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Specific heat of a three dimensional Ising ferromagnet above the Curie temperature II

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Abstract. High temperature series expansions for the specific heat of the Ising model of a ferromagnet are given for the face-centred cubic, body-centred cubic, and simple cubic lattices. From a numerical study it is concluded that the critical index (α) is lattice independent and that in three dimensions $\alpha \simeq \frac{1}{8}$. A numerical representation of the specific heat in the range $T_C \leqslant T \leqslant \infty$ is given in each case, together with estimates of the critical energy, entropy, and free energy. Asymptotic forms for the specific heat and energy are given.

1. Introduction

In this paper we continue our investigation of the behaviour of the specific heat of the three dimensional Ising model above the Curie temperature. We have already given a general introduction in a previous paper (Sykes *et al* 1967, to be referred to as I). In I the investigation was restricted to the series expansion for the specific heat of the face-centred cubic (FCC) lattice to twelfth order; it was concluded that the expansion was sufficiently well behaved to enable the critical behaviour to be inferred, and that the smoothness of behaviour justified the derivation of further coefficients. We have extended the series to fourteenth order and derived the corresponding series for the body-centred cubic (BCC) lattice to sixteenth order and for the simple cubic (SC) lattice to eighteenth order.

The starting point of our investigation is the high temperature expansion for the configurational free energy. In terms of the standard high temperature counting variable $v = \tanh K$ we find

$$\text{SC} \qquad \ln \Lambda(v) = \ln 2 - 3\ln(1+v) + 3v^4 + 22v^6 + 187\tfrac{1}{2}v^8 + 1980v^{10} + 24044v^{12} + 319170v^{14} + 4514757\tfrac{3}{4}v^{16} + 67003469\tfrac{1}{3}v^{18} + \ldots \tag{1.1}$$

$$\text{BCC} \qquad \ln \Lambda(v) = \ln 2 - 4\ln(1+v) + 12v^4 + 148v^6 + 2496v^8 + 52168v^{10} + 1242078v^{12} + 32262852v^{14} + 892367762v^{16} + \ldots \tag{1.2}$$

$$\text{FCC} \qquad \ln \Lambda(v) = \ln 2 - 6\ln(1+v) + 8v^3 + 33v^4 + 168v^5 + 930v^6 + 5664v^7 + 37018\tfrac{1}{2}v^8 + 254986\tfrac{2}{3}v^9 + 1827768v^{10} + 13520328v^{11} + 102607720v^{12} + 795503400v^{13} + 6279937374v^{14} + \ldots. \tag{1.3}$$

From these expansions the specific heat in zero-field can be obtained as a series in ascending powers of K or v. We have found the extrapolations quite insensitive to a choice between these variables and we therefore present our treatment in v only. In general it is more convenient to work in v, which variable arises quite naturally in the derivation of high temperature expansions for the spin $\frac{1}{2}$ Ising model. There is one exception; to facilitate comparison with experimental results we present our numerical representations of the specific heat on the direct temperature scale by using K.

We will describe the actual derivation of the expansions (1.1–3) elsewhere; the complex configurational problems involved have no direct relevance to our present objective which is to study the specific heat numerically. For three dimensional lattices a particularly difficult problem is the determination of the number of embeddings of self-avoiding rings of large size (Sykes *et al* 1972b).

Most published data contain small errors, never large enough to be seriously misleading. The expansion for the simple cubic lattice has had a particularly chequered career. Wakefield (1951) gave the coefficients of v^{10} and v^{12} incorrectly; Wakefield found agreement with Trefftz (1950) as the result of a misprint (her expansion for the energy is correct to v^{10}). The error in v^{10} was noticed and corrected by Domb and Sykes (1957), who also improved the coefficient of v^{12}. This latter was finally corrected by Rushbrooke and Eve (1962) who added the coefficient of v^{14}, apparently incorrectly.

2. Specific heat

From the expansions (1.1–3) we derive the specific heat expansion in the form

$$\frac{C_H}{R} = \sum_{n=2}^{\infty} a_n v^n \tag{2.1}$$

where the coefficients have the values given in table 1. Following I we make the hypothesis that asymptotically

$$\frac{C_H}{R} \sim A(1 - T_C/T)^{-\alpha} \qquad \text{as } T \to T_C+ \tag{2.2}$$

where α and A are constants. In terms of $\tanh K$ this is equivalent to

$$\frac{C_H}{R} \sim B(1 - v/v_C)^{-\alpha} \qquad \text{as } v \to v_C- \tag{2.3}$$

where B is a constant. To estimate α for the face-centred cubic lattice we form the sequence

$$\alpha_n = n\left(\frac{a_n}{a_{n-1}}\right)v_C - n + 1. \tag{2.4}$$

Table 1. Coefficients in the specific heat expansion in powers of $v = \tanh K$

	SC	BCC	FCC
a_2	3·0000000000000	4·0000000000000	6·0000000000000
a_3	—	—	48·000000000000
a_4	35·000000000000	142·66666666667	394·00000000000
a_5	—	—	3248·0000000000
a_6	587·53333333333	4151·3777777778	27107·066666667
a_7	—	—	231752·53333333
a_8	9370·1238095238	132137·23174603	2024833·8476190
a_9	—	—	17963727·847619
a_{10}	161411·16761904	4470221·1631746	161151521·84000
a_{11}	—	—	1458236803·7486
a_{12}	2899560·8114863	156689508·28706	13288901035·269
a_{13}	—	—	121822923193·11
a_{14}	53326199·747121	5624621332·6678	1122468713132·8
a_{15}	—	—	
a_{16}	997927863·96704	205475336857·47	
a_{17}	—	—	
a_{18}	18927473467·877		

For the loose-packed lattices, for which only even terms are present, we use the modified form

$$\alpha_n = n\left(\frac{a_{2n}}{a_{2n-2}}\right)v_C^2 - n + 1 \tag{2.5}$$

To form these sequences we adopt the most recent estimates for v_C, based on the corresponding high temperature susceptibility expansions (Sykes *et al* 1972a). These are

$$\begin{aligned}
&\text{SC} && \frac{1}{v_C} = 4{\cdot}5844 \pm 0{\cdot}0002 && K_C = 0{\cdot}22169 \pm 0{\cdot}00001 \\
&\text{BCC} && \frac{1}{v_C} = 6{\cdot}4055 \pm 0{\cdot}0010 && K_C = 0{\cdot}15740 \pm 0{\cdot}00003 \\
&\text{FCC} && \frac{1}{v_C} = 9{\cdot}8290 \pm 0{\cdot}0005 && K_C = 0{\cdot}10209 \pm 0{\cdot}00001.
\end{aligned} \tag{2.6}$$

We illustrate the three sequences in figure 1.

There is a close similarity in the behaviour of the three sequences; they seem consistent with the view that α is determined by the dimensionality of the lattice and not by its detailed structure. They are also still consistent with our earlier conclusions that α is very close to $\frac{1}{8}$. The sequences illustrated are calculated for the middle values of (2.6); to gauge the sensitivity to variations in the critical point we quote the value of α_{18} for the simple cubic lattice corresponding to the middle and two extremes of (2.6)

$$\begin{aligned}
&\frac{1}{v_C} = 4{\cdot}5846 && \alpha_{18} \simeq 0{\cdot}12144 \\
&\frac{1}{v_C} = 4{\cdot}5844 && \alpha_{18} \simeq 0{\cdot}12215 \\
&\frac{1}{v_C} = 4{\cdot}5842 && \alpha_{18} \simeq 0{\cdot}12285.
\end{aligned} \tag{2.7}$$

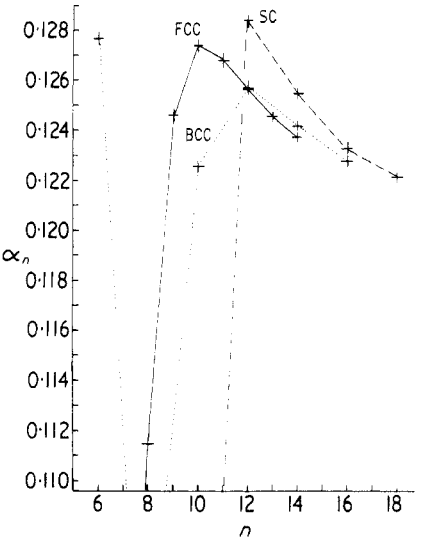

Figure 1. Estimates for the critical index (α) for the face-centred cubic, body-centred cubic, and simple cubic lattices calculated from (2.4) and (2.5).

If the highest value in the range is chosen for each lattice (which choice corresponds to the highest critical *temperature*) the three graphs in figure 1 all move up by less than 1%; to obtain a value of α_{18} for the simple cubic lattice of 0·1250 requires $1/v_C = 4{\cdot}5836$; thus if the limit is exactly $\frac{1}{8}$ the sequences probably pass through a minimum.

3. Representation for specific heat

To obtain a specific representation for the specific heat we follow the technique of I and write for the face-centred cubic lattice

$$\frac{C_H}{R} = 1{\cdot}089\left((1-t)^{-1/8} - 1 - \frac{1}{8}t\right) + \phi_{fcc}(t) \qquad t = \frac{K}{K_C} \tag{3.1}$$

where the first factor is determined from the last available coefficient and the correction polynomial $\phi(t)$ accounts for the departure of all the earlier coefficients from the expansion of the first part. Correct to four decimal places

$$\phi_{fcc}(t) = -0{\cdot}0140t^2 - 0{\cdot}0031t^3 + 0{\cdot}0005t^5 + 0{\cdot}0002t^6. \tag{3.2}$$

For the loose packed lattices using a similar technique we represent the specific heat by the modified forms

SC
$$\frac{C_H}{R} = 1{\cdot}232\{(1-t^2)^{-1/8} - 1\} + \phi_{sc}(t) \tag{3.3}$$

BCC
$$\frac{C_H}{R} = 1{\cdot}200\{(1-t^2)^{-1/8} - 1\} + \phi_{bcc}(t) \tag{3.4}$$

where, correct to four decimal places

$$\phi_{sc}(t) = -0{\cdot}0065t^2 - 0{\cdot}0069t^4 + 0{\cdot}0030t^6 + 0{\cdot}0001t^8 \tag{3.5}$$

$$\phi_{bcc}(t) = -0{\cdot}0508t^2 + 0{\cdot}0016t^4 + 0{\cdot}0005t^6. \tag{3.6}$$

The corresponding critical behaviour is

$$\frac{C_H}{R} \sim A(1 - T_C/T)^{-1/8} + a \tag{3.7}$$

where the constants A, and particularly a, are relatively insensitive to lattice structure. We give the values that correspond to the above representations

$$\begin{array}{lll} \text{SC} & A = 1{\cdot}136 & a = -1{\cdot}242 \\ \text{BCC} & A = 1{\cdot}106 & a = -1{\cdot}248 \\ \text{FCC} & A = 1{\cdot}089 & a = -1{\cdot}241. \end{array} \tag{3.8}$$

A similar insensitivity is found in two dimensions (I § 2) although the amplitudes (A) there increase with coordination number. The values (3.8) correspond to the last available coefficient; strictly the absolute values of A and a should be determined by an extrapolation but we have not done this because of the uncertainty on the critical point. This may account for the nonmonoticity of the estimates for a.

The energy and entropy can be derived directly from the relations

$$U(K) = \int_0^K \frac{C_H}{RK^2}\,dK \tag{3.9}$$

$$S(K) = R\ln 2 - \int_0^K \frac{C_H}{K}\,dK \tag{3.10}$$

$$\ln \Lambda_C = \frac{S_C}{R} - (U_0 - U_C)K_C \tag{3.11}$$

and we calculate the critical values

	SC	BCC	FCC	
U_C	$0{\cdot}99218 \pm 0{\cdot}00015$	$1{\cdot}0928 \pm 0{\cdot}0006$	$1{\cdot}4845 \pm 0{\cdot}0003$	
$\frac{S_C}{R}$	$0{\cdot}55793 \pm 0{\cdot}00003$	$0{\cdot}58203 \pm 0{\cdot}00010$	$0{\cdot}59023 \pm 0{\cdot}00003$	(3.12)
$\ln \Lambda_C$	$0{\cdot}11280 \pm 0{\cdot}00002$	$0{\cdot}12443 \pm 0{\cdot}00007$	$0{\cdot}12921 \pm 0{\cdot}00002$	

where the uncertainties quoted correspond exactly to the extremes of (2.6). Near the critical point

$$\frac{2}{q}U(v) \sim \begin{cases} 0{\cdot}3307 - 2{\cdot}045(1 - v/v_C)^{7/8} & \text{SC} \\ 0{\cdot}2731 - 2{\cdot}040(1 - v/v_C)^{7/8} & \text{BCC} \\ 0{\cdot}2475 - 2{\cdot}017(1 - v/v_C)^{7/8} & \text{FCC} \end{cases} \tag{3.13}$$

where q denotes the coordination number of the lattice. In terms of the absolute temperature (3.13) becomes

$$\frac{2}{q}U(T) \sim \begin{cases} 0{\cdot}3307 - 1{\cdot}987(1 - T_C/T)^{7/8} & \text{SC} \\ 0{\cdot}2731 - 2{\cdot}010(1 - T_C/T)^{7/8} & \text{BCC} \\ 0{\cdot}2475 - 2{\cdot}005(1 - T_C/T)^{7/8} & \text{FCC.} \end{cases} \tag{3.14}$$

Again the estimates for the amplitude of the second term could be improved by extrapolation in each case if the critical point were known precisely enough. It is evident that this amplitude is insensitive to the detailed structure of the lattice.

The estimates (3.11) differ only slightly from those collected from the literature by Fisher (1963), who gives an extensive bibliography; earlier estimates are based on the assumption that the specific heat diverges logarithmically. It should be emphasized that the errors quoted in (3.12) are of course only realistic if $\alpha = \frac{1}{8}$ and the critical temperature is correct to within the limits given in (2.6).

4. General conclusions

The hypothesis that the specific heat of a three dimensional Ising model of a ferromagnet diverges at the critical temperature, from above, inversely as an one eighth power was made in I; in our opinion the extended series presented in this paper appear consistent with this hypothesis. Convergence is slow and higher coefficients difficult to derive; the hypothesis must therefore remain a tentative one. However the evidence that α is close to 0·125 is strong.

We have estimated the critical entropy and energy of three three dimensional lattices from extended series expansions for the specific heat; although there should be some improvement in precision the values do not differ much from earlier estimates based on fewer terms and an incorrect asymptotic form. We conclude that the critical values are known accurately enough for most practical purposes. Estimates of the amplitude of the specific heat singularity are much more sensitive to small changes in the assumed values of α and T_C.

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