The smoothness postulate and the Ising antiferromagnet

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Abstract. The validity of the smoothness postulate is tested for the Ising antiferromagnet in two and three dimensions. The field dependence of the staggered susceptibility above the critical temperature is studied by means of series extrapolation, and the curvature of the phase boundary in zero field is deduced. The results are compared with those found from initial susceptibility and specific heat data.

1. Introduction

Most of the exact results which have been obtained for the Ising model in the critical region apply only in zero magnetic field. With one or two noteworthy exceptions the bulk of our knowledge of the properties in nonzero field has been obtained from various types of series expansion (Fisher 1967, Domb 1970). It is known that the Ising ferromagnet will not undergo a transition in the presence of a uniform field (Yang and Lee 1952); for the antiferromagnet, however, the phase transition persists so long as the field does not exceed a certain limiting value. The question posed is what is the nature of this transition?

An analysis of the energy and susceptibility series expansions for the antiferromagnet in zero field (Sykes and Fisher 1962) suggested that to leading order their singular parts are of the same form. A more general theoretical treatment of the correlation functions (Fisher 1962) confirmed this conclusion. Experimentally, the critical behaviour of the specific heat of an antiferromagnet is unaltered in the presence of a field and the field dependence of the transition temperature is almost quadratic (Schelleng and Friedberg 1969).

In an attempt to unify these and similar results for other problems the postulate of smoothness was introduced by Griffiths (1970). The application of this postulate to the antiferromagnet is based on the observation that the boundary between the antiferromagnetic and paramagnetic phases is really no more than a line of critical points, and there appears to be no a priori reason to single out the particular point corresponding to zero field. On this basis it becomes possible to postulate the functional form of the free energy at points near the critical line, and the critical properties in nonzero field follow immediately. This argument is, of course, restricted to weak fields; in a strong field the nature of the lowest energy state changes.

The absence of any exact solutions which could be used to verify the smoothness postulate for the Ising model means that one must look for confirmation to the results of series studies. In this paper we report on the results of a number of such tests. The high temperature expansions of the staggered susceptibility of the antiferromagnet and its field derivatives in zero field are computed and the result of their analysis compared with the predictions of the smoothness postulate. In a repeat of an earlier investigation (Bienenstock 1966, Bienenstock and Lewis 1967, to be referred to as BL), the staggered susceptibility in the presence of a field is also studied, but this time longer series are used. A further test is made which relies on available results for the specific heat and antiferromagnetic susceptibility. For the two lattices we have examined, the simple quadratic in two dimensions and the

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2684
simple cubic in three, we find that to within the limits of confidence in the results of our series analysis the smoothness postulate is verified.

2. Prediction of the smoothness postulate

Applied to the antiferromagnet the smoothness postulate states that the phase boundary is a smooth curve, and in the neighbourhood of any point on this curve the singular part of the free energy has essentially the same form. The field dependence of the singular part of the free energy is restricted to a smooth variation of the parameters representing the amplitudes of the critical singularities. The simple form proposed for the free energy near the phase boundary which complies with these requirements is (Griffiths 1970)

\[ F(H, T) = F_0(H, T) + \phi(H) \{ \theta(H)[T - T(H)] \} \]

where \( F_0, \phi, \theta \) and \( T_c \) are smooth functions of their respective arguments. \( T_c(H) \) is the critical temperature in field \( H \)—the equation of the phase boundary is just \( T_c = T_c(H) \); \( T(0) \) is the Néel temperature. The functions \( \phi \) and \( \theta \) are defined to be unity at \( H = 0 \). Written in this form the singular part of \( F \) is proportional to a function of a single variable \( f(\tau) \), where, for a given \( H, \tau \) is the distance of \( T \) from the appropriate critical temperature. The ‘unit’ in which this temperature difference is measured is scaled with respect to its value in zero field by the function \( \theta(H) \).

Since \( F \) is an even function of \( H \), for small \( H \)

\[ T_c(H) = T_c + \frac{1}{2!} T_c^{(2)} H^2 + \frac{1}{4!} T_c^{(4)} H^4 + \ldots \]

where \( T_c = T_c(0), T_c^{(2)} = d^2/dH^2 T_c(H) \), etc. The specific heat and the temperature derivative of the susceptibility in zero field follow immediately

\[ T^{-1} C = -\frac{\partial^2}{\partial T^2} F_0 - \frac{\partial^2}{\partial T^2} f(T - T_c) \]

and

\[ \frac{d}{dT} \chi = \chi' = T_c^{(2)} \frac{d^2}{dT^2} f(T - T_c) \]

so that the ratios of the amplitudes of the singularities of \( \chi' \) and \( C \) is \( -T_c^{(2)}/T_c \). In nonzero field the singular parts of \( C \) and \( \chi \) turn out to be proportional, a result which also arises out of the exact solution of the superexchange model of an antiferromagnet (Fisher 1960).

For a ferromagnet, the quantity whose high temperature series are most amenable to analysis is the zero field susceptibility \( \chi_0 \). The susceptibility of the antiferromagnet is only weakly singular in zero field, but the staggered susceptibility in zero staggered field, \( \chi_s \), is identical to the \( \chi_0 \) of the corresponding ferromagnet, so that for \( H = 0 \) and \( T \geq T_c \),

\[ \chi_s \sim \frac{m^2}{k_B T_c} C^+ \left( \frac{T}{T_c} - 1 \right)^{-\gamma} \]

where \( \gamma \) and \( C^+ \) are the usual exponent and amplitude of \( \chi_0 \) (Fisher 1967). Here \( m \) is the magnetic moment per spin and \( k_B \) is the Boltzmann constant. The staggered susceptibility was originally used in the study of the Heisenberg antiferromagnet (Rushbrooke and Wood 1963), and later by BL in their investigation of the shape of the phase boundary.

The smoothness postulate suggests that in nonzero field, the form of the staggered susceptibility in the critical region should be

\[ \chi_s(H) \sim \frac{m^2}{k_B T_c(H)} C^+(H) \left( \frac{T}{T_c(H)} - 1 \right)^{-\gamma} \]
where, once again, the field affects only the amplitude and location of the singularity, but not the exponent. For convenience we introduce the reduced quantity

\[ \tilde{\chi}_s = \left( \frac{m^2}{k_BT} \right)^{-1} \chi_s \]

then since \( C^+(H) \) is assumed to be a smooth function of \( H \) and to have the expansion

\[ C^+(H) = C^+ + \frac{1}{2!} C^{+(2)} H^2 + \ldots \]

we find that

\[ \tilde{\chi}_s(H) \sim \left( C^+ + \frac{1}{2!} C^{+(2)} H^2 + \ldots \right) -\gamma \left( 1 + \frac{T_c^{(2)}}{T_c} H^2 + \ldots \right)^{\gamma - 1} \left( 1 - \frac{1}{2!} \frac{T_c^{(2)}}{T_c} H^2 t^{-1} \ldots \right)^{-\gamma} \]

where \( t = T/T_c - 1 \). If we expand \( \tilde{\chi}_s(H) \) in terms of \( H \),

\[ \tilde{\chi}_s(H) \sim \tilde{\chi}_s^{(0)} + \frac{1}{2!} \tilde{\chi}_s^{(2)} H^2 + \frac{1}{4!} \tilde{\chi}_s^{(4)} H^4 + \ldots \]

\[ \tilde{\chi}_s^{(0)} = \tilde{\chi}_s \]

(6)

the derivatives of \( \tilde{\chi}_s \) are seen to have the critical behaviour

\[ \tilde{\chi}_s^{(2n)} \sim G_2 \gamma^{(2n)} + O(t^{-\gamma^{(2n)} + 1}). \]

(7)

The exponent of \( \tilde{\chi}_s^{(2n)} \) is a linear function of \( n \)

\[ \gamma^{(2n)} = \gamma + n \]

(8)

and the amplitudes can be shown to satisfy the relation

\[ \frac{G_{2n+2}}{G_{2n}} = (2n + 1)(n + \gamma) \frac{T_c^{(2)}}{T_c} \]

\[ G_0 = C^+. \]

(9)

To conclude this section we summarize the predictions made by the smoothness postulate which will be studied in subsequent sections: (1) at \( H = 0 \) the ratio of the amplitudes of \( \chi' \) and \( C \) is proportional to \( T_c^{(2)} \); (2) \( \tilde{\chi}_s \) and all its even field derivatives diverge at \( T_c \) for \( H = 0 \); (3) the exponent of \( \tilde{\chi}_s^{(2n)} \) is \( \gamma + n \); (4) the ratios of the amplitudes of successive \( \tilde{\chi}_s^{(2n)} \) are proportional to \( T_c^{(2)} \), and (5) the exponent \( \gamma \) is a constant independent of \( H \).

3. Generation of the expansions

A convenient method of obtaining high temperature Ising series in nonzero field is the application of a transformation to the already known low temperature results. The series produced by this technique are of course shorter than the zero field high temperature series found by more direct methods (Domb 1960). Since we are only interested in the expansions for the staggered susceptibility we are limited to loose packed lattices, for it is only for this class of lattice that \( \chi_s \) is defined. The sites of a loose packed lattice may be regarded as belonging to one of two regular sublattices; the field at sites on one of the sublattices will be denoted by \( H_A \), that at the other by \( H_B \). If \( Z_{2N} \) is the partition function for the lattice of \( 2N \) sites, then

\[ Z_{2N} = (\mu v)^{-N/2} u^{-qN/4} \Lambda_{2N} \]

where \( \mu = \exp(-2\beta m H_A) \), \( v = \exp(-2\beta m H_B) \), \( u = \exp(-4\beta|J|) \) (\( J \) is the exchange integral) and we have the expansion

\[ \ln \Lambda = \lim_{N \to \infty} (2N)^{-1} \ln \Lambda_{2N} = \sum_{i=1}^{\infty} \sum_{j=0}^{i} f_{i-j,j}(u) \mu^{i-j} v^{i} \]

(10)
where \( f_{ij}(u) \) is a polynomial in \( u \). The coefficients of this expansion can be found via the code method (Sykes et al. 1965). The high temperature expansion then has the form
\[
\ln \Lambda = \frac{1}{2} \ln \{(1 + \mu)(1 + \nu)\} + \frac{1}{2} \sum_{\lambda=1}^{\infty} \frac{(u - 1)^{\lambda}}{\lambda!} \{\ln(1 + \mu)(1 + \nu)\}_{\lambda}
\times \sum_{i=1}^{\lambda} \sum_{j=0}^{\lambda} a_{i-j}^\lambda (\mu^{i-j} + \mu^{i-1} \nu^{j-i} + \nu^{j-i}).
\]

This last equation is an unpublished result of Sykes quoted by BL.

In order to complete the first \( \lambda \) terms of the high temperature series, a total of \( \lambda + [\lambda^2/4] \) constants \( a_{ij}^\lambda \) must be evaluated (the symmetry conditions \( a_{ij}^\lambda = a_{ji}^\lambda \) has halved the number of unknowns). The method of doing this is described by BL. Briefly stated, it involves evaluating the first \( \lambda \) \( u \)-derivatives of both the high and low temperature expansions at \( u = 1 \). The coefficients of \( \mu^{i-j} \) in the two series are equated and a set of simultaneous equations is obtained, one equation for each pair of \( s \) and \( t \). For the correct choice of the order of the values taken by \( s \) and \( t \) the coefficient matrix is triangular and the solution is easily found. Note that the \( a_{ij}^\lambda \) may be numbers with 20 or more digits (see for example the table in BL). Because of the large amount of cancellation which must occur when the \( a_{ij}^\lambda \) are used to find the terms of the high temperature expansion, care must be taken to prevent any numerical rounding at this stage of the problem.

In the presence of both a field \( H \), and a staggered field \( h \) whose direction alternates between the two sublattices, we can set
\[
H_A = H + h \quad H_B = -H + h
\]
The staggered susceptibility per spin at \( h = 0 \) is defined as
\[
\chi_s = k_B T \frac{\partial^2}{\partial h^2} \ln \Lambda \Big|_{h=0}
\]
and a straightforward calculation yields the expansion
\[
\tilde{\chi}_s = (\cosh x)^{-2} + \sum_{\lambda=1}^{\infty} \frac{(u - 1)^{\lambda}}{\lambda!} 2^{\lambda-2} \sum_{i=1}^{\lambda} \sum_{j=0}^{\lambda} a_{i-j}^\lambda \cosh (2i - 4j)x
\times \left( (\lambda - i)^2 (\cosh x)^{-2\lambda} - \frac{\lambda}{2} (\cosh x)^{-2\lambda-2} \right)
\]
where \( x = \beta mH \). The odd derivatives of \( \tilde{\chi}_s \) with respect to \( H \) are seen to be zero at \( H = 0 \). The even derivatives are
\[
\frac{\partial^{2n}}{\partial H^{2n}} \tilde{\chi}_s \bigg|_{H=0} = (\beta m)^{2n} \tilde{\chi}_s^{(2n)} \quad \tilde{\chi}_s = \tilde{\chi}_s^{(0)}
\]
where
\[
\tilde{\chi}_s^{(2n)} = Y_{2n}^{(2n)} + \sum_{\lambda=1}^{\infty} \frac{(u - 1)^{\lambda}}{\lambda!} 2^{2\lambda-2} \sum_{r=0}^{n} \binom{2n}{2r} \sum_{i=1}^{\lambda} \sum_{j=0}^{\lambda} a_{i-j}^\lambda \cosh (2i - 4j)^{2n-2r} \left( (\lambda - i)^2 Y_{2\lambda}^{(2r)} - \frac{\lambda}{2} Y_{2\lambda+2}^{(2r)} \right)
\]
and the quantities \( Y_{\mu}^{(n)} \) satisfy the recurrence relation
\[
Y_{\mu}^{(n+2)} = \mu^2 Y_{\mu}^{(n)} - \mu(\mu + 1) Y_{\mu+2}^{(n)} \quad Y_{\mu}^{(0)} = 1.
\]

4. The staggered susceptibility

Using equations (15) and (16), together with the coefficients \( a_{ij}^\lambda \), we have computed the series expansions of \( \chi_s^{(n)} \) with \( n = 0, 2, 4, 6, 8 \), for the simple cubic (SC) and simple quadratic...
(SQ) lattices. A simple substitution leads to series in the more commonly used high temperature variable \( w = \tanh K \). For the SC lattice terms up to \( w^{12} \) were obtained, and up to \( w^{15} \) for the SQ. The series for \( \gamma^{(2)} \) contain only even powers of \( w \), whereas the terms of the higher derivatives oscillate in sign. The obvious method of analysing such series is by the Padé approximant technique (e.g. Baker 1965).

A straightforward calculation of the Padé approximants to the logarithmic derivatives of the series failed to produce conclusive results. We therefore proceeded by assuming that each of the \( \gamma^{(n)} \) has its physical singularity at the same value \( w_c \). Then with the values of \( w_c \) of 0.21814 for the SC (Gaunt and Guttman 1971) and 0.414214 for the SQ, we found estimates of the exponents \( \gamma^{(n)} \) by evaluating the Padé approximants of the functions

\[
(w_c - w) \frac{d}{dw} \ln \gamma^{(n)}
\]

at \( w = w_c \). The values produced by the approximants \([D, N]\) for a range of \( D \) values, with \( N = D \pm 1 \), are given in tables 1 and 2. (The \( n = 8 \) results are omitted because of too much scatter.) These results are seen to be in reasonable agreement with the prediction that the exponent of \( \gamma^{(2n)} \) should be

\[
\gamma^{(2n)} = \gamma + n
\]

where, of course, \( \gamma \) is \( 2/3 \) (SC) and \( 2/3 \) (SQ). The SC results appear to be better behaved than those for the SQ, even though the series for the latter are longer.

|  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|
| \( D \) | \( N \) | 0 | 2 | 4 | 6 |
| 4 | 3 | 1.2501 | 2.256 | 3.286 | 4.541 |
| 4 | 4 | 1.2501 | 0 | 2.753 | 5.615 |
| 4 | 5 | 1.2501 | 2.260 | 3.244 | 3.855 |
| 5 | 4 | 1.2501 | 2.258 | 3.247 | 4.031 |
| 5 | 5 | 1.2499 | 2.258 | 3.254 | 4.252 |
| 5 | 6 | 1.2499 | 2.257 | 3.252 | 4.241 |
| 6 | 5 | 1.2499 | 2.258 | 3.253 | 4.241 |
| 6 | 6 | 1.2499 | 2.267 | 3.254 | 4.252 |

Table 1. Padé estimates of the exponents \( \gamma^{(n)} \) for the SC lattice. Compare with the predicted result \( \gamma^{(2n)} = 1.25 - n \).

Table 2. Padé estimates of the exponents \( \gamma^{(n)} \) for the SQ lattice. Compare with the predicted result \( \gamma^{(2n)} = 1.75 + n \).
The smoothness postulate and the Ising antiferromagnet

Table 3. Padé estimates of the amplitude $Q_n$ for the SC lattice.

<table>
<thead>
<tr>
<th>D</th>
<th>N</th>
<th>0</th>
<th>2</th>
<th>4</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3</td>
<td>0.15171</td>
<td>-0.018654</td>
<td>0.01329</td>
<td>-0.017142</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>0.15168</td>
<td>-0.018662</td>
<td>0.012578</td>
<td>-0.025674</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>0.15168</td>
<td>-0.018714</td>
<td>0.012482</td>
<td>-0.03535</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>0.15168</td>
<td>-0.018650</td>
<td>0.012514</td>
<td>-0.021248</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>0.15168</td>
<td>-0.018385</td>
<td>0.012516</td>
<td>-0.019430</td>
</tr>
<tr>
<td>5</td>
<td>6</td>
<td>0.15167</td>
<td>-0.018786</td>
<td>0.012523</td>
<td>-0.020810</td>
</tr>
<tr>
<td>6</td>
<td>5</td>
<td>0.15167</td>
<td>-0.018695</td>
<td>0.012513</td>
<td>-0.020122</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0.15168</td>
<td>-0.018766</td>
<td>0.012556</td>
<td>-0.020231</td>
</tr>
</tbody>
</table>

We next turned to a study of the amplitudes, $Q_n$, of the critical singularities of the $\tilde{\gamma}^{(n)}$. Estimates of $Q_n$ were obtained by assuming both the linear $n$ dependence of $\gamma^{(n)}$ and the value of $w_c$, and evaluating the Padé approximants of

$$(w_c - w)^{(n)} \tilde{\gamma}_c$$

at $w_c$. The results are shown in tables 3 and 4. The values of $Q_n$ lie within 0.1% of the estimates of the $\chi_0$ amplitudes (Fisher 1967, where the values and references to their sources will be found). Not surprisingly the estimates become less reliable as $n$ increases. From successive pairs of amplitudes we computed sets of estimates of $T_c^{(2)}$ with the aid of the formula derived from the smoothness postulate

$$T_c^{(2)} = \frac{T_c}{(2n + 1)(n + \gamma)} \frac{G_{2n+2}}{G_{2n}}$$

(17)

and since $Q_n$ is the amplitude for an expansion in terms of the variable $w$, we have that

$$\frac{G_{2n+2}}{G_{2n}} = \frac{K_c}{1 - w_c^2} \frac{Q_{2n+2}}{Q_{2n}}$$

(18)

The values of $Q_n$ and the estimates of $T_c^{(2)}$ which follow are shown in tables 5 and 6. We have also examined series for $\tilde{\gamma}_c^{(2n+2)}/\tilde{\gamma}_c^{(2n)}$ and were led to results of comparable accuracy. Within the limits of confidence which can be ascribed to the Padé estimates, we may safely say that the three values of $T_c^{(2)}$ are the same. Since the results from the lowest derivatives

Table 4. Padé estimates of the amplitudes $Q_n$ for the SQ lattice.

<table>
<thead>
<tr>
<th>D</th>
<th>N</th>
<th>0</th>
<th>2</th>
<th>4</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>4</td>
<td>0.16509</td>
<td>-0.04211</td>
<td>0.05253</td>
<td>-0.1723</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>0.16508</td>
<td>-0.04246</td>
<td>0.04756</td>
<td>-0.0983</td>
</tr>
<tr>
<td>5</td>
<td>6</td>
<td>0.16505</td>
<td>-0.04184</td>
<td>0.04756</td>
<td>-0.1448</td>
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<tr>
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<td>0.16508</td>
<td>-0.04027</td>
<td>0.04756</td>
<td>-0.1226</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0.16509</td>
<td>-0.04117</td>
<td>0.04756</td>
<td>-0.1278</td>
</tr>
<tr>
<td>6</td>
<td>7</td>
<td>0.16508</td>
<td>-0.04128</td>
<td>0.04797</td>
<td>-0.1311</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>0.16509</td>
<td>-0.04132</td>
<td>0.04898</td>
<td>-0.1453</td>
</tr>
<tr>
<td>7</td>
<td>7</td>
<td>0.16508</td>
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<td>0.04852</td>
<td>-0.2002</td>
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<tr>
<td>7</td>
<td>8</td>
<td>0.16509</td>
<td>-0.04129</td>
<td>0.04851</td>
<td>-0.1322</td>
</tr>
<tr>
<td>8</td>
<td>7</td>
<td>0.16507</td>
<td>-0.04132</td>
<td>0.04851</td>
<td>-0.1460</td>
</tr>
</tbody>
</table>
Table 5. Estimates of \( Q_s \) (SC lattice) from the Padé results in table 3, with the resulting values of \( T_c^{(2)} \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \left( \frac{J}{m} \right)^{-n} Q_n )</th>
<th>( \left( \frac{J}{m} \right)^{-2} \frac{T_c^{(2)}}{T_c} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.15168</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-0.01875</td>
<td>-0.02302</td>
</tr>
<tr>
<td>4</td>
<td>0.01252</td>
<td>-0.02303</td>
</tr>
<tr>
<td>6</td>
<td>-0.0203</td>
<td>-0.023</td>
</tr>
</tbody>
</table>

(ie\( \gamma_s^{(2)} \) and \( \gamma_s \) itself) appear to be the most accurate we find that the equations of the phase boundary are

\[
T_c(H) = T_c(1 - 0.0115 \frac{(m/J)^2 H^2}{H^2}) + O(H^4) \quad \text{SC}
\]

and

\[
T_c(H) = T_c(1 - 0.0380 \frac{(m/J)^2 H^2}{H^2}) + O(H^4) \quad \text{SQ}.
\]

In their study of the equation of the phase boundary, BL looked into the behaviour of \( \chi_s \) in nonzero field. A least squares fit of the data to a function of the form

\[
T_c(H) = T_c(1 - (m/J)^2 H^2)^\xi
\]

(\( q \) = coordinate number) led to the result \( \xi = 0.36 \) for SC and \( 0.87 \) for SQ. Thus for small \( H \)

\[
\frac{T_c^{(2)}}{T_c} = -0.010 \frac{(m/J)^2}{SC}
\]

\[
-0.054 \frac{(m/J)^2}{SQ}.
\]

The value for the SQ is in disagreement with our estimate, and in an attempt to discover the reason for this we have repeated the calculation using series obtained from equation (13). These series are slightly longer than those used by BL.

Table 6. Estimates of \( Q_s \) (SQ lattice) from the Padé results in table 4, with the resulting values of \( T_c^{(2)} \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \left( \frac{J}{m} \right)^{-n} Q_n )</th>
<th>( \left( \frac{J}{m} \right)^{-2} \frac{T_c^{(2)}}{T_c} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.16508</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-0.04130</td>
<td>-0.07605</td>
</tr>
<tr>
<td>4</td>
<td>0.0485</td>
<td>-0.0757</td>
</tr>
<tr>
<td>6</td>
<td>-0.136</td>
<td>-0.079</td>
</tr>
</tbody>
</table>

In tables 7 and 8 we give the estimates of \( w_c(H) \) and \( \gamma \) produced by a Padé analysis of the series for \( d/dw \ln \chi_s \) for various values of the field variable \( x \). Since we are only interested in the quadratic term in the expansion of \( T_c(H) \) we are restricted to weak fields in order to minimize the effects of the quartic and higher order terms. There is no obvious variation of \( \gamma \) with \( H \) (or \( x \)). In trying to estimate the value of \( w_c \) corresponding to a given \( H \), we have assumed that of the last few approximants, those which give a value of \( \gamma \) closest to the expected
The smoothness postulate and the Ising antiferromagnet

Table 7. Padé estimates of the SC critical point $w_c(x)$ and exponent $\gamma$ (in parentheses) for various values of the field $x = \beta_c mH$.

<table>
<thead>
<tr>
<th>$D$</th>
<th>$N$</th>
<th>$x$</th>
<th>0</th>
<th>0.05</th>
<th>0.10</th>
<th>0.15</th>
<th>0.20</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
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Table 8. Padé estimates of the SQ critical point $w_c(x)$ and exponent $\gamma$ (in parentheses) for various values of the field $x$.

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one will also produce the best estimate for $w_c(H)$. On this basis we find that for small $H$ the results can be fitted by a parabola, and

$$T_c(H) = T_c(1 - 0.012 (m/J)^2 H^2) + O(H^4) \quad \text{SC}$$

$$T_c(H) = T_c(1 - 0.037 (m/J)^2 H^2) + O(H^4) \quad \text{SQ}.$$  

The accuracy of this approach is lower than the method which uses derivatives because the result of the subtraction of the nearly equal quantities $\xi_c(H)$ and $w_c$ used to find $T_c^{(2)}$ is a number little larger than the uncertainty in $w_c$ itself. Nevertheless, the results agree moderately well with those found earlier.

We suggest that the reason for the discrepancy between the BL results and those given here is that the parameter $\xi$ was determined by fitting over a wide range of $H$ values, and thus the small $H$ behaviour is incorrectly described.
5. Results from the susceptibility and specific heat

In §2 we pointed out that one of the predictions of the smoothness postulate is that in zero field the ratio of the critical amplitudes of $\chi'$ and $C$ is proportional to $T_c^{(2)}$. We shall now see how the value produced in this manner compares with that obtained via the staggered susceptibility.

The critical amplitudes of the specific heat require little discussion. For the SQ lattice we have the exact result

$$\frac{C}{k_B} \sim -0.4945 \ln \left(\frac{T}{T_c} - 1\right) \quad T \gtrsim T_c.$$  

The result for the SC lattice is derived from series analysis. We shall adopt the value obtained by Hunter (1969) which, after a change of variable, becomes

$$\frac{C}{k_B} \sim 1.132 \left(\frac{T}{T_c} - 1\right)^{-1/8} \quad T \gtrsim T_c.$$  

In determining the amplitudes of the susceptibility we face the problem of finding the weak singularity in a series whose asymptotic behaviour is dominated by a strong ferromagnetic singularity. The problem has been discussed in an article by Domb (1970). On the assumption that the higher order terms in the susceptibility series will be well represented by the function

$$A_0^+ \left(1 - \frac{w}{w_c}\right)^{-\gamma} + A_1^+ \left(1 - \frac{w}{w_c}\right)^{-\gamma+1} + \bar{A}_0^+ \left(1 + \frac{w}{w_c}\right)^{-\gamma},$$

the series are analysed by equating the ratio $n a_n/(n + \gamma - 1) a_{n-1}$ (where $a_n$ is the nth term in the series) to

$$w_c^{-1}(1 + a/n^2 + (-1)^b/n^{\gamma+\gamma})$$

and solving for $w_c$, $a$ and $b$ for each set of four terms. The amplitude of the antiferromagnetic singularity is then

$$\bar{A}_0^+ = \frac{1}{2} \Gamma(\gamma) A_0^+ b / \Gamma(\gamma)$$

where $A_0^+$, the ferromagnetic amplitude, is known relatively accurately. (As given, these formulae are suitable for analysing the SC series: for the SQ they need modification to accommodate the logarithmic singularity.) An alternative method of evaluating $b$ consists of feeding in the value of $w_c$ and solving for $a$ and $b$ using successive sets of three terms of the series. The value finally adopted for $b$ is the average of the values from the last few sets of terms. We eventually find that the susceptibility of the antiferromagnet in the critical region is

$$\chi \sim 0.613 \frac{m^2}{k_B T_c} \left(\frac{T}{T_c} - 1\right)^{7/8} \quad \text{SC}$$

and

$$-0.190 \frac{m^2}{k_B T_c} \left(\frac{T}{T_c} - 1\right) \ln \left(\frac{T}{T_c} - 1\right) \quad \text{SQ}.$$  

The amplitudes of the derivatives $\chi'$ follow, and as a consequence of equations (2) and (3),

$$T_c(H) = T_c(1 - 0.0116 \frac{(m/J)^2 H^2}{H^4}) + O(H^4) \quad \text{SC}$$

$$T_c(1 - 0.0373 \frac{(m/J)^2 H^2}{H^4} + O(H^4) \quad \text{SQ}.$$  

The difference between the results of this and the preceding section lies well within the limits of uncertainty in the values of the amplitudes themselves.

For the SQ lattice we can use the value of $T_c^{(2)}$ provided by $\chi_s$, together with the exact value of the specific heat amplitude to derive the amplitude of the singular part of $\chi$. The
truth of the smoothness postulate must, of course, be assumed; the value which follows for the amplitude is 0.194.

We have been informed by Sykes (private communication) that the estimates of the antiferromagnetic amplitudes are currently under review, and are being revised in the light of extended series. However, we do not expect the pattern of results described here to be affected significantly.

6. Review

Two different approaches have been used in the study of $\chi_s$: one involved assuming the smoothness postulate applies to $\chi_s$ and testing the predicted behaviour; the other was an investigation of $\chi_s$ in nonzero field, from whose results one might be led to the smoothness postulate. The order may appear logically incorrect, but the accuracy of the first method is considerably greater than the second. Both methods predict the zero field curvature of the phase boundary. This quantity can also be found from the amplitudes of $\chi'$ and $C$, a result which has also been found to apply experimentally (Schelleng and Friedberg 1969). The values of the curvature obtained by each of the methods are sufficiently close to be regarded as being the same, subject of course, to the reliability of the techniques used to analyze the series.

The work can obviously be extended to include other lattices and low temperature expansions, and it may also be possible to find higher order corrections to the equation of the phase boundary. These points are being investigated further. One consequence of the smoothness postulate is that since the specific heat of the two dimensional Ising antiferromagnet is symmetrical about $T_c$, the amplitudes of the singular part of the susceptibility will be the same above and below $T_c$. The amplitudes below $T_c$ are not known at all accurately, but for the SQ lattice its estimated value (Fisher 1967) lies within 10% of the value obtained from the high temperature series.

We should perhaps clarify the relation between this work and other types of expansion about critical points. Three different situations have been distinguished.

The critical point of a ferromagnet (or a fluid) gives rise to a gap index, $\Delta$, which is usually nonintegral (Domb and Hunter 1965, Essam and Hunter 1968). Each term in the free energy expansion in terms of $H$ diverges with an exponent which is a linear multiple of $\Delta$. However, since the free energy in the presence of a field is known to be an analytic function of temperature, it is possible to resum (at least formally) this kind of divergent series to obtain an analytic function describing behaviour in the critical region. This type of critical point corresponds to the termination of the equilibrium line between two phases.

In the case of an antiferromagnet and similar problems where the presence of an additional parameter in the Hamiltonian serves only to define a line of critical points along which no fundamental change of critical behaviour is expected, Griffiths (1970) introduced the smoothness postulate which attempts to predict the relation between the singular parts of the free energy with and without the perturbation. The terms of the perturbation expansion about the zero value of the parameter diverge as the critical point is approached, and the smoothness postulate enables us to determine the singular behaviour of these divergent terms. If we start with this perturbation series and resum (eg Herman and Dorfman 1968) we must be led to a function of similar form to the unperturbed free energy if the smoothness postulate is valid.

The third case corresponds to a point on a transition line at which there is a change in critical behaviour and critical indices; for example, if the expansion parameter corresponds to the interaction between planes of Ising spins to produce a three dimensional Ising system, we should expect a change in critical indices from two dimensional to three dimensional values. Scaling arguments have been used to predict the shift in critical point as the parameter changes, and also to describe the way in which the critical amplitudes vary (Abe 1970, Suzuki 1971, Coniglio 1971). An example of this type where the perturbation series can be exactly resummed is the four dimensional spherical model regarded as a perturbation about the three dimensional model (Rapaport 1971).
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References

CONIGLIO, A., 1971, to be published.
RAPAPORT, D. C., 1971, to be published.