Statistical mechanics of the 1D ferromagnetic ANNNI chain under an external field: revisited

1991 J. Phys. A: Math. Gen. 24 3927

(http://iopscience.iop.org/0305-4470/24/16/027)

J. Phys. A: Math. Gen. 24 (1991) 3927-3934. Printed in the UK

Statistical mechanics of the 1D ferromagnetic ANNNI chain under an external field: revisited

Nibedita Bhattacharyya and Subinay Dasgupta

Department of Pure Physics, University of Calcutta, 92 Acharyya Prafulla Chandra Road, Calcutta 700009, India

Received 30 November 1990

Abstract. This paper presents an analysis of the exact solution for the statistical mechanics of the one-dimensional ferromagnetic ANNNI chain under an external magnetic field by the transfer matrix method. Expressions in closed form are derived for the free energy, magnetic moment, disorder line, susceptibility and the temperature and field derivatives of susceptibility. The variation of the wavevector and correlation length with the external field shows interesting features.

Among the periodic frustrated Ising models, the ANNNI models are the most important, and the only member of this family for which the statistical mechanics has been solved exactly is the 1D ANNNI chain (for a review, see [1, 2]). Surprisingly, there seems to be an omission for the non-zero external field case, presumably because of algebraic complexity. This paper presents the detailed exact solution for the statistical mechanics of the 1D ANNNI chain under an external magnetic field; the free energy and magnetic moment (and hence susceptibility) are determined for arbitrary values of the external field by the transfer matrix approach. An expression is determined (again for arbitrary values of the external field) for the line across which the decay of two-spin correlation changes from monotonous to oscillatory. The wavevector (for the modulated phase) and correlation are found to display interesting behaviour as a function of the field. Previous works were confined to the case of zero field [3-7], except for studies on the ground state [8, 9], a numerical study [10] on the *anti*ferromagnetic chain and an application of interface method to the 2D case [11].

The ANNNI chain is described by the Hamiltonian

$$\mathscr{H} = -\sum_i s_i(J_1 s_{i+1} + J_2 s_{i+2} + H) \tag{1}$$

where $s_i = \pm 1$ is the spin at site i and H is the external magnetic field. We shall confine ourselves to the ferromagnetic chain by choosing $J_1 > 0$, $J_2 < 0$. In a straightforward manner one can write down the transfer matrix V by the conventional method of breaking up the lattice into cells, each containing two consecutive spins [12]:

$$V = \begin{array}{c} \\ ++ \\ +- \\ -- \\ -+ \end{array} \begin{array}{c} \begin{array}{cccc} ++ & +- & -- & -+ \end{array} \\ \begin{pmatrix} 1/(xyz) & 1/\sqrt{(xz)} & y & \sqrt{(x/z)} \\ \sqrt{(x/z)} & (x/y) & \sqrt{(z/x)} & y \\ y & \sqrt{(xz)} & (z/xy) & \sqrt{(z/x)} \\ 1/\sqrt{(xz)} & y & \sqrt{(xz)} & (x/y) \end{pmatrix} \end{array} \tag{2}$$

where

$$V(s_i, s_j, s_k, s_l) = \exp[(K_1/2)(2s_j s_k + s_i s_j + s_k s_l) + K_2(s_i s_k + s_j s_l) + h(s_i + s_j + s_k + s_l)/2] \tag{3}$$

0305-4470/91/163927+08\$03.50

$x=\exp(-2K_1)$, $y=\exp(-2K_2)$, $z=\exp(-2h)$, $K_1=J_1/k_BT$, $K_2=J_2/k_BT$, $h=H/k_BT$, k_B = Boltzmann's constant. The characteristic equation for V is quite cumbersome but a remarkable simplification is obtained from the important observation that $V=x^{-1}y^{-1}W^2$, where

$$W=\begin{pmatrix} 1/\sqrt{z} & y\sqrt{x} & 0 & 0 \\ 0 & 0 & y\sqrt{x} & x/\sqrt{z} \\ 0 & 0 & \sqrt{z} & y\sqrt{x} \\ y\sqrt{x} & x\sqrt{z} & 0 & 0. \end{pmatrix} \tag{4}$$

This form of transfer matrix has been mentioned previously several times [13-15]. The matrix W has a rather simple characteristic equation (that also has been mentioned earlier [14]):

$$\det(W-aI)=a^4-2Ca^3+\alpha a^2+2\beta Ca-\beta^2/x^2=0 \tag{5}$$

and the free energy per spin is given by

$$F=-J_1-J_2-k_BT\ln a_1 \tag{6}$$

where $C=\cosh h$, $\alpha=1-x^2$, $\beta=x^2(1-y^2)$ and a_1 is the largest root of equation (5).

We shall now discuss the behaviour of susceptibility and then go over to correlation. The magnetic moment per spin is obtained immediately as

$$M=-\partial F/\partial H=(1/a_1)(\mathrm{d}a_1/\mathrm{d}h)=S(a_1^2-\beta)A \tag{7}$$

where $S=\sinh h$ and $A=[2a_1^3+\alpha a_1+C(\beta-3a_1^2)]^{-1}$. This in turn gives the susceptibility χ (per spin),

$$\begin{aligned} k_BT\chi &= -M^2+(1/a_1)(\mathrm{d}^2a_1/\mathrm{d}h^2) \\ &= -M^2+A[C(a_1^2-\beta)+2MS(3a_1^2-\beta)-M^2a_1(6a_1^2-6a_1C+\alpha)] \end{aligned} \tag{8}$$

and the field derivative of susceptibility,

$$\begin{aligned} k_B^2T^2(\mathrm{d}\chi/\mathrm{d}H) & \\ &= (1/a_1)(\mathrm{d}^3a_1/\mathrm{d}h^3)-3Mk_BT\chi-M^3 \\ &= -3Mk_BT\chi-M^3+A[(k_BT\chi+M^2)3a_1M(6a_1C-6a_1^2-\alpha) \\ &\quad +6a_1^2M^3(C-2a_1)+3S(3a_1^2-\beta)(k_BT\chi+M^2) \\ &\quad +18a_1^2M^2S+3MC(3a_1^2-\beta)+S(a_1^2-\beta)]. \end{aligned} \tag{9}$$

It can be seen that at zero field, equation (8) reduces to the expression of Stephenson [4]. Some typical numerical results are displayed in figure 1. There exists a maximum of susceptibility for variation of temperature as well as the field. However, as for the zero field case [4], the lines of these maxima are not related in any way to the disorder line.

Before we investigate the correlation, a comment is in order. For $H=0$ the line across which the correlation changes from monotonous to oscillatory coincides with the one where the correlation length shows a spike-like minimum, and this line is called the disorder line. Although there is no *a priori* guarantee for this coincidence, it also occurs for decorated chains ([2], section 2.2). In the present case of a non-zero external field, the former line exists but not the latter (correlation length does not show

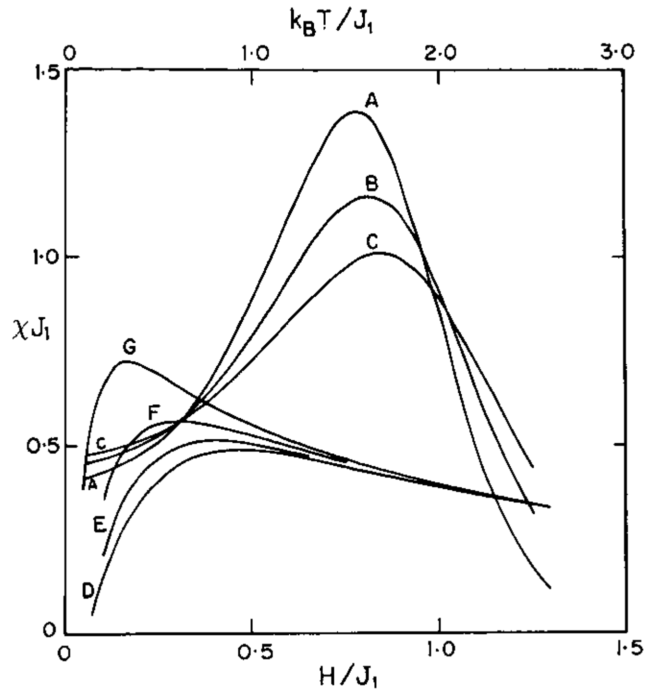

Figure 1. Plot of susceptibility as a function of field and temperature for $-J_2/J_1=0.8$. $k_BT/J_1=0.5$, 0.6, 0.7 for A, B, C respectively, $H/J_1=0$, 0.2, 0.3, 0.4 for D, E, F, G respectively.

any sharp minimum), as has also been observed earlier [10]; still, we propose to call the former line a *disorder line* since this line expresses an important characteristic of correlation. This line will perhaps be a disorder line of the 'third kind' since disorder lines of the first and second kinds have already found entry in the literature [1, 2].

Let us now calculate the correlation. The two-spin correlation in the thermodynamic limit can be easily obtained by working out the standard prescription (see for example [16]):

$$\langle s_i s_{i+r}\rangle = U_{11}^2 + \mathrm{Re}[U_{12}U_{21}(a_2/a_1)^r] \tag{10}$$

for large r. Here a_2 is the second largest root (considering the modulus for complex roots if any) of equation (5), U = similarity transform of the matrix [(1, 0, 0, 0), (0, 1, 0, 0), (0, 0, −1, 0), (0, 0, 0, −1)] by the matrix that diagonalizes W (to one having first and second diagonal elements as a_1 and a_2 respectively). Now, the decay of $\langle s_i s_{i+r}\rangle$ with respect to r (at large r) will change from monotonous to oscillatory when the nature of a_2 changes from real to complex. Incidentally, it turns out that for the parameter range considered below, if a_2 is real, all the four roots are real. Hence, we can fortunately locate the disorder line by finding the switchover of the nature of eigenvalues from 'all real' to 'two real, two complex'. This implies [17] that the equation for the disorder line is given by $\Delta=0$ where Δ is the discriminant of the quartic equation (5):

$$\Delta = -(X^2/16)(16XY^3 - \alpha^2Y^2 + 18\alpha^2XYZ - \alpha^4Z + 27\alpha^2X^2Z^2) = 0 \tag{11}$$

where $X = 1 - y^{-2}$, $Y = x^2y^2(y^2+S^2)$ and $Z = x^2y^4S^2$. (For $H=0$, this equation reduces to the previously known form [1-4].) Moreover, for a monotonically decaying correlation, the correlation length ξ is given by

$$\xi^{-1} = \ln(a_1/a_2) \tag{12}$$

while for an oscillatorily decaying correlation the correlation length and wave vector are given by

$$\xi^{-1} = \ln(a_1/|a_2|) \qquad q = \mathrm{Arg}(a_2). \tag{13}$$

Thus, the correlation at a large distance can be written as

$$\langle s_i s_{i+r}\rangle \sim M^2 + A_\mathrm{m}\exp(-r/\xi)\cos(qr) \tag{14}$$

where A_m is the amplitude. For a monotonous correlation $q=0$.

It is interesting to investigate where the disorder line intersects the $T=0$ line. As $T\to 0$, $x\to 0$ and $y\to\infty$, so that $\alpha\to 1$, $X\to 1$ and $Y\to 0$ and the only feasible solution of equation (11) is $Z=\frac{1}{27}$. This in turn gives $\varkappa \equiv -J_2/J_1 = \varkappa_- + [\ln(\frac{27}{4})]/(4\ln x) \to \varkappa_-$ as $T\to 0$ with

$$\varkappa_- = [1-(H/2J_1)]/2. \tag{15}$$

The disorder line for some non-zero values of the applied field is displayed in figure 2. As the field increases the line comes down and a larger portion of the $\varkappa - T$ plane corresponds to an oscillatorily decaying correlation (however, see [10]). The most interesting feature of this figure is the indication that at an infinitesimally small temperature the correlation is oscillatory for $\varkappa > \varkappa_-$, but according to studies [8, 9] on the ground state the ferromagnetic state extends up to

$$\varkappa_+ = [1+(H/J_1)]/2. \tag{16}$$

In order to understand this contradiction, let us look at the significance of the point $\varkappa_+$ in the behaviour of correlation length ξ. Figure 3 shows the variation of ξ^{-1} with temperature, and figure 4 that of ξ^{-1} and M with $\varkappa$. These figures show that at low

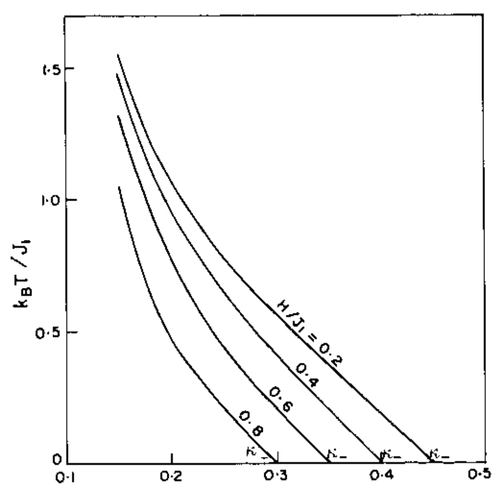

Figure 2. The disorder line for various values of the external field H. The location of $\varkappa_+$ points for $H/J_1 = 0.2$, 0.4, 0.6, 0.8 are 0.6, 0.7, 0.8 and 0.9 respectively.

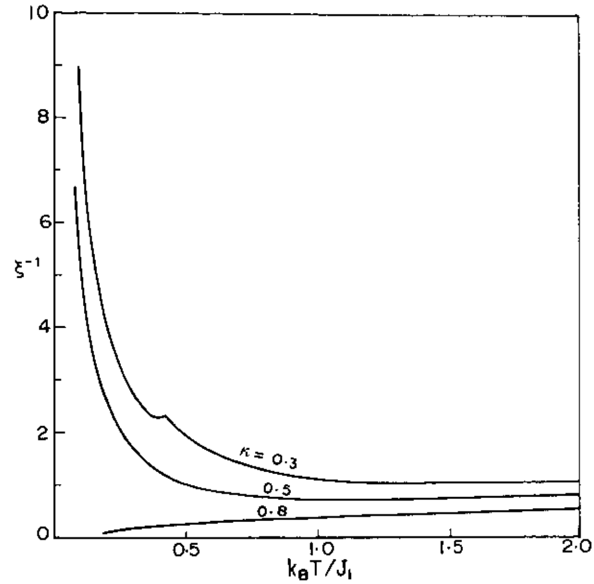

Figure 3. Plot of inverse correlation length ξ^{-1} as a function of temperature for various values of $\varkappa$ with $H/J_1 = 0.4$.

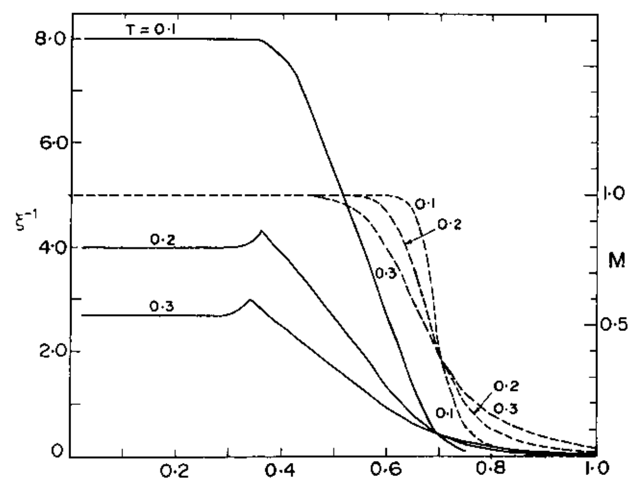

Figure 4. Plot of magnetization per spin M (broken line) and inverse correlation length ξ^{-1} (full line) as a function of $\varkappa$ at $H/J_1 = 0.4$ for various temperatures. The change in M at $\varkappa = \varkappa_+$ becomes sharper as the temperature is lowered.

temperatures ξ^{-1} and M remain high (∞ and 1 respectively) for $\varkappa < \varkappa_+$ and vanish for $\varkappa > \varkappa_+$. Therefore, equation (14) tells us that at a low enough temperature

$$\begin{aligned} \langle s_i s_{i+r} \rangle &\sim M^2 \qquad && \text{for } \varkappa < \varkappa_+ \\ &\sim 0 && \text{for } \varkappa > \varkappa_+ \end{aligned}$$

and this is precisely the result of ground state analysis. This reconciles the apparent contradiction mentioned above and indicates that there is no sudden change in correlation at $T = 0$ at a fixed H.

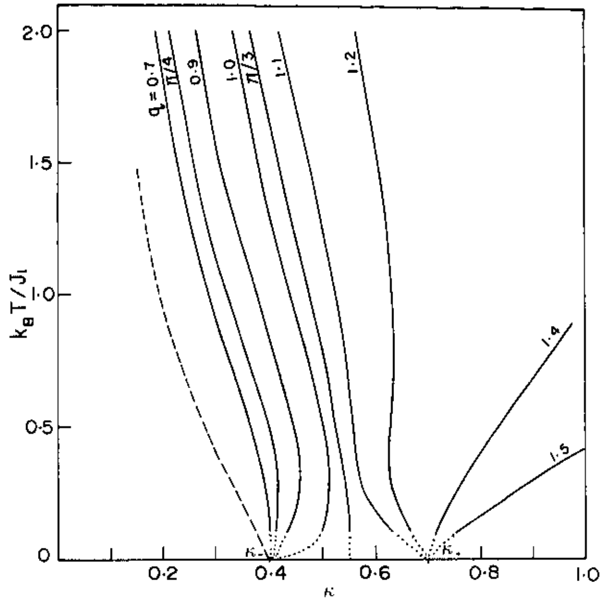

Figure 5. Constant-q curves (full line) and the disorder line (broken line) in the $T-\varkappa$ plane for $H/J_1 = 0.4$. Dotted regions of the lines are shown for guidance.

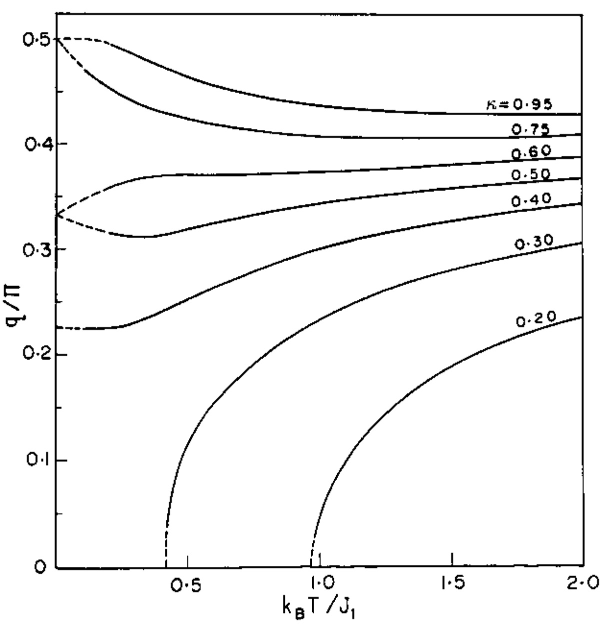

Figure 6. Plot of wavevector q as a function of T and $\varkappa$ for $H/J_1 = 0.4$. Broken lines are shown for guidance.

The behaviour of the wavevector (for modulated correlation) is displayed in figures 5 and 6. For $H=0$, there was a single degenerate 'singular' point from which all constant-q lines in the $\varkappa - T$ plane emerge [1, 2]. But for $H \neq 0$ we find that there are two degenerate 'singular' points on the $T=0$ line (figure 5); one is the $\varkappa=\varkappa_-$ point from which constant-q lines with $0 \leqslant q < \pi/3$ emerge and the other is the $\varkappa = \varkappa_+$ point from which the lines for $\pi/3 < q \leqslant \pi/2$ emerge. The $q = \pi/3$ line cuts the $\varkappa$-axis normally at $\varkappa = (\varkappa_+ + \varkappa_-)/2$. Thus, the $q - T$ curve cuts the $T=0$ line at $\pi/3$ for $\varkappa_- < \varkappa < \varkappa_+$ and at $\pi/2$ for $\varkappa > \varkappa_+$ (figure 6).

Obviously a dramatic change also occurs in the $\xi^{-1} - T$ curve as the external field is switched on; the cusp disappears and the curve (for $\varkappa < \varkappa_+$) goes up, instead of

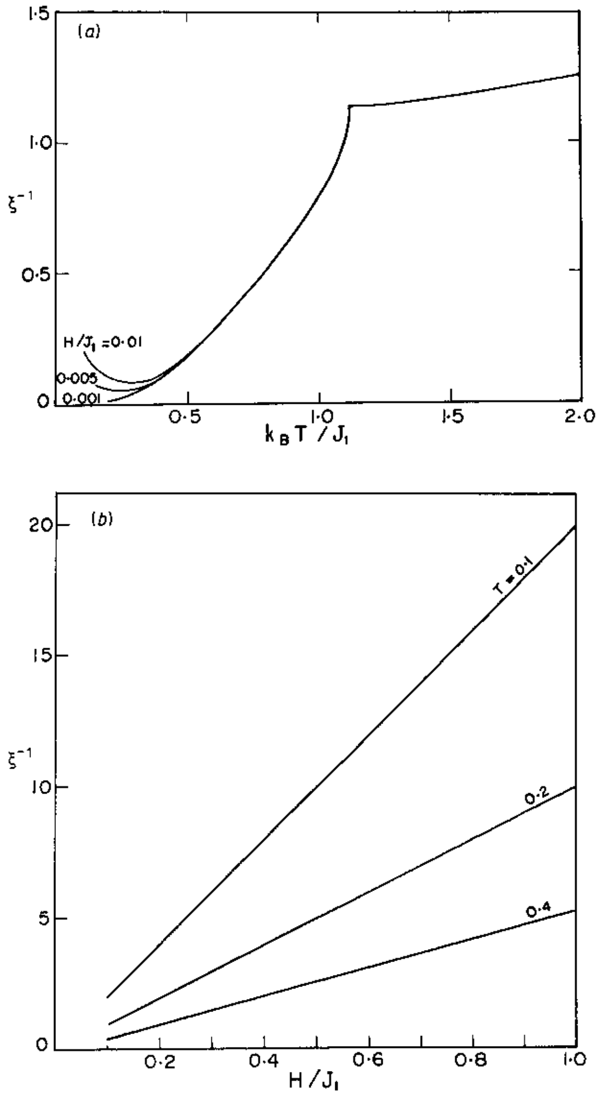

Figure 7. (a) Plot of inverse correlation length ξ^{-1} as a function of temperature for a low external field at $\varkappa = 0.2$. The curves are nearly coincident for $k_BT/J_1 > 0.4$. (b) Plot of inverse correlation length ξ^{-1} as a function of external field at low temperatures for $\varkappa = 0.2$.

coming down as $T \to 0$. Now we shall see that although the correlation length is an important parameter for the description of correlation, this behaviour of ξ^{-1} does not imply any non-analyticity in the field dependence of correlation itself (which is of course the actual physical quantity involved) at $H = 0$ at a non-zero temperature. The $\xi^{-1} - T$ curve at a low H nearly coincides with the curve for $H = 0$, except at very low temperatures (figure 7(*a*)). The departure is in the form of a rise ($\xi^{-1} \to \infty$ as $T \to 0$) and this begins at a temperature that decreases with decreasing field and at $H = 0$ this rise is not obtained. Thus, the rate of change of ξ^{-1} with H increases with lowering of temperature (figure 7(*b*)) and at $T \to 0$, the $\xi^{-1} - H$ curve is vertical.

In short, the correlation tends to the zero-temperature limit $\langle s_i s_{i+r} \rangle \to 1$ (for $\varkappa < \varkappa_+$), in two different ways, depending on the external field. For $H = 0$, $M = 0$ at $T \neq 0$, and this limit is achieved by a vanishing ξ^{-1}. For $H \neq 0$, the limit is approached through $\xi^{-1} \to \infty$ with M being non-zero at a low temperature. For $\varkappa > \varkappa_+$ the limit $\langle s_i s_{i+r} \rangle \to 0$ is always approached through $\xi^{-1} \to 0$, whether the external field is present or not.

We conclude with the remark that it is indeed difficult to derive analytically the characteristics of q and ξ mentioned above. Nevertheless, we have been able to write down a fairly simple equation for the partition function and the disorder line (equations (5) and (11)). However, it is difficult to extend the above treatment to further neighbour interactions and derive therefrom the effect of the range of interaction on the disorder line. This is because, for equations of degree higher than four, one cannot write down a closed-form expression for the line where the second-largest root changes its nature from real to complex. However, numerical approaches are obviously possible and will soon be reported.

Acknowledgments

The authors are grateful to Professor S Sengupta for encouragement and helpful discussions. The work of one of us (NB) was financed by the University Grants Commission through a junior research fellowship (pre-doctoral).

References

[1] Selke W 1988 *Phys. Rep.* **170** 213
[2] Liebmann R 1986 *Statistical Mechanics of Periodic Frustrated Ising Systems* (Berlin: Springer) section 2.1
[3] Hornreich R M, Liebmann R, Schuster H G and Selke W 1979 *Z. Phys.* B **35** 91
[4] Stephenson J 1970 *Can. J. Phys.* **48** 1724
[5] Stephenson J 1970 *Phys. Rev.* B **1** 4405
[6] Dobson J F 1969 *J. Math. Phys.* **10** 40
[7] Marsh J S 1966 *Phys. Rev.* **145** 251
[8] Morita T and Horiguchi T 1972 *Phys. Lett.* **38A** 223
[9] Yokoi C S O, Coutinho-Filho M D and Salinas S R 1981 *Phys. Rev.* B **24** 4047
[10] Rujan P, Selke W and Uimin G V 1983 *Z. Phys.* B **53** 221
[11] Rottman C 1990 *Phys. Rev.* B **41** 2547
[12] Montroll E W 1942 *J. Chem. Phys.* **10** 61
[13] Oguchi T 1965 *J. Phys. Soc. Japan* **20** 2236
[14] Katsura S and Ohminami M 1972 *J. Phys. A: Math. Gen.* **5** 95
[15] Kassan-Ogly F A, Kormil'tsev E V, Naish V E and Sagaradze I V 1989 *Sov. Phys. Solid State* **31** 939
[16] Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (London: Academic) section 2.2
[17] Barnard S and Child J M 1936 *Higher Algebra* (London: Macmillan) ch XII