

Domain Structure in a Second-Neighbour Ising Chain

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Two different methods of obtaining the partition function for a spin $\frac{1}{2}$ open ended Ising chain with interactions between nearest and second nearest neighbour spins are presented. These are non-matrix methods, in that they do not require the diagonalization of a transfer matrix, and they provide a useful representation for studying the analytical structure of the partition function. The pair correlation functions are also derived, using the second of these methods. These correlation functions are utilized in a study of the ground state and the finite temperature spin configurations. An interesting application of these results to the problem of out-of-phase domain structure in binary alloys is discussed.

§ 1. Introduction

The Ising chain is of interest in statistical mechanics because it can be solved exactly and because it can be incorporated into some interesting problems of statistical physics. This paper presents exact solutions for the partition function and pair correlation functions of a spin $\frac{1}{2}$ Ising chain with both nearest and second nearest neighbour interactions. The motivation for this work was two-fold in nature.

Firstly, within a statistical mechanical context, it was our desire to obtain methods of solving for the partition function and pair correlation functions of an open ended*) spin $\frac{1}{2}$ chain of any length which did not rely upon the standard matrix technique. The nearest neighbour Ising chain has so simple a solution that in order to learn how to achieve this goal it is necessary to study a chain with more than nearest neighbour interactions. Section 2 presents an inductive, non-matrix method of solving for the partition function. There we present a series representation which generates the appropriate polynomial solution for a chain of arbitrary length. With this series representation we are able to see the analytical structure of the partition function. Such transparency is not directly displayed by the matrix method which has been used in the past^{1),2)} to calculate the partition function.

Section 3 describes a second method. We present a difference equation for the partition function and readily solve it to obtain a result in agreement with that of § 2. In § 4 we calculate the pair correlation functions of Ising chain; these results are new and are obtained using the difference equation method in-

*) An open ended Ising chain is one in which periodic boundary conditions are not imposed: the chain begins with site 1 and ends with site N .

introduced in § 3. An interesting isomorphism between the nearest neighbour spin $\frac{1}{2}$ Ising chain in an external magnetic field and this second neighbour chain can be derived and is discussed in Appendix A. Appendix B describes the extension of the techniques of § 3 to the third nearest neighbour Ising chain.

Secondly, we were interested in using our model to study some aspects of the problem of the formation of long period superlattices³⁾ in binary alloys. It is well known that an isomorphism exists between the Ising model and the binary alloy.⁴⁾ If the problem of a three dimensional binary alloy could be reduced to an effectively one dimensional model, then our results could be used to give some guide to the type of behaviour to be expected. Such a model has been proposed by Cowley and will be discussed in § 7. We have therefore used our formulae for the pair correlation functions to study, in § 5, the ground state spin configurations, and in § 6 the temperature dependence of the spin correlations. Section 7 contains a discussion of these results in the light of these motivating forces.

§ 2. Partition function—series method

Consider a one dimensional chain of N spins, where each spin $s_i = \pm 1$. We will assume that the only interactions present in the system are those between nearest neighbour and second nearest neighbour spins, the former having the form $-J_1 s_i s_{i+1}$ and the latter the form $-J_2 s_i s_{i+2}$. The Hamiltonian of the system is then

$$H_N = -J_1 \sum_{i=1}^{N-1} s_i s_{i+1} - J_2 \sum_{i=1}^{N-2} s_i s_{i+2}. \quad (1)$$

J_1 and J_2 are the interaction strengths—with our sign convention a positive interaction strength corresponds to a ferromagnetic interaction between spins. The partition function, Q_N , is the sum over all 2^N possible spin configurations of the function $\exp(-H_N/kT)$:

$$Q_N = \sum_{\{s_i\}} \exp(K_1 \sum_{i=1}^{N-1} s_i s_{i+1} + K_2 \sum_{i=1}^{N-2} s_i s_{i+2}), \quad K_i = J_i/kT.$$

Using the identity

$$\exp(Kss') = \cosh K \cdot (1 + ss' \cdot \tanh K)$$

we can rewrite the partition function as

$$Q_N = \cosh^{N-1} K_1 \cdot \cosh^{N-2} K_2 \cdot \sum_{\{s_i\}} \left\{ \prod_{i=1}^{N-1} (1 + \alpha s_i s_{i+1}) \cdot \prod_{i=1}^{N-2} (1 + \beta s_i s_{i+2}) \right\},$$

where $\alpha = \tanh K_1$ and $\beta = \tanh K_2$.

We introduce a new set of variables t_i , defined in terms of the s_i variables by the equations

$$t_0 = s_1; \quad t_i = s_i s_{i+1}, \quad i = 1, 2, \dots, N-1.$$

There is a one-to-one correspondence between the sets $\{s_i\}$ and $\{t_i\}$ because each s_i is uniquely expressible as a product of t_i :

$$s_1 = t_0; \quad s_i = t_0 t_1 \cdots t_{i-1}, \quad i > 1.$$

The partition function becomes

$$Q_N = 2^N \cosh^{N-1} K_1 \cdot \cosh^{N-2} K_2 \cdot Q_N, \quad (2)$$

where the function Q_N is defined in terms of the t_i as

$$Q_N = 2^{-N} \sum_{\{t_i\}} \left\{ \prod_{i=1}^{N-1} (1 + \alpha t_i) \cdot \prod_{i=1}^{N-2} (1 + \beta t_i t_{i+1}) \right\}. \quad (3)$$

We must now expand the products in (3) and sum over each of the t_i . It is obvious that, since each t_i can take the values $+1$ and -1 , the only terms of the expanded form of the product which contribute to (3) are those which are either independent of t_i or contain t_i twice (because $t_i^2 = 1$) for each value of i . The final expression for Q_N will be a polynomial in α and β whose first term is unity; our problem is to determine the coefficients of the remaining terms.

If N is small the problem of finding the polynomials is trivial: the first few are

$$Q_2 = 1, \quad Q_3 = 1 + \alpha^2 \beta, \quad Q_4 = 1 + 2\alpha^2 \beta + \alpha^2 \beta^2.$$

We continue this sequence until a definite pattern emerges. We are then able to write down the general form of Q_N :

$$Q_N = \sum_{m=0}^{(N-1)/2} \sum_{i=m}^{N-m-1} \binom{N-i-1}{m} \binom{i-1}{m-1} \alpha^{2m} \beta^i,$$

where $[x]$ denotes the greatest integer $\leq x$. Using the identity $\binom{L}{\lambda} = \binom{L}{L-\lambda}$ and relabelling, we obtain

$$Q_N = \sum_{m=0}^{(N-1)/2} \alpha^{2m} \beta^m \sum_{i=0}^{N-2m-1} \binom{N-i-m-1}{N-i-2m-1} \binom{i+m-1}{i} \beta^i.$$

Now since

$$(1-z)^{-p-1} = \sum_{r=0}^{\infty} \binom{p+r}{r} z^r,$$

the term

$$\sum_{i=0}^{N-2m-1} \binom{N-i-m-1}{N-i-2m-1} \binom{i+m-1}{i} \beta^i$$

is just the coefficients of z^{N-2m-1} in the power series expansion of

$$(1-\beta z)^{-m} (1-z)^{-m-1}.$$

This coefficient may also be expressed in the form of a contour integral

$$J_m(N, \beta) = \frac{1}{2\pi i} \oint_C \frac{dz}{z^{N-2m} (1-\beta z)^m (1-z)^{m+1}},$$

where the contour C encloses only the pole at the origin. Thus

$$Q_N = \sum_{m=0}^{[(N-1)/2]} \alpha^{2m} \beta^m J_m(N, \beta),$$

and if we reverse the order of summation and integration we find that

$$Q_N = \frac{1}{2\pi i} \oint_C \frac{dz}{z^N} \frac{1-\beta z - (\alpha^2 \beta z^2 / (1-z)) (\alpha^2 \beta z^2 / (1-\beta z) (1-z))^{[(N-1)/2]}}{(1-\beta z) (1-z) - \alpha^2 \beta z^2}.$$

The third term of the numerator makes no contribution to the value of Q_N ; we can then evaluate Q_N by expanding the remainder of the integrand in terms of partial fractions. Let

$$a = \beta + 1, \quad b = \{(\beta - 1)^2 + 4\alpha^2 \beta\}^{1/2},$$

the final result is then

$$Q_N = \frac{1}{b} \left\{ \left(1 - \frac{a-b}{2}\right) \left(\frac{a+b}{2}\right)^{N-1} - \left(1 - \frac{a+b}{2}\right) \left(\frac{a-b}{2}\right)^{N-1} \right\}. \tag{4}$$

As $N \rightarrow \infty$, $\{(a-b)/(a+b)\}^N \rightarrow 0$, so that in the thermodynamic limit

$$Q_N \sim \frac{1}{b} \left(1 - \frac{a-b}{2}\right) \left(\frac{a+b}{2}\right)^{N-1}.$$

The partition function of the infinite chain is therefore

$$\begin{aligned} \ln Q &= \lim_{N \rightarrow \infty} (N^{-1} \ln Q_N) \\ &= K_2 + \ln \{ \cosh K_1 + (\cosh^2 K_1 - 2e^{-2K_2} \sinh 2K_2)^{1/2} \}. \end{aligned} \tag{5}$$

By applying the binomial theorem to (4) we obtain a more useful form of Q_N :

$$Q_N = \left(\frac{a}{2}\right)^{N-1} \left\{ \sum_{r=0}^{(N-1)/2} \binom{N}{2r+1} \left(\frac{b^2}{a^2}\right)^r - 2 \left(1 - \frac{1}{a}\right) \sum_{r=0}^{(N-2)/2} \binom{N-1}{2r+1} \left(\frac{b^2}{a^2}\right)^r \right\}. \tag{6}$$

This result will be used when we later require an expression for Q_N where α is replaced by its reciprocal, in which case b is imaginary.

§ 3. Partition function—difference equation method

In order to obtain a recurrence relation for Q_N we separate out the first term of each of the products in (3):

$$Q_N = 2^{-N} \sum_{\{t_i\}} \{ (1 + \alpha t_1) (1 + \beta t_1 t_2) \prod_{i=2}^{N-1} (1 + \alpha t_i) \cdot \prod_{i=2}^{N-2} (1 + \beta t_i t_{i+1}) \}$$

$$\begin{aligned}
&= 2^{-N} \sum_{\{t_i\}} \left\{ \prod_{i=2}^{N-1} (1 + \alpha t_i) \cdot \prod_{i=2}^{N-2} (1 + \beta t_i t_{i+1}) \right\} \\
&\quad + \alpha 2^{-N} \sum_{\{t_i\}} \left\{ t_1 \prod_{i=2}^{N-1} (1 + \alpha t_i) \cdot \prod_{i=2}^{N-2} (1 + \beta t_i t_{i+1}) \right\} \\
&\quad + \alpha \beta 2^{-N} \sum_{\{t_i\}} \left\{ t_2 \prod_{i=2}^{N-1} (1 + \alpha t_i) \cdot \prod_{i=2}^{N-2} (1 + \beta t_i t_{i+1}) \right\} \\
&\quad + \beta 2^{-N} \sum_{\{t_i\}} \left\{ t_1 t_2 \prod_{i=2}^{N-1} (1 + \alpha t_i) \cdot \prod_{i=2}^{N-2} (1 + \beta t_i t_{i+1}) \right\}. \tag{7}
\end{aligned}$$

We introduce a function X_N , defined as

$$X_N = 2^{-N} \sum_{\{t_i\}} \left\{ t_1 \prod_{i=1}^{N-1} (1 + \alpha t_i) \cdot \prod_{i=1}^{N-2} (1 + \beta t_i t_{i+1}) \right\}.$$

The second and fourth terms of (7) are zero because they contain an unpaired t_1 ; if the indices of the remaining two terms are reduced by one we obtain the result

$$Q_N = Q_{N-1} + \alpha \beta X_{N-1}. \tag{8}$$

Similarly,

$$X_N = \alpha Q_{N-1} + \beta X_{N-1}. \tag{9}$$

In (8) and (9) we have a pair of simultaneous linear difference equations. To solve for Q_N we introduce the operator E having the property that $Ef(N) = f(N+1)$. X_N can be eliminated between the two equations, the resulting second order difference equation is

$$\{E^2 - (\beta + 1)E + \beta(1 - \alpha^2)\} Q_N = 0. \tag{10}$$

The solution to (10) can be written down immediately, it is

$$Q_N = A \lambda_+^N + B \lambda_-^N,$$

where

$$\lambda_{\pm} = \frac{1}{2} \{ \beta + 1 \pm [(\beta - 1)^2 + 4\alpha^2 \beta]^{1/2} \}$$

and A, B are constants which depend on the boundary conditions—in this case the expressions for Q_2 and Q_3 which were obtained earlier. Finally

$$Q_N = [(\beta - 1)^2 + 4\alpha^2 \beta]^{-1/2} [\lambda_+^N - \lambda_-^N - \beta(\lambda_+^{N-1} - \lambda_-^{N-1})];$$

it is a simple matter to show that this reduces to (4), the result obtained from the series method.

§ 4. The spin correlation functions

The correlation between the spins s_i and s_{i+r} on a chain of length N is defined as

$$\mathcal{S}_{s_l s_{l+r}}^N = Q_N^{-1} \sum_{\{s_i\}} s_l s_{l+r} \exp(K_1 \sum_{i=1}^{N-1} s_i s_{i+1} + K_2 \sum_{i=1}^{N-2} s_i s_{i+2}) \tag{11}$$

in the notation of § 2. Equivalently,

$$\begin{aligned} Q_N \mathcal{S}_{s_l s_{l+r}}^N &= 2^{-N} \sum_{\{t_i\}} \left\{ \sum_{i=l}^{l+r-1} t_i \cdot \prod_{i=1}^{N-1} (1 + \alpha t_i) \cdot \prod_{i=1}^{N-2} (1 + \beta t_i t_{i+1}) \right\} \\ &= 2^{-N} \sum_{\{t_i\}} \left\{ \left[\prod_{i=1}^{l-1} (1 + \alpha t_i) \cdot \prod_{i=1}^{l-2} (1 + \beta t_i t_{i+1}) \right] \cdot (1 + \beta t_{l-1} t_l) \right. \\ &\quad \times \left[\prod_{i=l}^{l+r-1} t_i (1 + \alpha t_i) \cdot \prod_{i=l}^{l+r-2} (1 + \beta t_i t_{i+1}) \right] \cdot (1 + \beta t_{l+r-1} t_{l+r}) \\ &\quad \left. \times \left[\prod_{i=l+r}^{N-1} (1 + \alpha t_i) \cdot \prod_{i=l+r}^{N-2} (1 + \beta t_i t_{i+1}) \right] \right\}; \tag{12} \end{aligned}$$

should the lower limit of any of the products in (12) exceed the upper limit then that product is replaced by unity. (By definition $\mathcal{S}_{s_1 s_2}^1 = 0$.) Since

$$t_i (1 + \alpha t_i) = \alpha \left(1 + \frac{1}{\alpha} t_i \right)$$

we find that (12) can be expressed as

$$\begin{aligned} Q_N \mathcal{S}_{s_l s_{l+r}}^N &= \alpha^r Q_l Q_{r+1} \left(\frac{1}{\alpha} \right) Q_{N+1-l-r} \left[1 + \beta \mathcal{S}_{s_1 s_2}^l \mathcal{S}_{s_1 s_2}^{r+1} \left(\frac{1}{\alpha} \right) \right. \\ &\quad \left. + \beta \mathcal{S}_{s_1 s_2}^{r+1} \left(\frac{1}{\alpha} \right) \mathcal{S}_{s_1 s_2}^{N+1-l-r} + \beta^2 \mathcal{S}_{s_1 s_2}^l \mathcal{S}_{s_1 s_2 s_r s_{r+1}}^{r+1} \left(\frac{1}{\alpha} \right) \mathcal{S}_{s_1 s_2}^{N+1-l-r} \right], \tag{13} \end{aligned}$$

where we have defined the four spin correlation function $\mathcal{S}_{s_1 s_2 s_r s_{r+1}}^{r+1}$ as the obvious generalization of (11). (Note that $\mathcal{S}_{s_1 s_2 s_1 s_2}^2 = 1$ and $\mathcal{S}_{s_1 s_2 s_2 s_3}^3 = \mathcal{S}_{s_1 s_3}^3$.) The correlation functions and the Q_M are polynomials in α and β , except where the arguments of these functions are given explicitly as $1/\alpha$, in which case each α in the polynomial is replaced by its reciprocal—as an example

$$Q_3 \left(\frac{1}{\alpha} \right) = 1 + \frac{1}{\alpha^2} \beta.$$

Treating Q_N itself in the same way we obtain

$$\begin{aligned} Q_N &= Q_l Q_{r+1} Q_{N+1-l-r} \left[1 + \beta \mathcal{S}_{s_1 s_2}^l \mathcal{S}_{s_1 s_2}^{r+1} \right. \\ &\quad \left. + \beta \mathcal{S}_{s_1 s_2}^{r+1} \mathcal{S}_{s_1 s_2}^{N+1-l-r} + \beta^2 \mathcal{S}_{s_1 s_2}^l \mathcal{S}_{s_1 s_2 s_r s_{r+1}}^{r+1} \mathcal{S}_{s_1 s_2}^{N+1-l-r} \right]. \tag{14} \end{aligned}$$

$\mathcal{S}_{s_l s_{l+r}}^N$ is then found by dividing (13) by (14).

For the special case $l=r=1$,

$$\mathcal{S}_{s_1 s_2}^N = \frac{\alpha + \beta \mathcal{S}_{s_1 s_2}^{N-1}}{1 + \alpha \beta \mathcal{S}_{s_1 s_2}^{N-1}}$$

since $Q_2 = 1$ and $\mathcal{S}_{s_1 s_2}^2 = \alpha$. We let $N \rightarrow \infty$ and define the quantity x as

$$x = \lim_{N \rightarrow \infty} \mathcal{S}_{s_1 s_2}^N,$$

then x satisfies the equation

$$x = \frac{\alpha + \beta x}{1 + \alpha \beta x}$$

whose solution is

$$x = \frac{\beta - 1 + [(\beta - 1)^2 + 4\alpha^2\beta]^{1/2}}{2\alpha\beta} \quad (15)$$

(the second solution is unphysical).

We now consider the general case and let $N \rightarrow \infty$ —replacing $\mathcal{S}_{s_1 s_2}^N$ by x ,

$$\begin{aligned} \langle s_l s_{l+r} \rangle &= \lim_{N \rightarrow \infty} \mathcal{S}_{s_l s_{l+r}}^N \\ &= a^r \frac{Q_{r+1}(1/\alpha)}{Q_{r+1}} \left[\frac{1 + \beta \mathcal{S}_{s_1 s_2}^{r+1}(1/\alpha) \cdot (x + \mathcal{S}_{s_1 s_2}^l) + \beta^2 x \mathcal{S}_{s_1 s_2 s_r s_{r+1}}^{r+1}(1/\alpha)}{1 + \beta \mathcal{S}_{s_1 s_2}^{r+1} \cdot (x + \mathcal{S}_{s_1 s_2}^l) + \beta^2 x \mathcal{S}_{s_1 s_2 s_r s_{r+1}}^{r+1}} \right]. \end{aligned} \quad (16)$$

The four-spin correlation function may be expanded in a form similar to (12) and expressed in terms of the partition function and the correlation functions of a shorter chain:

$$Q_{r+1} \mathcal{S}_{s_1 s_2 s_r s_{r+1}}^{r+1} = \alpha^2 Q_{r-1} + 2\alpha\beta Q_{r-1} \mathcal{S}_{s_1 s_2}^{r-1} + \beta^2 Q_{r-1} \mathcal{S}_{s_1 s_2 s_{r-2} s_{r-1}}^{r-1}.$$

Also

$$Q_{r+1} = Q_{r-1} + 2\alpha\beta Q_{r-1} \mathcal{S}_{s_1 s_2}^{r-1} + \alpha^2 \beta^2 Q_{r-1} \mathcal{S}_{s_1 s_2 s_{r-2} s_{r-1}}^{r-1};$$

hence

$$Q_{r+1} \mathcal{S}_{s_1 s_2 s_r s_{r+1}}^{r+1} = \frac{1}{\alpha^2} Q_{r+1} + \left(\alpha^2 - \frac{1}{\alpha^2} \right) Q_{r-1} + 2\beta \left(\alpha - \frac{1}{\alpha} \right) Q_{r-1} \mathcal{S}_{s_1 s_2}^{r-1},$$

where $r \geq 3$. We eliminate $\mathcal{S}_{s_1 s_2}^{r-1}$ by using (9) (from the definitions, $X_M \equiv \mathcal{S}_{s_1 s_2}^M$) and obtain

$$Q_{r+1} \mathcal{S}_{s_1 s_2 s_r s_{r+1}}^{r+1} = \frac{1}{\alpha^2} Q_{r+1} + 2 \left(1 - \frac{1}{\alpha^2} \right) Q_r + \left(\alpha - \frac{1}{\alpha} \right)^2 Q_{r-1}. \quad (17)$$

Considering (16) we see that the spin index l appears only in the correlation function $\mathcal{S}_{s_1 s_2}^l$. It might be argued that by taking the limit $l \rightarrow \infty$ and replacing $\mathcal{S}_{s_1 s_2}^l$ by x we would obtain the correlation function for two spins both of which are an infinite distance from the ends of the chain. This is in fact the case when both nearest and second nearest neighbour interactions are ferromagnetic (J_1 and $J_2 > 0$), but if either (or both) are antiferromagnetic there is a tendency, as we shall soon see, for sublattices to appear for certain ranges of J_1 and J_2 , and the index l must be retained in order to indicate which particular sublattice is being considered.

§ 5. Ground state configurations

The four possible zero temperature configurations are shown in Fig. 1. States I and IV are strictly equivalent, differing only in the location of the domain boundaries relative to one end of the chain. Neglecting end effects, the ground state energies are

$$E_{\text{I}}^0 = E_{\text{IV}}^0 = 2J_2,$$

$$E_{\text{II}}^0 = -2J_1 - 2J_2,$$

$$E_{\text{III}}^0 = 2J_1 - 2J_2.$$

If $J_2 > -\frac{1}{2}|J_1|$, states II and III are stable for $J_1 > 0$ and $J_1 < 0$ respectively. If $J_2 < -\frac{1}{2}|J_1|$, states I and IV are stable for $J_1 > 0$ and $J_1 < 0$ respectively; the choice of state in this case depends only on the relative directions of the first two spins of the chain which, from a further simple energy argument, can be shown to depend only on the sign of J_1 . These results can be displayed on a phase diagram, Fig. 2, the J_1 - J_2 plane is divided into four regions, each corresponding to a different ground state configuration.

The $T=0$ behaviour may also be deduced from the limiting forms of the correlation functions. Rather than considering the general expressions for the correlation functions we will discuss three particular examples, and for simplicity we shall assume that $J_1 > 0$ and $J_2 < 0$. The expression for $\langle s_1 s_2 \rangle$ appears in (15) and from (16) we can obtain the expressions for the two other correlation functions we propose to consider, namely

$$\langle s_1 s_3 \rangle = \frac{\beta + \alpha x}{1 + \alpha \beta x}, \quad (18)$$

$$\langle s_2 s_3 \rangle = \frac{\alpha \beta + x}{1 + \alpha \beta x}. \quad (19)$$

For sufficiently small values of T , K_1 and K_2 are large, so

$$\alpha = \tanh K_1 \sim 1 - 2e^{-2K_1} + 2e^{-4K_1}, \quad K_1 > 0,$$

$$\beta = \tanh K_2 \sim -1 + 2e^{2K_2} - 2e^{4K_2}, \quad K_2 < 0.$$

Substituting these expansions into (15) we obtain to lowest order

$$\langle s_1 s_2 \rangle = 1 - 2e^{-K_1}, \quad J_2 > -\frac{1}{2}J_1,$$

$$1 - 4e^{4K_2}, \quad J_2 < -\frac{1}{2}J_1;$$

in both cases $\langle s_1 s_2 \rangle = 1$ at zero temperature. If we now use these expansions in the evaluation of the limits of (18) and (19) we see that to lowest order the numerators and denominators are zero. On retaining the higher order terms we find that at $T=0$,

$$\langle s_1 s_3 \rangle = \langle s_2 s_3 \rangle = 1, \quad J_2 > -\frac{1}{2}J_1,$$

$$\langle s_1 s_3 \rangle = \langle s_2 s_4 \rangle = -1, \quad J_2 < -\frac{1}{2} J_1.$$

These results agree with those reached earlier, and also with those of Obokata and Oguchi⁵⁾ which were obtained by taking the zero temperature limit of the expression for the energy of the system.

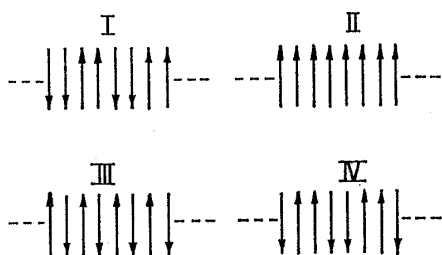


Fig. 1. The allowed ground state ($T=0^\circ\text{K}$) spin configurations.

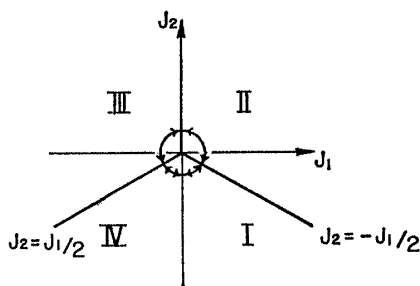


Fig. 2. The ground state phase diagram.

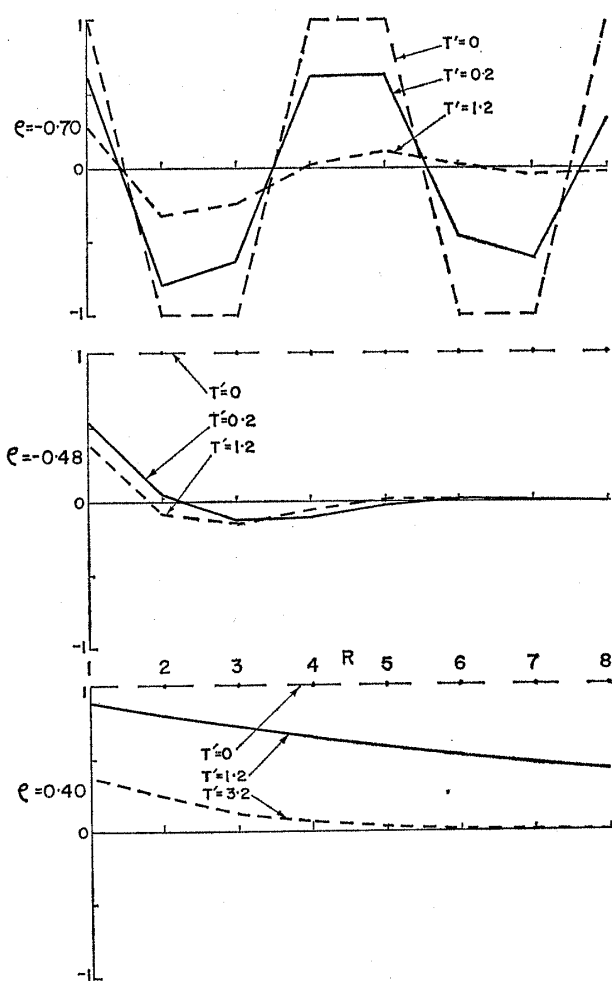


Fig. 3. The spin correlation function $\langle s_1 s_{1+R} \rangle$ for different values of the ratio $\rho (=J_2/|J_1|)$ and the temperature $T' (=kT/|J_1|)$. $J_1 > 0$.

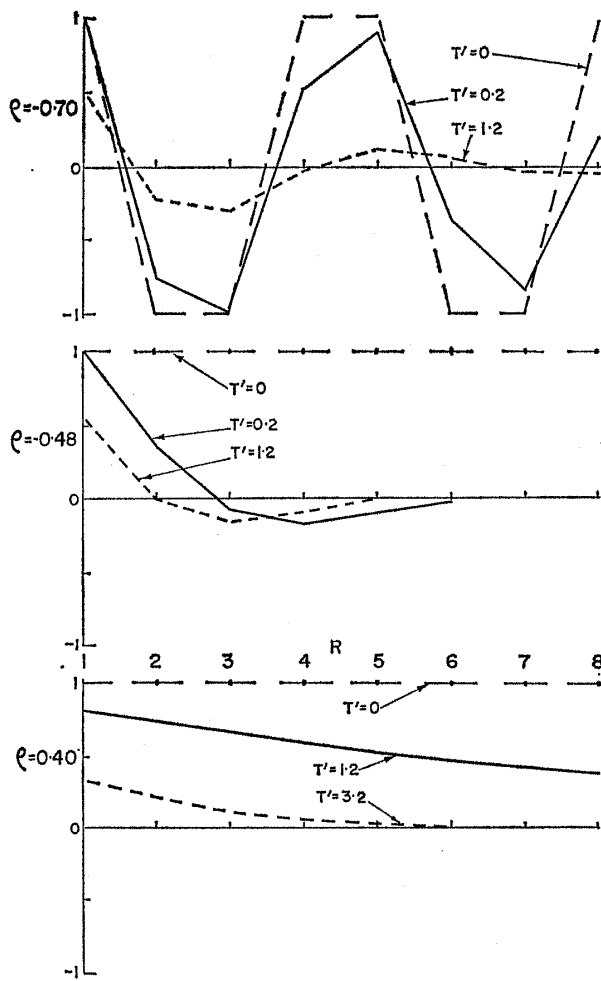


Fig. 4. The spin correlation function $\langle s_5 s_{5+R} \rangle$ for different values of the ratio $\rho (=J_2/|J_1|)$ and the temperature $T' (=kT/|J_1|)$. $J_1 > 0$.

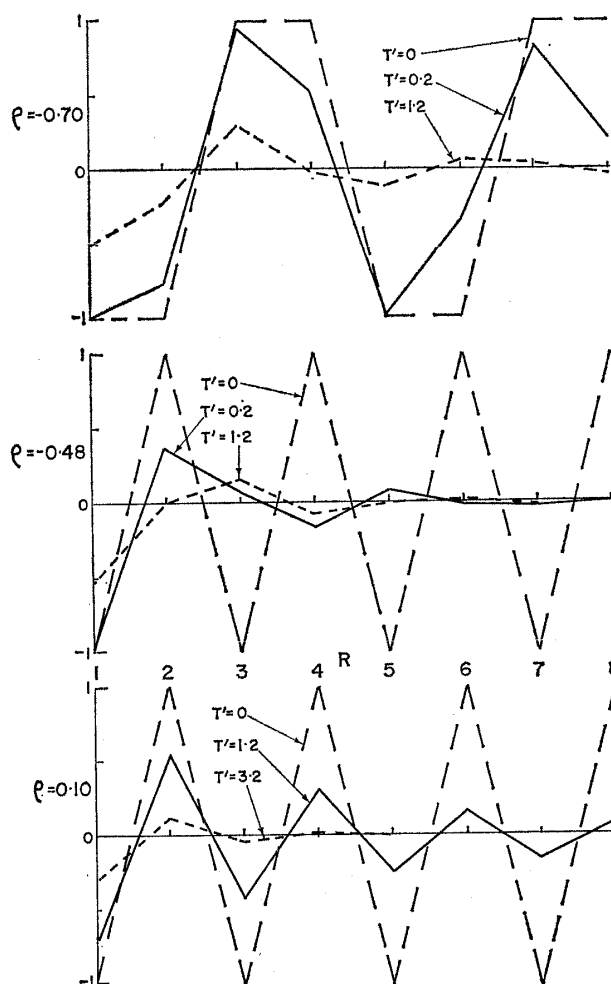


Fig. 5. The spin correlation function $\langle s_1 s_{1+R} \rangle$ for different values of the ratio $\rho (=J_2/|J_1|)$ and the temperature $T' (=kT/|J_1|)$. $J_1 < 0$.

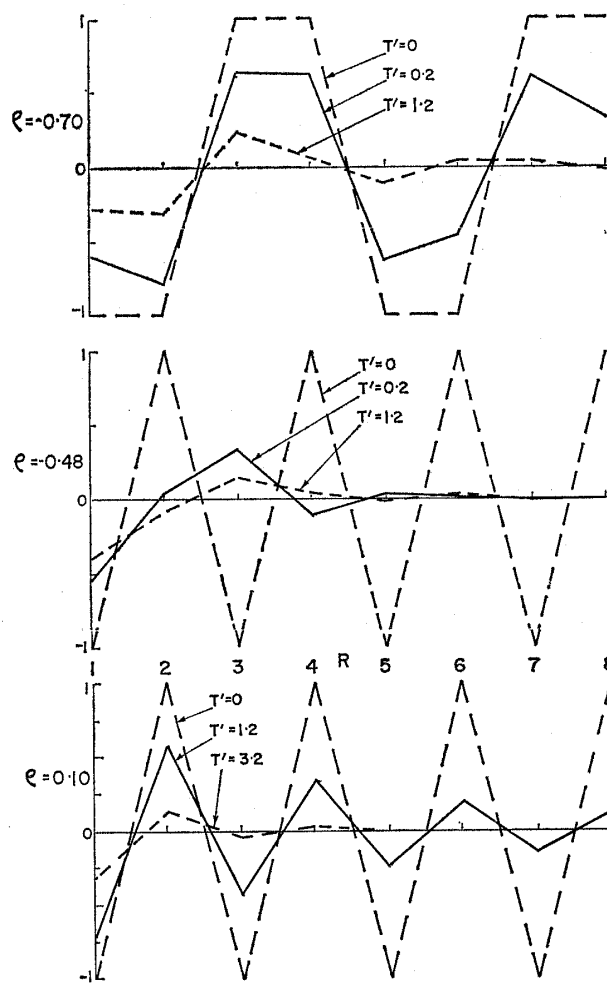


Fig. 6. The spin correlation function $\langle s_5 s_{5+R} \rangle$ for different values of the ratio $\rho (=J_2/|J_1|)$ and the temperature $T' (=kT/|J_1|)$. $J_1 < 0$.

§ 6. Numerical results

Using Eqs. (6), (15), (16) and (17), we have numerically evaluated the spin correlation function $\langle s_L s_{L+R} \rangle$ over a range of temperatures for both positive and negative J_1 and various values of the ratio $\rho = J_2/|J_1|$. In Figs. 3 to 6 we display the results obtained for $L=1$ and $L=5$; the graphs show how the correlation between spins varies with the distance, R , between them—for various values of the temperature $T' = kT/|J_1|$.

From the numerical results the general properties of the system may be deduced. When J_2 is positive the behaviour is qualitatively the same as the nearest neighbour Ising chain: the ground state is ferromagnetic if $J_1 > 0$ and anti-ferromagnetic if $J_1 < 0$. For $T > 0$ the correlations are all positive for $J_1 > 0$ and oscillate in sign for $J_1 < 0$. Should J_2 be negative, the behaviour will depend

on whether or not ρ exceeds $-\frac{1}{2}$. If $\rho > -\frac{1}{2}$ the ground state configuration is identical to that for $J_2 > 0$; as the temperature increases from zero some of the correlation functions change sign one or more times and, of course, eventually approach zero. On the other hand, if $\rho < -\frac{1}{2}$, the spins group in parallel pairs at $T=0$, with successive pairs antiparallel; depending on the sign of J_1 this configuration may correspond to either I or IV. This domain structure disappears for $T > 0$ and the signs of some of the correlation functions change—the behaviour at higher temperatures is similar to that of the previous case. Even though both positive and negative correlations exist for $T > 0$ there is no resemblance between them and the domain structure of the ground state; in fact when the temperature is greater than zero all spin sites are equivalent, apart from end effects—a result which follows from the absence of long-range order when $T > 0$.

As this calculation considers spins close to one end of an infinite chain we have been able to investigate the effects of the open boundary conditions. A comparison of the results for $L=1$ and $L=5$ will indicate the increased importance of end effects at lower temperatures (except, of course, $T=0$) and also that where the ground state is a simple ferro- or antiferromagnetic configuration the end effects are less pronounced than for the case in which spin pairing occurs; in each case however, the end effects decrease steadily as L increases.

The reason why, in general, L is not allowed to become infinite should by now be apparent. We have seen that for certain values of J_1 and J_2 domain structure exists at $T=0$. The correlation functions therefore oscillate between $+1$ and -1 as L changes. Hence no unique limit of $\langle s_L s_{L+R} \rangle$ exists (for general R) as $L \rightarrow \infty$ and the value of L (or at least its value modulo 2) must be retained.

Bitterlich and Jelitto⁶⁾ have made a numerical study of the two-dimensional model with second nearest neighbour interactions. They found that the system exhibited only a single phase transition, but there was a choice of three possible ordered ground states, depending on the ratio of the interaction strengths. Of the three ground states one was ferromagnetic and the other two were antiferromagnetic; their phase diagram was identical in form to the one given here. The ground state configurations of the three dimensional model are discussed by Clapp and Moss.⁷⁾

§ 7. Discussion

We have presented two different methods of solution for the partition function in §§ 2 and 3. These methods are non-matrix methods, in that they do not require the diagonalization of any matrix, but our final result agrees with that of the matrix methods, as it must. However, the series representation of the partition function in § 2 and the recurrence relation given in § 3 provide a direction in which to search for a new analytical representation of the problem.

In particular, it appears possible to use these results to establish the relationship between the solution of this and other Ising chains to the class of orthogonal and bi-orthogonal polynomials. With an analytical representation of these solutions in terms of known functions it should then be possible to obtain differential equations that the partition functions satisfy. While this is an ambitious undertaking, we are encouraged by preliminary results presently at hand to continue this line of study as well as to attempt to extend it to higher dimensional Ising models. The ultimate desire is that if the appropriate differential equations could be obtained, the analytical properties of the Ising model would then be more amenable to study. Work in this direction is presently underway.

The pair correlation functions derived in § 4 have been used in a study of the spin configurations as a function of temperature for all the values (both sign and magnitude) of the nearest and second nearest neighbour interaction strengths in §§ 5 and 6. It was pointed out in the introduction that these results could be used in studying an effectively one dimensional binary alloy problem. It is our intention to discuss this problem now.

The superlattice reflections in x-ray and electron diffraction patterns from certain ordered binary alloys below their critical temperatures show splittings, as do the diffuse maxima from certain disordered binary alloys above their critical temperatures. The splittings in the long-range ordered state of the alloy below the critical temperature are attributed to the presence of a long period superlattice composed of a periodic alternation of out-of-phase domains. The splittings in the disordered state above the critical temperature are attributed to the presence of finite but relatively large regions of the alloy where superlattice (out-of-phase) structure exists.⁹⁾ These are small ordered regions in the disordered structure which are a manifestation of the short-range order in the alloy above its critical temperature. This is particularly true as the critical temperature is approached from above in which case the amount of short-range order in the system increases. The separation of the split maxima is determined by the period of the domain structure.

Cowley⁹⁾ has proposed an interesting model of the binary alloy in order to interpret this phenomenon. He assumes that the alloy is composed of ordered planes of atoms, as in the ordered structure. This is certainly correct for the ordered state of the alloy, and the presence of a considerable amount of short-range order in the alloy near and above the critical temperature would indicate that it is a good approximation there as well. At an anti-phase domain boundary in the alloy there is a shift of the ordered planes by an amount equal to one half the face diagonal of a unit cell. An unshifted ordered plane will be called an *A*-centered ordered plane, and a shifted plane will be called a *B*-centered ordered plane. Thus Cowley visualizes the alloy as a one dimensional array of *A*- and *B*-centered ordered planes. There will be an interaction between the planes arising from the interactions between the atoms of the alloy.

If we denote an A -centered ordered plane by the spin up direction and a B -centered plane by the spin down direction, and assume there exists only nearest and second nearest neighbour planar interactions, then we have an isomorphism between the Cowley model and our Ising chain.

At this point it is important to stress that in the Cowley model the ordering of out-of-phase domains is a *separate* problem, involving weak, long-range energy terms (oscillatory potentials due to electron energies) from that of the in-plane ordering. The Cowley model requires first of all the solving of the ordering problem arising from short-range interactions. This gives a state of order in the usual sense. For Cu_3Au and other similar alloys this implies (both from approximate theory and experiment) out-of-phase boundaries parallel to 100 type planes—hence relative stability of planes of atoms perpendicular to cube axes. Now having established this over all state of order with antiphase boundaries, Cowley introduces long-range, weak oscillatory potentials to get ordering of anti-phase boundaries.*) This is the one dimensional problem which we are interested in here.

Although there will be no phase transition in this model because the second neighbour Ising chain has no phase transition, we expect the ground state of the Ising chain to correspond to that of the alloy. We would also expect that the temperature dependence of the spin configuration above $T=0^\circ\text{K}$ (the effective T_c for the Ising chain) would provide some indication of the type of ordered plane (domain) structure to be expected in the alloy above its critical temperature.

Thus, by studying the temperature dependence of the pair correlation functions of the Ising chain for different values of the interaction strengths, we can learn something about the ordered plane configurations. A configuration of all spins up (or equivalently, all spins down) corresponds to a configuration of all A -centred planes (all B -centred planes) and hence no out-of-phase domain structure. A periodic configuration of up and down spins corresponds to a periodic configuration of A - and B -centred ordered planes, and therefore represents a periodic out-of-phase domain structure for the binary alloy.

The spin configurations of the Ising chain were given in §§ 5 and 6; the results are displayed in Figs. 1 through 6. Depending on the magnitude and sign of the two interaction strengths, it is possible to find the following types of domain structure: (i) no out-of-phase domain structure at $T=0^\circ\text{K}$ but the presence of such structure at temperatures above zero; this corresponds to values of the interaction strengths in a portion of section II of the phase diagram; (ii) out-of-phase domain structure at both $T=0^\circ\text{K}$ and $T>0^\circ\text{K}$ —the different types of domain structure correspond to the sectors I, III and IV of the phase diagram. Accordingly, the presence or absence of splittings in the diffraction patterns would be determined by the values of the interaction strengths corresponding

*) Moss¹⁰⁾ has recently used the Friedel oscillatory potential to interpret the splitting of the diffuse spots from Cu-Au alloys above T_c .

to the appropriate sector of the phase diagram.

It is also interesting to contrast the domain structure which occurs at the ends of the chain with that which occurs within the chain. The difference can be clearly seen in Figs. 3 through 6. The spins (ordered planes) at the ends of the chain are more strongly ordered than those away from the ends. This is a manifestation of the end effects which occur in an open ended chain.

In short, we see that it is the competition between ferromagnetic and anti-ferromagnetic coupling which gives rise to the different types of domain structure. These results, however, should only be taken as instructive, as it is well known that forces of longer range play an important role in binary alloys. Nevertheless, Cowley's picture of the binary alloy makes for an interesting physical application of the analytical results presented in this paper.

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Appendix A

It is a simple matter to demonstrate that the solution to the nearest neighbour Ising problem in a magnetic field can be obtained from our results. The Hamiltonian of a chain of $N-1$ sites in a field B is

$$H'_{N-1} = -J \sum_{i=1}^{N-2} s_i s_{i+1} - \mu_0 B \sum_{i=1}^{N-1} s_i .$$

The partition function is then

$$Q'_{N-1} = \sum_{\{s_i\}} \exp(\beta J \sum_{i=1}^{N-2} s_i s_{i+1} + \beta \mu_0 B \sum_{i=1}^{N-1} s_i) .$$

If we replace βJ by our K_2 and $\beta \mu_0 B$ by our K_1 we see that

$$Q'_{N-1} = \frac{1}{2} Q_N ,$$

Q_N being the partition function of a chain of N sites with second nearest neighbour interactions. The spin correlation functions for the two systems are clearly identical in form if the same change of variable is made.

Appendix B

We can extend the difference equation method to the third neighbour problem. If $-J_3 s_i s_{i+3}$ is the interaction between spins s_i and s_{i+3} we modify the Hamiltonian in (1) by the addition of a term

$$-J_3 \sum_{i=1}^{N-3} s_i s_{i+3}.$$

The polynomial part of the partition function is then

$$Q_N = 2^{-N} \sum_{\{s_i\}} \{ (1 + \alpha s_1 s_2) (1 + \beta s_1 s_3) (1 + \gamma s_1 s_4) \cdot \prod_{i=2}^{N-1} (1 + \alpha s_i s_{i+1}) \\ \times \prod_{i=2}^{N-2} (1 + \beta s_i s_{i+2}) \cdot \prod_{i=2}^{N-3} (1 + \gamma s_i s_{i+3}) \},$$

where $\gamma = \tanh(\beta J_3)$ (no advantage is gained by expressing Q_N in terms of the t_i variables). We introduce the functions

$$X_N = Q_N \mathcal{S}_{s_1 s_2}^N, \quad Y_N = Q_N \mathcal{S}_{s_1 s_3}^N, \quad Z_N = Q_N \mathcal{S}_{s_2 s_3}^N,$$

where $\mathcal{S}_{s_i s_j}^N$ is the spin correlation function—

$$\mathcal{S}_{s_i s_j}^N = 2^{-N} \sum_{\{s_i\}} \{ s_i s_j \cdot \prod_{i=1}^{N-1} (1 + \alpha s_i s_{i+1}) \cdot \prod_{i=1}^{N-2} (1 + \beta s_i s_{i+2}) \cdot \prod_{i=1}^{N-3} (1 + \gamma s_i s_{i+3}) \},$$

and obtain a set of linear difference equations—

$$\begin{aligned} (1-E)Q_N + \alpha\beta X_N + \alpha\gamma Y_N + \beta\gamma Z_N &= 0, \\ \alpha Q_N + (\beta-E)X_N + \gamma Y_N + \alpha\beta\gamma Z_N &= 0, \\ \beta Q_N + \alpha X_N + (\alpha\beta\gamma-E)Y_N + \gamma Z_N &= 0, \\ \alpha\beta Q_N + X_N + \beta\gamma Y_N + (\alpha\gamma-E)Z_N &= 0. \end{aligned}$$

These reduce to a single fourth order difference equation

$$\begin{aligned} \{ E^4 - (\beta+1)(\alpha\gamma+1)E^3 + \beta(1-\alpha^2)(1-\gamma^2)E^2 \\ + \gamma(\alpha-\gamma)(1-\beta)(1-\alpha^2)(1-\beta^2)E + \gamma^2(1-\alpha^2)(1-\beta^2) \} Q_N = 0. \end{aligned}$$

We shall not proceed any further with the third nearest neighbour problem as it requires solving a quartic equation. In any case, the second nearest neighbour chain displays all the features in which we are interested; nothing essentially new is provided by the solution to the more difficult problem.

In conclusion we should point out that Fisher and Temperley⁹⁾ have discussed the second and third nearest neighbour problems. Their results are expressed in the form of algebraic equations but, whereas our equations are of second and fourth order for the second and third neighbour problems respectively, their equations are of fourth and eighth order. A similar observation has been made⁹⁾ in connection with the transfer matrix approach to this problem, namely that the introduction of the t_i variables reduces the matrices to half their original size.

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