromagnetic critical temperature the behaviour indicated by (3.12) is

$$\chi \sim 0{\cdot}159374-0{\cdot}2003(1+t)\ln|1+t| \qquad t \to -1. \tag{3.16}$$

We estimate that

$$\chi_{\mathrm{a}} = 0{\cdot}1594 \pm 0{\cdot}0010. \tag{3.17}$$

The antiferromagnetic amplitude is difficult to estimate with precision, owing to the presence of the ferromagnetic singularity. From table 2 we conclude that

$$a_{+} = 0{\cdot}22 \pm 0{\cdot}01. \tag{3.18}$$

The estimate of A_{+} is in good agreement with the earlier estimate of Sykes and Fisher (1962), from 16 terms, that $A_{+} = 0{\cdot}77184 \pm 0{\cdot}00025$, the discrepancy being inside the quoted error limits. For χ_{a} their estimate of 0·15695 is some 1·5% lower, and their estimate $a_{+} = 0{\cdot}317$ some 44% higher. As we have already stated these rather large discrepancies appear to result partly from the slow convergence of ln Q, and partly from the assumption that the dominant singularity may be divided out; the result (3.15) suggests the latter does not hold precisely.

4. Antiferromagnetic susceptibility of triangular lattice

A detailed study of the antiferromagnetic susceptibility was made by Sykes and Zucker (1961). Their investigation effectively assumes that the ferromagnetic singularity occurs as a factor; as we have seen this is apparently very nearly the case. We follow them in first transforming the expansion (2.1) into a form convergent over the whole temperature range ($T > 0$) of the antiferromagnet. Fisher (1959b) has shown that if χ_{T} denotes the susceptibility of the triangular lattice and χ_{H} that of the honeycomb lattice, then

$$\chi_{\mathrm{T}}(v) = \tfrac{1}{2}(\chi_{\mathrm{H}}(w)+\chi_{\mathrm{H}}(-w)) \tag{4.1}$$

for

$$w^2 = \frac{v(1+v)}{1+v^3}. \tag{4.2}$$

We obtain

$$\begin{aligned}\chi_{\mathrm{T}}(w) = {} & 1+6w^2+24w^4+90w^6+318w^8+1098w^{10}+3696w^{12} \\ & +12270w^{14}+40224w^{16}+130650w^{18}+421176w^{20} \\ & +1348998w^{22}+4299018w^{24}+13635630w^{26} \\ & +43092888w^{28}+135698970w^{30}+426144654w^{32} \ldots .\end{aligned} \tag{4.3}$$

As v varies from 0 to -1, w^2 varies from 0 to $-\frac{1}{3}$. The ferromagnetic critical point corresponds to $w^2 = +\frac{1}{3}$. We divide by the dominant singularity by writing

$$\chi_{\mathrm{T}}(w) = (1-3w^2)^{-1{\cdot}75}Q(w) \tag{4.4}$$

$$Q(w) = 1+0{\cdot}75w^2-1{\cdot}5937w^4+0{\cdot}91406w^6-2{\cdot}5063w^8+5{\cdot}6744w^{10}$$
$$-9{\cdot}9498w^{12}+13{\cdot}7967w^{14}-17{\cdot}3852w^{16}+9{\cdot}3517w^{18}$$
$$+32{\cdot}4408w^{20}-214{\cdot}18w^{22}+782{\cdot}166w^{24}-2648{\cdot}07w^{26}$$
$$+8095{\cdot}03w^{28}-24769{\cdot}21w^{30}+72499w^{32}-\ldots \qquad (4.5)$$

Once again the quotient shows clearly the overriding dominance of the ferromagnetic singularity; there is a break in the sign pattern after the coefficient of w^{18} but it seems likely that a steady alternation persists thereafter and the radius of convergence is probably $w^2 = \frac{1}{3}$.

At absolute zero the behaviour of the energetic approximation can be calculated from the known value of the energy (Houtappel 1950) and we find

$$\chi_E \simeq \frac{1}{9}-\frac{\sqrt{3}}{18\pi}(1+v)^2\ln(1+v) \qquad v \to -1 \qquad (4.6)$$

or in the variable w

$$\chi_E \simeq \frac{1}{9}-\frac{\sqrt{3}}{12\pi}(1+3w^2)\ln(1+3w^2) \qquad w^2 \to -\frac{1}{3}. \qquad (4.7)$$

In other words: *in the variable* w^2, but not in v, the singularity is of the same form as for a loose-packed antiferromagnet. In the variable v the singularity is weaker. We therefore begin by fitting (4.3) to a form analogous to (3.11) by writing

$$\chi_{2,1}(w) = A_2(1-3w^2)^{-1{\cdot}75}+B_2(1-3w^2)^{-0{\cdot}75}$$
$$-a_1(1+3w^2)\ln|1+3w^2|. \qquad (4.8)$$

We give the successive solutions in table 3. The first two columns appear to be converging to constant values

$$A_2 \simeq 1{\cdot}089$$
$$B_2 \simeq 0{\cdot}072 \qquad (4.9)$$

Table 3. Successive approximations for triangular lattice in special variable w^2

m	A_2	B_2	a_1
6	1·0899	0·0699	+0·0795
7	1·0878	0·0882	+0·0614
8	1·0900	0·0662	+0·0348
9	1·0886	0·0821	+0·0124
10	1·0898	0·0677	−0·0106
11	1·0890	0·0781	−0·0291
12	1·0897	0·0686	−0·0477
13	1·0892	0·0757	−0·0629
14	1·0896	0·0689	−0·0786
15	1·0893	0·0742	−0·0918
16	1·0895	0·0690	−0·1056

These values, which correspond to the ferromagnetic singularity, are in reasonable agreement with the more precise estimates already made in § 2; thus it follows from (4.2) that

$$(1-t) = \frac{\sqrt{3}}{2}(1-3w^2)+\frac{2\sqrt{3}-3}{8}(1-3w^2)^2 + \frac{2\sqrt{3}-3}{8}(1-3w^2)^3+\ldots \tag{4.10}$$

and on substitution in (2.8) we obtain

$$\chi(w) \sim 1{\cdot}08955(1-3w^2)^{-1{\cdot}75}+0{\cdot}067877(1-3w^2)^{-0{\cdot}75} - 0{\cdot}078448(1-3w^2)^{0{\cdot}25}. \tag{4.11}$$

The third column does not appear to be converging. The data seem *inconsistent* with the assumption (4.8) which we have based on the *energetic approximation.* Since (4.11) should be a fairly accurate representation of the ferromagnetic singularity we subtract it from the total susceptibility (4.3) to obtain the following series (with coefficients correct to five figures):

$$\begin{aligned} &-0{\cdot}07898+0{\cdot}06830w^2-0{\cdot}06266w^4+0{\cdot}29832w^6-0{\cdot}56164w^8 \\ &+1{\cdot}1095w^{10}-1{\cdot}0495w^{12}+2{\cdot}4968w^{14}+1{\cdot}1760w^{16}+2{\cdot}3309w^{18} \\ &+36{\cdot}511w^{20}-36{\cdot}194w^{22}+378{\cdot}95w^{24}-482{\cdot}58w^{26}+3375{\cdot}5w^{28} \\ &-4639{\cdot}8w^{30}+28708w^{32}\ldots. \end{aligned} \tag{4.12}$$

This appears to be a very slowly convergent series. The signs alternate but with a change in phase after eight terms; it is difficult to represent the behaviour of the coefficients by any simple function and it would seem that further data are required. We conclude however that the energetic approximation is not a good one for the triangular lattice near $v = -1$. The antiferromagnetic ground state of the triangular lattice is highly degenerate (Wannier 1950); since the energy is singular at absolute zero it seems likely the susceptibility will be also; the series (4.12) is quite consistent with such a conjecture. The earlier conclusions of Sykes and Zucker (1961) are not confirmed by the new data.

The estimation of χ_a is difficult because an estimate of the remainder in (4.12) is required; however this remainder is probably not large. The value indicated by truncating (4.12) and adding (4.11) is 0·141; on the assumption that any singularity in (4.12) is no stronger than that of (4.7) we estimate

$$0{\cdot}141 < \chi_a < 0{\cdot}150 \tag{4.13}$$

but the upper limit is very uncertain because of the possibility of a stronger singularity. The earlier estimate of Sykes and Zucker (1961) is slightly lower, at $\chi_a = 0{\cdot}139$, but this was based on the assumption that the dominant ferromagnetic singularity occurs as a factor.

5. Ferromagnetic and antiferromagnetic susceptibility of honeycomb lattice above T_c

We have derived the expansion of the reduced susceptibility of the honeycomb lattice through v^{32}. We find

$$\begin{aligned}\chi(v) = {} & 1+3v+6v^2+12v^3+24v^4+48v^5+90v^6+168v^7+318v^8 \\ & +600v^9+1098v^{10}+2004v^{11}+3696v^{12}+6792v^{13} \\ & +12270v^{14}+22140v^{15}+40224v^{16}+72888v^{17} \\ & +130650v^{18}+234012v^{19}+421176v^{20}+756624v^{21} \\ & +1348998v^{22}+2403840v^{23}+4299018v^{24}+7677840v^{25} \\ & +13635630v^{26}+24206220v^{27}+43092888v^{28} \\ & +76635984v^{29}+135698970v^{30}+240199320v^{31} \\ & +426144654v^{32}+\ldots \end{aligned} \tag{5.1}$$

We have found this series difficult to represent satisfactorily. The behaviour of the coefficients is consistent with the presence of the expected ferromagnetic and antiferromagnetic singularities, but is complicated by the presence of a pair of singularities in the complex plane at $v = \pm i/\sqrt{3}$. The precise nature of these singularities is hard to determine but without some approximate allowance for their effect it is not possible to estimate A_+ and a_+ by the methods we have used so far. After much numerical experiment with representations of the general type

$$\begin{aligned}\chi \sim {} & A_2(1-t)^{-1\cdot 75}+B_2(1-t)^{-0\cdot 75}-a_1(1+t)\ln|1+t| \\ & +R(1+t^2)^{\xi}+St(1+t^2)^{\eta}\end{aligned} \tag{5.2}$$

we have found no set of the parameters R, S, ξ, η, which gives a wholly satisfactory result. A similar difficulty was found by Sykes and Fisher (1962) who divided out the ferromagnetic singularity and included in the representation of the quotient a term effectively equivalent to taking $\xi = -\frac{1}{8}$, $S = 0$, in (5.3). However the sequences obtained for A_2 and a_1 are not very sensitive to the values of ξ and η adopted in the range $|\xi| \leqslant \frac{1}{8}$, $|\eta| \leqslant \frac{1}{8}$ and indicate

$$A_+ \simeq 0\cdot 6478 \qquad a_+ \simeq 0\cdot 23. \tag{5.3}$$

We do not consider the quality of the data justifies our quoting any evidence explicitly; we simply report that in general the range of estimates for a_+ obtained in this way is some 40 %–50 % lower than the estimate of Sykes and Fisher of $a_+ \simeq 0\cdot 332$. An average of various extrapolations indicates

$$\chi_a = 0\cdot 1230 \pm 0\cdot 0010 \tag{5.4}$$

while Sykes and Fisher found 0·121, some 1·6 % lower. The discrepancies are of the same order, and in the same sense, as we have already found for the square lattice; they are probably accounted for in the same way. Since the even terms of the series (5.1) have already been examined in § 4, with only partial success, we shall not present any further analyses; our understanding of this series is incomplete.

At present the best available estimate for the ferromagnetic amplitude of the honeycomb lattice is that obtained by the theory of transformations (Fisher 1959b); using the result

$$\frac{A_+(\text{triangular})}{A_+(\text{honeycomb})} = \frac{1}{2}(3)^{7/8} \tag{5.5}$$

we calculate from (2.10)

$$A_+(\text{honeycomb}) = 0{\cdot}64786 \pm 0{\cdot}00002 \tag{5.6}$$

in good agreement with (5.3)

The best available estimate of a_+ is probably obtained by assuming symmetry and adopting the estimate of a_- we make in the next section.

The expansion (5.1) can be used to evaluate the antiferromagnetic susceptibility of the Kagomé lattice. The method is described by Sykes and Zucker (1961); the new data are consistent with their conclusion that for the honeycomb lattice

$$\chi(-\tfrac{1}{3}) = 0{\cdot}397193 \pm 0{\cdot}000002 \tag{5.7}$$

from which it follows, after correcting their arithmetic, that for the Kagomé lattice:

$$\chi(-1) = 0{\cdot}20098 \pm 0{\cdot}0001. \tag{5.8}$$

6. Antiferromagnetic susceptibility of square and honeycomb lattices below T_N

Since the investigation of Sykes and Fisher (1962) the low temperature series expansions for the antiferromagnetic susceptibility of the square lattice have been extended by four coefficients, and for the honeycomb lattice by three coefficients (Sykes *et al* 1965, 1973). In terms of the standard variable $y = \exp(2J/kT)$ the series are for the square lattice

$$\begin{aligned}\chi(y) = {} & 4y^4 + 16y^8 + 32y^{10} + 156y^{12} + 608y^{14} + 2688y^{16} + 12064y^{18} \\ & + 55956y^{20} + 266656y^{22} + \ldots \end{aligned} \tag{6.1}$$

and for the honeycomb lattice

$$\begin{aligned}\chi(y) = {} & 4y^3 + 12y^5 + 8y^6 + 48y^7 + 96y^8 + 320y^9 + 888y^{10} + 2748y^{11} \\ & + 8384y^{12} + 26340y^{13} + 83568y^{14} + 268864y^{15} \\ & + 873648y^{16} + \ldots \end{aligned} \tag{6.2}$$

We follow the original investigation and try to represent the remainders in (6.1) and (6.2) by

$$\sum_{n=12}^{\infty} \frac{E(y/y_c)^{2n}}{(n+\theta)(n+\theta+1)} \tag{6.3}$$

$$\sum_{n=17}^{\infty} \frac{F(y/y_c)^{n}}{(n+\theta')(n+\theta'+1)} \tag{6.4}$$

respectively. The constants E and F are determined from the last known coefficients and the constants θ and θ' are chosen to give the best representation of the available terms. The method assumes a singularity of the energetic type; allowing for the change of variable $E \to \frac{1}{2}a_-$ and $F \to a_-/\sqrt{3}$ as the number of known coefficients increases.

For the square lattice the value $\theta = 0$ gives about the optimum sequence of estimates for a_-, the last six being 0·23876, 0·22352, 0·22606, 0·22382, 0·22264, 0·22248. Although slightly irregular these seem to be converging to a limit which we estimate as

$$a_- = 0{\cdot}222 \pm 0{\cdot}002 \tag{6.5}$$

which is close to the estimate $a_+ = 0{\cdot}22 \pm 0{\cdot}01$ of § 3. We conclude that the amplitudes are symmetric and some 5% higher than those of the energetic approximation ($a^{\mathrm{E}} = 0{\cdot}2097\ldots$). Using the last value for E and summing the series (6.3) at

$$y = y_{\mathrm{a}} = \exp(2J/kT_{\mathrm{N}})$$

we estimate

$$\chi_{\mathrm{a}} = 0{\cdot}1589 \pm 0{\cdot}0005 \tag{6.6}$$

which is inside the limits of error of the corresponding high temperature estimate (3.17)

For the honeycomb lattice $\theta' = \frac{1}{2}$ gives about the optimum sequence of estimates for a_-, the last six being 0·24209, 0·24019, 0·24070, 0·24020, 0·24020, 0·24013. We estimate the limit as

$$a_- = 0{\cdot}240 \pm 0{\cdot}001 \tag{6.7}$$

which is close to the rather imprecise estimate of $a_+ = 0{\cdot}23$ we made in § 5. We conclude that the amplitudes are probably symmetric and very close to the energetic approximation ($a^{\mathrm{E}} = 0{\cdot}2375\ldots$). Using the last value of F and summing (6.4) at $y = y_{\mathrm{c}}$ we estimate

$$\chi_{\mathrm{a}} = 0{\cdot}1224 \pm 0{\cdot}0003 \tag{6.8}$$

which is inside the limits of error of the corresponding high temperature estimate (5.4).

For these low temperature expansions the dominant singularity is the antiferromagnetic singularity. The coefficients can be fitted to a sequence of approximations of the type (3.10); we have found the successive estimates converge only slowly but are consistent with the conclusions of this section; in particular the estimates for the critical susceptibility χ_{a} are within the quoted error limits.

7. General conclusions

We have not reviewed the whole problem; rather we have described only those parts where new data have resulted in new conclusions.

The simplest situation is presented by the high temperature expansion for the susceptibility of the triangular lattice in the counting variable v. Asymptotically

$$\chi \sim (1 - v/v_{\mathrm{f}})^{-1{\cdot}75}\Phi(v) + \Psi(v) \tag{7.1}$$

where Φ and Ψ are regular in the disc $|v| \leqslant v_{\mathrm{f}}$. The ratio $\Psi(v_{\mathrm{f}})/\Phi(v_{\mathrm{f}})$ is only about $-0{\cdot}03$; the dominant singularity cannot therefore be removed completely by division. This latter conclusion holds, *mutatis mutandis*, for the square and honeycomb lattices; as a result we are not in detailed agreement with Sykes and Fisher (1962) whose methods effectively assume factorization of the ferromagnetic singularity. Expanding Φ as a

Taylor series yields successive approximations which can be used for numerical representations. We have estimated the ferromagnetic amplitude A_+ for the triangular lattice on the basis of (7.1).

The corresponding expansion for the square lattice is complicated by the presence of the antiferromagnetic singularity at $v_a = -v_f$. Asymptotically

$$\chi \sim (1-v/v_f)^{-1\cdot 75}\Phi_f(v) - (1+v/v_f)\ln|1+v/v_f|\Phi_a(v) + \Psi(v) \tag{7.2}$$

where Φ_f, Φ_a and Ψ are regular in the disc $|v| \leqslant v_f$. Expanding Φ_f and Φ_a as Taylor series yields successive approximations which can be used for numerical representations. We have estimated the ferromagnetic amplitude A_+ and the antiferromagnetic amplitude a_+ on the basis of (7.2); we have estimated the amplitude a_- from extended low temperature expansions. As a result we have made quantitive rather than qualitative modifications to the conclusions of Sykes and Fisher (1962); the antiferromagnetic singularity is still found to be of the energetic type

$$\chi \sim \chi_a - a_\pm(1+v/v_f)\ln|1+v/v_f| \qquad v \to -v_f \tag{7.3}$$

but consistent with $a_+ = a_-$. In other words the singularity has the same symmetry as the energy; we have also found this amplitude to be close to that of the energetic approximation.

The corresponding expansion for the honeycomb lattice is further complicated by the presence of singularities on the same radius of convergence but in the complex plane; additional terms are required to construct the analogue of the representation (7.2). We have not been able to find a completely satisfactory one.

To investigate the antiferromagnetic susceptibility of the triangular lattice we have studied the expansion in the variable $w^2 = v(1+v)/(1+v^3)$. Again we have found that the ferromagnetic singularity, although very nearly a factor, cannot be removed completely by division. From extended data we have concluded, in disagreement with Sykes and Zucker (1961), that the susceptibility of the antiferromagnet could well be singular at absolute zero and that there is some justification in writing $v_a = -1$; however the behaviour there does not seem in accord with a singularity of the energetic type. The problem remains unresolved.

For convenience of reference we summarize the dominant amplitudes converted to the temperature scale. Near T_C the ferromagnetic susceptibility behaves as

$$\chi \sim A_T(1-T_C/T)^{-1\cdot 75} \qquad T \to T_C+ \tag{7.4}$$

with

$$A_T = 0\cdot 92421 \pm 0\cdot 00003 \qquad \text{(triangular)}$$
$$A_T = 0\cdot 96259 \pm 0\cdot 00003 \qquad \text{(square)}$$
$$A_T = 1\cdot 04642 \pm 0\cdot 00003 \qquad \text{(honeycomb).}$$

Near T_N the antiferromagnetic susceptibility behaves approximately as

$$\chi \sim \chi_a - a_T(1-T_N/T)\ln|1-T_N/T| \qquad T \to T_N \tag{7.5}$$

with

$$a_{\mathrm{T}} = 0{\cdot}196 \pm 0{\cdot}002 \qquad \text{(square)}$$

$$a_{\mathrm{T}} = 0{\cdot}182 \pm 0{\cdot}001 \qquad \text{(honeycomb).}$$

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