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Phase transitions in a one dimensional model of a ferromagnet: a transfer-matrix approach

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Abstract. It is shown that a transfer-matrix method provides a particularly direct solution for a ferromagnetic version of a one dimensional model originally invented by Fisher. An essential feature of this model is the many body potential, leading to a phase transition. All the thermodynamical properties of the model may be written down once the dominant eigenvalue and eigenvector of the matrix are known; in particular, surface properties may be obtained in terms of the dominant eigenvector. Typical phase diagrams are obtained, and the singularities at the phase boundaries discussed.

1. Introduction and summary

It is now some years since Fisher (1967a) invented a 'physically natural' one dimensional model of a fluid with both liquid and gaseous phases. The essential feature of this model is that a set of particles which are in a certain sense not too far apart interact to form a *cluster*, with its own characteristic energy; the interaction is short range in that distinct clusters do not interact. The possibility of a phase transition arises from the many body nature of the interactions. Fisher and Felderhof (1970a,b), Felderhof and Fisher (1970) and Felderhof (1970a,b) have shown that cluster models can show a great variety of transition behaviour, according to the interaction chosen; as these authors supply a good list of references, we mention here only those papers that impinge directly on this work.

The purpose of this paper is to consider the ferromagnet (or equivalently, the one dimensional lattice gas) which is in essence a discrete version of the Fisher cluster model. The precise form of the model is given in § 2, and we show in § 3 and § 4 that a 'transfer-matrix' method provides a particularly simple route to the complete thermodynamics (cf Lassettre and Howe 1941). In fact, not only is the 'partition function per spin' the dominant eigenvalue of the transfer matrix, but the surface correction for a semi-infinite chain can be simply written in terms of the dominant eigenvector (§ 7). Similarly we may obtain full information on other features, such as the statistics of cluster sizes in the model, though we do not discuss these in this paper (but see Felderhof 1972). This directness and the versatility of the matrix approach are not affected by the fact that the transfer matrix is of infinite dimension (as it has to be, since a system with a finite-dimensional transfer matrix may be expected to show no phase change).

In §§ 3-5 it is shown that as many as three phase regions may exist in the (T, H) plane; for convenience, we call these the paramagnetic and the (+) or (-) ferromagnetic regions. The ferromagnetic regions are characterized by the presence of a cluster of infinite size. The mechanism of the transition as a phase boundary is crossed depends

on which way the boundary is approached. On the paramagnetic side there is a breakdown of convergence of certain infinite series; on the ferromagnetic side there are no mathematical singularities of this type, the transition here arising from a breakdown in the physical interpretation of the eigenvector. The nature of the singularities on the paramagnetic side of a phase boundary is discussed in § 6, and some comments are made on the probable irrelevance of the cluster model for the Ising model in higher dimensions.

2. The model

The model consists of a chain of 'spins', whose two possible values are +1 and -1; any assignment of these values to the spins of the chain constitutes a typical *configuration*. The energy associated with any configuration is to be computed as follows.

An (m+) cluster of the configuration is a set of *m* consecutive spins which have all been assigned the value +1, flanked by spins with value -1; an (m-) cluster is similarly defined. Thus a configuration is an alternating sequence of (+) and (-) clusters of various sizes. The energy of a configuration is then the sum of the energies of the individual clusters in the configuration; these in turn are given by

energy of an
$$(m +)$$
 cluster $= -m(J + H) + \eta_m$
energy of an $(m -)$ cluster $= -m(J - H) + \eta_m$ (2.1)

where J > 0, and the η must satisfy $\eta_m/m \to 0$ as $m \to \infty$. Clearly $J \pm H$ are bulk energies per spin of the clusters, while the η_m may be thought of as size-dependent 'surface corrections' (though such a description is less appropriate in one dimension than in two or three).

The usual one dimensional Ising model (with an unimportant overall energy shift +J) is obtained by setting every $\eta_m = 2J$. It is well known that there is then no phase change. The point of the more general prescription (2.1) is that it is possible to obtain a model exhibiting a phase change by a proper choice of the energies η_m . The precise circumstances under which this happens are examined in § 5; they depend on the convergence properties of a certain series involving η_m . Roughly it may be said that the η are to be chosen so that the formation of large clusters becomes energetically favourable, though this is not the whole story.

It is convenient to divide the solution of the model into two sections, depending on whether an infinite cluster is absent or present; we shall call the two possibilities 'paramagnetic' and 'ferromagnetic'. In §5 we shall find that for every temperature and magnetic field one or other of these possibilities holds, and thus that the complete solution is obtained. Throughout, we write $\beta = 1/kT$.

3. The transfer matrix

We shall find it convenient to consider the semi-infinite chain (rather than the infinite chain), with the advantages that a simple transfer-matrix treatment is possible and that the surface properties as well as the bulk properties can be determined (§ 7). In this section we consider the problem of finding the form of the transfer matrix T.

Write $\Lambda_N(\beta, H)$ for the canonical partition function for a finite chain of N spins. Further, write $\Lambda_N(\beta, H; m+)$ for the contribution to this partition function from all those configurations which have exactly an (m+) cluster at (say) the right hand end of the chain; similarly for $\Lambda_N(\beta, H; m-)$. These contributions are mutually exclusive and leave nothing out.

We shall take the limit $N \to \infty$ by allowing the left hand end of the chain to grow indefinitely. In this limit we define for each $m \ge 1$

$$p_m^+ \equiv p_m^+(\beta, H) \equiv$$
 proportion of configurations in the statistical ensemble
with exactly an $(m+)$ cluster at the right hand end

$$= \lim_{N \to \infty} \frac{\Lambda_N(\beta, H; m+)}{\Lambda_N(\beta, H)}.$$
(3.1)

Analogously

$$p_m^- = \lim_{N \to \infty} \frac{\Lambda_N(m-)}{\Lambda_N}.$$
(3.2)

(We shall often omit the arguments β and H.) We also introduce what we may loosely describe as the bulk partition function per spin

$$\Lambda \equiv \Lambda(\beta, H) = \lim_{N \to \infty} \frac{\Lambda_{N+1}}{\Lambda_N}.$$
(3.3)

Naturally we assume that all these limits exist.

It may happen that in the limit the numbers p_m^{\pm} of equations (3.1) and (3.2) are not sufficient to provide a complete picture. For even though

$$\sum_{m=1}^{N} \left(\frac{\Lambda_N(m+)}{\Lambda_N} + \frac{\Lambda_N(m-)}{\Lambda_N} \right) = 1$$

for all finite N, it does not follow that in the limit $\sum_{m=1}^{\infty} (p_m^+ + p_m^-) = 1$ unless the interchange of two limiting operations can be justified. In fact, it is precisely those circumstances where the interchange is not valid which lead to the possibility of a phase change; the thermodynamic limit, as it were, acquires a feature not present in the finite case. This feature is the possible appearance of a semi-infinite (+) or (-) cluster (possibly with finite clusters to its right).

We must therefore introduce two further quantities

 $p_{\infty}^{+} \equiv p_{\infty}^{+}(\beta, H) =$ proportion in the statistical ensemble of configurations consisting solely of an infinite (+) cluster

and p_{∞}^- , similarly defined. All the *p* taken together now provide an exhaustive picture with

$$p_{\infty}^{+} + p_{\infty}^{-} + \sum_{m=1}^{\infty} (p_m^{+} + p_m^{-}) = 1.$$
 (3.4)

The transfer-matrix equations are obtained by considering the effect of adding a further spin to the right hand end of the chain. Before the limit $N \to \infty$ is taken, we have, for $m \ge 2$

$$\Lambda_{N+1}(m+) = \exp\{\beta(J+H-\eta_m+\eta_{m-1})\}\Lambda_N(m-1+)$$

this comes about since for $m \ge 2$ any configuration of N + 1 spins terminating in an

(m+) cluster is uniquely obtained from a corresponding configuration of N spins terminating in an (m-1+) cluster. The Boltzmann factor accounts for the energy difference of the two clusters. Dividing (3.5) by Λ_N and going to the limit gives

$$\Lambda p_{m}^{+} = \exp\{\beta(J + H - \eta_{m} + \eta_{m-1})\}p_{m-1}^{+} \qquad (m \ge 2)$$
(3.6)

by (3.1) and (3.3); similarly

$$\Lambda p_{m}^{-} = \exp\{\beta(J - H - \eta_{m} + \eta_{m-1})\}p_{m-1}^{-} \qquad (m \ge 2).$$
(3.7)

Further relations follow from noting that configurations ending in a (1 +) cluster are obtained from configurations ending in a (-) cluster of any length; note that we must include the possibility of an infinite (-) cluster:

$$\Lambda p_1^+ = \exp\{\beta(J + H - \eta_1)\} \left(p_{\infty}^- + \sum_{m=1}^{\infty} p_m^- \right)$$
(3.8)

and similarly

$$\Lambda p_1^- = \exp\{\beta(J - H - \eta_1)\} \left(p_{\infty}^+ + \sum_{m=1}^{\infty} p_m^+ \right).$$
(3.9)

To obtain an equation for p_{∞}^+ , we use (3.5) with m = N + 1; in the limit $N \to \infty$

$$\Lambda p_{\infty}^{+} = \exp\{\beta(J+H)\}p_{\infty}^{+}$$
(3.10)

and similarly

$$\Lambda p_{\infty}^{-} = \exp\{\beta(J-H)\}p_{\infty}^{-}.$$
(3.11)

(Strictly, this route assumes $\lim(\eta_m - \eta_{m-1}) = 0$, and this need not be true—though it is true for 'reasonable' models. However, there is no other physically acceptable possibility for (3.10) or (3.11), since the energy per spin of an infinite cluster is

$$\lim_{m\to\infty} m^{-1}\{-m(J\pm H)+\eta_m\}=J\pm H$$

by (2.1).)

Taken together, (3.6 to 11) form an infinite set of linear equations homogeneous in the variables p; they may be concisely written

$$\Lambda \boldsymbol{p} = \boldsymbol{T} \boldsymbol{p} \tag{3.12}$$

the infinite-dimensional transfer matrix T being defined by the right sides of the equations. As is to be expected, Λ is an eigenvalue of T. In the next section, we shall see that among the eigenvalues of T there are at least one and at most three which are real and positive, depending on the values of β and H.

4. The eigenvalues of the transfer matrix

The matrix T is extremely sparse: only two rows have more than one nonzero element. Consequently finding its eigenvalues is very straightforward. First, repeated use of (3.6) gives, for any $m \ge 1$

$$p_m^+ = [\Lambda^{-1} \exp\{\beta(J+H)\}]^{m-1} \exp\{-\beta(\eta_m - \eta_1)\}p_1^+;$$
(4.1)

substituting this in (3.9) then gives

$$p_{1}^{-} = p_{\infty}^{+} \Lambda^{-1} \exp\{\beta(J - H - \eta_{1})\} + p_{1}^{+} \exp(-2\beta H) \sum_{m=1}^{\infty} [\Lambda^{-1} \exp\{\beta(J + H)\}]^{m} \exp(-\beta \eta_{m}).$$
(4.2)

Here we see the first appearance of an infinite series which will occur repeatedly in the sequel, and which therefore merits a special notation:

$$\Omega(x,\beta) \equiv \sum_{m=1}^{\infty} x^m \exp(-\beta\eta_m)$$
(4.3)

certainly convergent for |x| < 1, and certainly divergent for |x| > 1. This is the analogue for this model of the *master function* of Fisher and Felderhof; its properties, in particular its convergence properties, determine the thermodynamics of the model. From (4.2) and (4.3)

$$p_{1}^{-} = p_{\infty}^{+} \Lambda^{-1} \exp\{\beta(J - H - \eta_{1})\} + p_{1}^{+} \exp(-2\beta H) \Omega(\Lambda^{-1} \exp\{\beta(J + H)\}, \beta).$$
(4.4)

By a similar route, (3.7) and (3.8) lead to

$$p_1^+ = p_{\infty}^- \Lambda^{-1} \exp\{\beta(J + H - \eta_1)\} + p_1^- \exp(2\beta H) \Omega(\Lambda^{-1} \exp\{\beta(J - H)\}, \beta).$$
(4.5)

These equations, when taken with equations (3.10) and (3.11) complete a set of four linear homogeneous equations for p_1^{\pm} and p_{∞}^{\pm} . In order that they possess a nontrivial solution, the eigenvalue A must satisfy a consistency condition, which may be written as

$$[1 - \Lambda^{-1} \exp\{\beta(J+H)\}][1 - \Lambda^{-1} \exp\{\beta(J-H)\}]\Delta(\Lambda; \beta, H) = 0$$
(4.6)

where we have put for convenience

$$\Delta(\Lambda;\beta,H) \equiv 1 - \Omega(\Lambda^{-1} \exp\{\beta(J+H)\},\beta)\Omega(\Lambda^{-1} \exp\{\beta(J-H)\},\beta).$$
(4.7)

In fact, one may show (though we shall not pursue this) that (4.6) is precisely the characteristic equation of T, that is

$$\det(I - \Lambda^{-1}T) = 0.$$

If T were a finite matrix, this would be enough. However, we are concerned here with an infinite matrix, and any Λ satisfying (4.6) is an eigenvalue only if the relevant convergence properties hold. In fact, (4.4) and (4.5) make sense only if both series converge; that is

$$\Omega(\Lambda^{-1} \exp\{\beta(J+H)\}, \beta) < \infty$$

$$\Omega(\Lambda^{-1} \exp\{\beta(J-H)\}, \beta) < \infty.$$
(4.8)

There are three factors in (4.6); we may thus expect that eigenvalues may appear in three different ways.

Firstly $\Lambda = \exp{\{\beta(J+H)\}}$ satisfies (4.6). The conditions (4.8) become

$$\Omega(1,\beta) < \infty$$
 $\Omega(\exp(-2\beta H),\beta) < \infty.$

We conclude

(i) If $\Omega(1, \beta)$ converges, and $H \ge 0$, $\Lambda = \exp\{\beta(J+H)\}$ is an eigenvalue.

A similar examination of $\Lambda = \exp\{\beta(J-H)\}$ gives

(ii) If $\Omega(1,\beta)$ converges, and $H \leq 0, \Lambda = \exp\{\beta(J-H)\}$ is an eigenvalue.

The remaining factor in (4.6) may also lead to eigenvalues; we search for those which are real and positive. In the range $0 \le x < 1$, $\Omega(x, \beta)$ is a convergent series of positive terms; its sum therefore increases monotonically with x from 0 (at x = 0) to either a finite value ω or to ∞ (at x = 1). Consequently, (4.7) shows that $\Delta(\Lambda; \beta, H)$ decreases monotonically from 1 as Λ^{-1} increases from 0, and may therefore exhibit not more than one zero. The condition for exactly one zero is that $\Delta(\Lambda; \beta, H) < 0$ when Λ^{-1} takes its largest value consistent with convergence. Thus we have

(iii) If $\Delta(\exp\{\beta(J+|H|)\}; \beta, H) < 0$, then there is a real eigenvalue Λ with $\exp\{\beta(J+|H|)\} < \Lambda < \infty$.

There are no other possibilities for real positive eigenvalues, though it is easy to construct models for which $\Delta = 0$ has complex roots.

It should be noted that there is always at least one real positive eigenvalue. If $\Omega(1, \beta)$ converges, then either (i) or (ii) applies; if $\Omega(1, \beta)$ diverges, then

$$\Delta(\exp\{\beta(J+|H|)\};\beta,H) \to -\infty$$

and (iii) applies. On the other hand, there may be as many as three such eigenvalues (two of them being a degenerate pair); the conditions for this, namely H = 0 and $1 < \Omega(1, \beta) < \infty$, are easily achieved in suitable models.

When more than one eigenvalue Λ exists, the thermodynamically correct one is always the largest, as might be expected. It is simple to verify that where more than one eigenvalue exists, all the *p* are positive only for the dominant eigenvalue; the others are thus ruled out on physical grounds. It follows that case (iii) always overrides cases (i) and (ii) when more than one case applies. When we take account of the dominant eigenvalue only, the cases (i-iii) may be characterized as follows:

(i) $p_{\infty}^+ \neq 0$, $p_{\infty}^- = 0$; every configuration of the ensemble contains an infinite (+) cluster (possibly with finite clusters to its right);

(ii) $p_{\infty}^+ = 0$, $p_{\infty}^- \neq 0$; every configuration of the ensemble contains an infinite (-) cluster;

(iii) $p_{\infty}^{+} = p_{\infty}^{-} = 0$; no configuration contains an infinite cluster of either kind.

The usual Ising model is obtained with $\eta_m = 2J$, for all m. In this case Ω may be summed in closed form

$$\Omega(x,\beta) = \exp(-2\beta J)x(1-x)^{-1} \qquad \text{(Ising)} \tag{4.9}$$

and it is instructive to see where this leads. Only case (iii) can apply here, since $\Omega(1, \beta)$ diverges for any β . In the absence of a magnetic field (H = 0), (4.6) is satisfied by

$$\Omega(\Lambda^{-1} \exp(\beta J), \beta) = \pm 1$$

leading directly to

 $\Lambda = 2 \cosh \beta J \qquad \text{or} \qquad 2 \sinh \beta J.$

Apparently therefore T has two eigenvalues of familiar form. However, the value $2 \sinh \beta J$ is to be rejected, since in this case $\Lambda^{-1} \exp(\beta J) > 1$, and Ω diverges. Thus T

has in fact just one real eigenvalue $2 \cosh \beta J$, and no complex eigenvalues at all. It should be noted that any possibility of analytic continuation of $\Omega(x, \beta)$ beyond its circle of convergence |x| = 1 is quite irrelevant here.

5. The phase boundaries

Following from the discussion of §4 we may distinguish three types of region in the (β, H) plane:

- (a) regions where there exists an eigenvalue of type (iii) and where therefore there is no infinite cluster; we call these regions *paramagnetic*;
- (b) regions where there is no eigenvalue of type (iii), but where there is one of type (i); here there is an infinite (+) cluster ((+) ferromagnetic regions);
- (c) regions where there is no eigenvalue of type (iii), but where there is one of type (ii); there is then an infinite (-) cluster ((-) ferromagnetic regions).

The whole (β, H) plane (for $\beta > 0$) is accounted for by regions of one kind or another. In locating the different types of region, it is convenient first to consider what happens as H varies along lines of fixed β . There are three cases, depending on the convergence

of $\Omega(1, \beta)$.

Case I: β is such that $\Omega(1, \beta)$ does not converge. Then whatever the value of H, there is an eigenvalue of type (iii), and the ordinate at β lies entirely in a paramagnetic region.

Case II: β is such that $\Omega(1, \beta)$ converges to $\omega > 1$. To fix ideas take H > 0, and note that

(a) $\Delta(\exp{\{\beta(J+H)\}}; \beta, H) = 1 - \omega \Omega(\exp(-2\beta H), \beta)$ is monotonic with H;

(b) $\Delta = 1 - \omega^2 < 0$ when H = 0;

(c) $\Delta \rightarrow +1$ as $H \rightarrow \infty$.

It follows that for small enough H there is an eigenvalue of type (iii), and for large enough H there is not. Thus we may conclude that as H varies, regions of all three types are encountered by the ordinate at β . The boundaries are defined by

$$\Delta(\exp\{\beta(J+|H|);\beta,H)=0.$$

Case III: β is such that $\Omega(1, \beta)$ converges to $\omega < 1$. This differs from case II only in that $\Delta = 1 - \omega^2 > 0$; this means that the ordinate at β meets only ferromagnetic regions. The boundary between the regions is H = 0.

It follows from these considerations that in order to draw the phase diagram it is sufficient to understand the convergence properties of $\Omega(1, \beta)$ as β varies. To this end, suppose that β_0^{-1} is the least upper bound of α for which K can be found with

$$\exp(-\eta_m) < \frac{K}{m^{\alpha}}$$
 for all m. (5.1)

Then a simple comparison of series shows that $\Omega(1, \beta)$ converges or diverges according as $\beta > \beta_0$ or $\beta \le \beta_0$. (Of course, β_0 may not exist; in such an event Ω converges or diverges everywhere.) In passing we remark that the most singular part of Ω (in the sense of Fisher 1967b p623) can be found by the same series comparison:

$$\Omega(x,\beta) \sim (1-x)^{(\beta/\beta_0)-1}$$
 as $x \to 1-$. (5.2)

This will be used in §6.

There are several possibilities:

(i) $\Omega(1,\beta)$ may diverge for all β (eg η_m = constant, independent of *m*). For all β , case I applies, the entire (β, H) plane is a single paramagnetic region, and there is no phase transition.

(ii) $\Omega(1,\beta)$ may converge for all $\beta > 0$ (example $\eta_m = m^{1/2}$). Cases II or III apply for all $\beta > 0$; that is, a phase change is possible at any temperature.

(iii) $\Omega(1,\beta)$ may converge only for $\beta > \beta_0$ (eg $\eta_m = \ln m$, $\beta_0 = 1$). Phase changes are possible for $\beta > \beta_0$; that is, for low enough temperatures.

We consider possibility (iii) in more detail; the relevant phase diagrams are sketched in figure 1(b). Since

$$\Omega(1,\beta) = \sum \exp(-\beta\eta_m)$$

is a series of positive terms

$$\Omega(1,\beta) > 0 \qquad \text{for all } \beta > \beta_0$$

and

$$\lim_{\beta\to\beta_0^+}\Omega(1,\beta)=\infty.$$

Since

$$\frac{\mathrm{d}^2 \Omega(1,\beta)}{\mathrm{d}\beta^2} = \sum \eta_m^2 \exp(-\beta \eta_m) > 0 \qquad \text{for all } \beta > \beta_0$$



Figure 1. (a) Typical possibilities for the form of $\Omega(1, \beta)$. (b) The corresponding typical possibilities for the phase boundaries in the (β, H) plane.

 $\Omega(1,\beta)$ is convex downwards. Finally, as $\beta \to \infty$

$$\begin{split} \Omega(1,\beta) &\to 0 & \text{if all } \eta_m > 0 \\ \Omega(1,\beta) &\to n & \text{if } \eta_m = 0 \text{ for } n \text{ values of } m \\ \eta_m > 0 \text{ otherwise} \\ \Omega(1,\beta) &\to \infty & \text{if any } \eta_m < 0. \end{split}$$

Some typical graphs of Ω are sketched in figure 1(a) to cover all qualitative behaviour.

Possibility (ii) is similar, except that now case I does not occur, the asymptote $\beta = \beta_0$ moving to the remote right of the diagrams.

6. The nature of the phase changes

It is of interest to examine the properties of the model at the phase boundaries. At a boundary common to two ferromagnetic regions the situation is clear: as H changes sign, the magnetization changes discontinuously and the transition is first order.

The behaviour at the boundary of a paramagnetic region is more complicated. Assume for convenience H > 0. On the ferromagnetic side, $\Lambda = \exp\{\beta(J+H)\}$, and $x \equiv \Lambda^{-1} \exp\{\beta(J+H)\} = 1$; thus all derivatives of x on the ferromagnetic side are zero. This suggests that it will be useful to examine the derivatives of x as (β, H) approaches the boundary from the paramagnetic side.

In the paramagnetic region, x satisfies

$$\Delta(x^{-1}\exp\{\beta(J+H)\};\beta,H) \equiv 1 - \Omega(x,\beta)\Omega(x\exp(-2\beta H),\beta) = 0$$
(6.1)

by (3.14). On the boundary x = 1 and $x \exp(-2\beta H)$ lies inside the circle of convergence of Ω . Thus the singular behaviour of the derivatives of x is determined by the singular behaviour of $\Omega(x, \beta)$ at x = 1 -, and this was indicated at (5.2).

We shall consider derivatives with respect to H (at constant β). Differentiating (6.1) once gives

$$\Omega'(x,\beta)\Omega(x\exp(-2\beta H),\beta)\frac{\partial x}{\partial H} + \Omega(x,\beta)\Omega'(x\exp(-2\beta H),\beta)\left(\frac{\partial x}{\partial H} - 2\beta x\right)\exp(-2\beta H) = 0$$
(6.2)

where

$$\Omega'(x,\beta) \equiv \frac{\partial \Omega(x,\beta)}{\partial x} \sim (1-x)^{(\beta/\beta_0)-2} \qquad \text{as } x \to 1-.$$
(6.3)

First suppose that $\beta_0 < \beta < 2\beta_0$; then by (5.2) and (6.3), $\Omega(1, \beta)$ converges and $\Omega'(1, \beta)$ diverges. Solving (6.2) then shows that $\partial x/\partial H \to 0$ as $x \to 1-$; in fact

$$\frac{\partial x}{\partial H} \sim (1-x)^{2-\beta/\beta_0}.$$

Integrating in the neighbourhood of H_0 – gives

$$(1-x) \sim (H_0 - H)^{\beta_0/(\beta - \beta_0)}$$

hence

$$\frac{\partial x}{\partial H} \sim (H_0 - H)^{-1 + \beta_0/(\beta - \beta_0)}.$$
(6.4)

More generally

$$\frac{\partial^n x}{\partial H^n} \sim (H_0 - H)^{-n + \beta_0 / (\beta - \beta_0)} \qquad \text{as } H \to H_0^-$$

In consequence, when β lies in the range

$$\frac{n+2}{n+1}\beta_0 < \beta < \frac{n+1}{n}\beta_0$$

exactly *n* derivatives of x are zero at $H = H_0$ (and therefore continuous over the boundary), while all the rest diverge on the paramagnetic side. Thus the 'order' of the transition increases indefinitely as $\beta \rightarrow \beta_0 + .$

Whether or not there are parts of the paramagnetic boundary for which $\beta > 2\beta_0$ clearly depends on the location of the triple point, if there is one. If such parts do exist, both Ω and Ω' converge there, and solving (6.2) gives a finite nonzero value for $\partial x/\partial H$ on the paramagnetic side, and consequently a discontinuity over the boundary, that is, the transition is then first order.

An interesting feature of the model is the fact that throughout either ferromagnetic region Λ is analytic in both β and H, and may be continued analytically beyond the boundary with the paramagnetic region. Moreover, all other quantities, such as p_{∞}^+ , p_n^{\pm} behave smoothly as the boundary into the paramagnetic region is crossed. It might be supposed that this implies some kind of metastability; this is not so, since outside a ferromagnetic region p_1^- and p_{∞}^+ have opposite signs, in conflict with their physical meaning. The phase transition from the ferromagnetic side comes about not on account of any mathematical singularity, but on account of a breakdown in the physical interpretation of the formalism.

It may be asked what light is thrown by the one dimensional cluster model on the critical behaviour of the Ising model in higher dimensions. The answer must be: not much. The phase diagrams are clearly very different; in particular, the fundamental result of Lee and Yang (1952) that for the Ising ferromagnet in nonzero field the thermodynamic functions are nowhere singular is certainly not true of the cluster model. Moreover, the phase boundary in the Ising ferromagnet terminates at a finite point in the (β, H) plane, and does not divide the plane into separate regions with distinct mathematical regimes. There is no such boundary in the case of the cluster model.

7. Surface properties

In models where the transfer-matrix method may be applied, the dominant eigenvalue leads to the bulk properties of the system. If the corresponding eigenvector is available, the surface properties are easily obtained (cf Lassettre and Howe 1941).

We assume that the limit

$$\lim_{N \to \infty} \frac{\Lambda_N(\beta, H)}{\Lambda^N} \equiv (\lambda(\beta, H))^2$$
(7.1)

exists and is not zero. (It will be seen that this is so at any point within the paramagnetic region of the phase diagram.) Then for large N we may write

$$\Lambda_N \sim \lambda \Lambda^N \lambda$$

that is λ may be regarded as a surface correction for a long chain: there is a factor λ for each of the two ends. From (7.1) there follows

$$\lim_{\substack{M \to \infty \\ N \to \infty}} \frac{\Lambda_{M+N}}{\Lambda_M \Lambda_N} = \lambda^{-2}.$$
(7.2)

In the paramagnetic region, the left side may be expressed in terms of the eigenvector of T. Firstly, Λ_{M+N} may be regarded as the partition function for two chains (of M and N spins) linked by one further bond. If we now group the configurations contributing to Λ_{M+N} according to the clusters on either side of this bond, we have

$$\Lambda_{M+N} = \sum_{m,n} \left(\Lambda_M(m+)\Lambda_N(n+) + \Lambda_M(m-)\Lambda_N(n-) \right) \exp\{-\beta(\eta_{m+n} - \eta_m - \eta_n)\} + \sum_{m,n} \left(\Lambda_M(m-)\Lambda_N(n+) + \Lambda_M(m+)\Lambda_N(n-) \right)$$

the Boltzmann correction in the first sum is necessary, since, for example, if the clusters adjacent to the bond are (m+) and (n+) respectively, they form in reality a single (m+n+) cluster. Using (7.2), (3.1) and (3.2) gives in the limit

$$\lambda^{-2} = \sum_{\substack{m=1\\n=1}}^{\infty} \left[(p_m^+ p_n^+ + p_m^- p_n^-) \exp\{-\beta(\eta_{m+n} - \eta_m - \eta_n)\} + (p_m^+ p_n^- + p_n^+ p_m^-) \right].$$
(7.3)

This is the required result.

To go further, we may determine the p from the work of § 3, taken with the normalizing condition $\Sigma(p_n^+ + p_n^-) = 1$; substituting in (7.3) gives, after considerable rearrangement

$$\lambda^{-2} = \frac{\Lambda^{-1} \exp\{\beta(J+H)\}\Omega'(\Lambda^{-1} \exp\{\beta(J+H)\}, \beta)}{\{1 + \Omega(\Lambda^{-1} \exp\{\beta(J+H)\}, \beta)\}^2} + \text{similar expression with } H \text{ replaced by } -H$$
(7.4)

where Λ is as before the bulk partition function per spin. As in the case of the bulk properties, the surface properties are completely determined by the behaviour of the master function Ω . The singularities in a paramagnetic neighbourhood of a boundary may now be investigated as in § 6.

For the Ising model, Ω is given by (4.9) and then (7.4) leads directly to

$$(\lambda(\beta, 0))^{-2} = \exp(\beta J) \cosh \beta J \qquad (H = 0)$$

and hence by (7.1)

$$\Lambda_N(\beta, 0) \sim (2 \cosh \beta J)^N \{ \exp(\beta J) \cosh \beta J \}^{-1}$$

for large N. In fact, the Ising model is special in that Λ_N is given exactly by this expression for every N.

Similar techniques may be applied in the ferromagnetic regions, though the development is complicated by the need to reckon with the infinite cluster.

References

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