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LETTER TO THE EDITOR

On the residual entropy of the one-dimensional Ising chain with competing interactions

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Abstract. We establish explicit relations between the residual entropy of the one-dimensional Ising chain with a nearest-neighbour ferromagnetic and kth-neighbour anti-ferromagnetic interaction, and the residual entropies of the one-dimensional Ising chain with many-neighboured antiferromagnetic interactions in the corresponding maximum critical fields. The obtained results are, in particular, relevant to the chains that appear in the axial next-nearest-neighbour Ising model.

The axial next-nearest-neighbour Ising (or ANNNI) model in d dimensions consists of $(d-1)$-dimensional layers of spins with nearest-neighbour ferromagnetic coupling, $J_0>0$, within layers but competing ferromagnetic, J_1, and antiferromagnetic, $J_2<0$, first- and second-neighbour axial coupling between layers (Fisher and Selke 1981). In other words, the ANNNI model consists of one-dimensional Ising chains with ferromagnetic inter-chain interaction and competing intra-chain interactions. The chains are stretched along the spatial axis that is perpendicular to the ferromagnetic layers. For $-J_2/J_1=\frac{1}{2}$, such a chain has an infinitely degenerate ground state accompanied by a non-zero residual entropy per spin. This makes the phase diagram of the ANNNI model appear very complex, and interesting, close to the multiphase point $(T=0, -J_2/J_1=\frac{1}{2})$. Therefore, Redner (1981) was stimulated to study a one-dimensional Ising chain with a nearest-neighbour ferromagnetic interaction J_1 and a competing kth-neighbour antiferromagnetic interaction J_k, in a zero field. He found that such a chain (hereafter we shall call it the (J_1, J_k) chain) has a highly degenerate ground state when $-J_k/J_1=1/k$. In this letter we demonstrate that the residual entropy of the (J_1, J_k) chain in a zero field is equal to the residual entropy of the Ising chain with a many-neighboured antiferromagnetic interaction of range $(k-1)$ in the corresponding maximum critical field (Hajduković and Milošević 1982), whereas the residual entropy of the (J_1, J_k) chain in the critical field $H=-2J_k-2J_1/k$ is equal to the ground state degeneracy of the Ising chain with an antiferromagnetic interaction of range $(2k-1)$ in the corresponding maximum critical field.

In order to verify the statement formulated above, we derive formulae for the ground state degeneracy of the (J_1, J_k) chain in a form that is suitable for comparison with the results recently obtained for the antiferromagnetic Ising chains (Hajduković and Milošević 1982). Thus we study the Hamiltonian

$$\mathcal{H}=-J_1\sum_{i=1}^{N}S_iS_{i+1}-J_k\sum_{i=1}^{N}S_iS_{i+k}-H\sum_{i=1}^{N}S_i, \tag{1}$$

where S_i is the conventional Ising spin variable ($S_i = \pm 1$), while J_1 and J_k respectively represent the nearest-neighbour ferromagnetic and kth-neighbour antiferromagnetic coupling ($J_1 > 0, J_k < 0$). The applied field is positive ($H > 0$), and it defines the positive (upward) direction of spins. Now we introduce new variables: $n(\downarrow)$ number of spins turned down, $n_1(-)$ number of negative terms in the first sum of (1), and $n_k(-)$ number of negative terms in the second sum of (1). Hence, assuming periodic boundary conditions, the Hamiltonian can be written in the form

$$H = -N(J_1 + J_k + H) + 2J_1 n_1(-) + 2J_k n_k(-) + 2Hn(\downarrow), \tag{2}$$

or

$$H = \text{constant} + Y + Z \tag{3}$$

where

$$Y = 2J_1 n_1(-) + 2J_k n_k(-), \tag{4}$$

$$Z = 2Hn(\downarrow). \tag{5}$$

Here we observe that in a zero field it is the minimum of the function Y which determines the ground state of the system, whereas in a non-zero field the ground state is determined by a minimum of the sum $Y + Z$. In both cases we adopt $n(\downarrow)$ as a basic variable. It varies from zero to N.

We start our discussion with the $H = 0$ case and with the configuration $n(\downarrow) = 0$. The first spin turned $\downarrow$ brings about the following change in Y:

$$\Delta Y_1 = 4J_1 + 4J_k. \tag{6}$$

As we are looking for the largest possible decrement of Y for a given increment $\Delta n(\downarrow)$, we assume that the second spin turned $\downarrow$ clings to the first one, and so on up to the kth spin turned down. In this way the change of the first term in Y stays fixed, while there appears a decreasing sequence of total changes

$$\Delta Y_i = 4J_1 + 4iJ_k, \qquad i = 1, 2, \ldots, k. \tag{7}$$

For any additional number of spins which are turned $\downarrow$ (as long as $N - n(\downarrow) \geqslant k$) and stuck to the domain of the first k of them, the change in Y is the same, that is to say ΔY_k. If ΔY_k is positive (i.e. $-J_k/J_1 < 1/k$) then all ΔY_i are positive as well, and there is no decreasing of Y by turning spins $\downarrow$. The ground state is ferromagnetic. On the other hand, if any of ΔY_i is negative, then ΔY_k is the most negative entry in the sequence (7), and the ground state is formed of domains of k spins. The domains are alternately aligned up and down. Following Redner (1981) we denote this phase as $\langle k \rangle$. It occurs when $-J_k/J_1 > 1/k$. At $-J_k/J_1 = 1/k$ the state $n(\downarrow) = 0$ is not affected by the appearance of a domain of k, or more, spins turned $\downarrow$, and thus the ground state degenerates into all possible sequences of domains such that each domain consists of at least k aligned spins and is followed by a domain of at least k spins aligned in the opposite direction.

In a non-zero field, functions Y and Z may have different effects in achieving a minimum of $\mathscr{H}$. When $-J_k/J_1 < 1/k$ both functions increase with increasing $n(\downarrow)$, and the ground state is at $n(\downarrow) = 0$ (a ferromagnetic ground state). However, Y decreases and Z increases, with increasing $n(\downarrow)$, when $J_k/J_1 < 1/k$. Then, if we expect a degenerate ground state, we should look for those values of H which compensate ΔY_i, yielding $\Delta Z_i = -\Delta Y_i$, and hence $\Delta\mathscr{H} = 0$ when $\Delta n(\downarrow) > 0$. For all values of H such that

$$H = -2J_k - 2J_1/k \tag{8}$$

the equality $\Delta Z_k = -\Delta Y_k$ holds, and $\mathcal{H}$ does not change (with respect to the state $n(\downarrow)=0$) if there appears any sequence of domains such that each domain composed of spins aligned $\downarrow$ has k elements and is followed by a domain composed of k, *or more*, spins aligned $\uparrow$. If there appeared a domain with $n(\downarrow)>k$ (or $n(\downarrow)<k$), when the field (8) is applied, the corresponding ΔY would be smaller than ΔZ and Δ would be positive. On the other hand, if a field smaller than (8) is applied, $|\Delta Y_k|$ will be greater than ΔZ_k and the ground state will be of the $\langle k\rangle$ type, whereas in the case of a field greater than (8), $|\Delta Y_k|$ will be smaller than ΔZ and the ground state will be ferromagnetic. Therefore, equation (8) defines a line in the plane $(-J_k/J_1, H/J_1)$. The line passes through the multiphase point $(1/k, 0)$. For any point that lies above this line the ground state of a system described by (1) is ferromagnetic. For points below the line the ground state is of the $\langle k\rangle$ type. On the line, the ground state is highly degenerate.

We first calculate the ground state degeneracy in the case $-J_k/J_1 = 1/k$ and $H=0$. This degeneracy is a sum of products of two binomial coefficients. The first binomial coefficient represents the number of ways in which a group of $n(\downarrow)$ spins can be divided into m domains each consisting of at least k elements. The second binomial coefficient represents the number of ways in which m domains of spins turned $\downarrow$ can break the group of remaining $N-n(\downarrow)$ spins so that there is no broken part with less than k elements and no touching of the $\downarrow$ domains. Hence the ground state degeneracy is given by

$$P = \sum_{n(\downarrow)=k}^{N} \sum_{m=1}^{[n(\downarrow)/k]}{}' \binom{n(\downarrow)-km+m}{m}\binom{N-n(\downarrow)-km+m}{m} \tag{9}$$

where $[n(\downarrow)/k]$ is the integral part of $n(\downarrow)/k$, while the prime on the second summation sign means that m must not be greater than $(N-n(\downarrow))/k$, i.e. no domain of spins pointed up may have less than k elements. It suffices to find the largest term in the sum (9) so as to obtain the residual entropy in the thermodynamic limit

$$\sigma = \lim_{N\to\infty} (1/N) \ln P. \tag{10}$$

The largest term is determined by $n(\downarrow)=N/2$ and $m = xN/2$, where x is the smallest positive root of the equation

$$(1-kx)^k = x(1-kx+x)^{k-1}, \tag{11}$$

and thereby the residual entropy turns out to be

$$\sigma = \ln\{[1-(k-1)x]/(1-kx)\}. \tag{12}$$

One can verify numerically for particular values of k, and analytically for arbitrary k, that formulae (11) and (12) yield the same entropies found by Redner (1981).

The ground state degeneracy in the critical field (8) is a sum of the degeneracy elements, each one being the number of ways in which a group of m domains with altogether mk spins turned $\downarrow$ can break the remaining group of spins aligned $\uparrow$ so that there is no broken part with less than k elements and no touching of the $\downarrow$ domains. This number is the binomial coefficient formed of the numbers $N-2km+m$ and m, and thus the ground state degeneracy is

$$P = \sum_{m=1}^{[N/2k]} \binom{N-2km+m}{m}, \tag{13}$$

whereas the concomitant residual entropy per spin is given by

$$\sigma = \ln\{[1-(2k-1)x]/(1-2kx)\}, \tag{14}$$

with x being the smallest positive root of the equation

$$(1-2kx)^{2k} = x(1-2kx+x)^{2k-1}. \tag{15}$$

In the case of the ANNNI chain, $k=2$, formulae (12) and (14), together with the corresponding equations for x, give $\sigma = \ln[(1+\sqrt{5})/2]$ and $\sigma = 0.3223$, respectively. The first result coincides with the well known residual entropy of the antiferromagnetic Ising chain, with the nearest-neighbour interaction, in its critical field (Domb 1960), whereas the latter coincides with the residual entropy of the antiferromagnetic Ising chain, with interaction of range $k=3$, in its maximum critical field (Hajduković and Milošević 1982). This coincidence is quite general. Indeed, Hajduković and Milošević (1982) found that an Ising chain with antiferromagnetic interaction of range k, in the maximum critical field

$$H = -2\sum_{j=1}^{k} J_j, \tag{16}$$

has the residual entropy

$$\sigma = \ln\{(1-kx)/[1-(k+1)x]\}, \tag{17}$$

where x is the smallest positive root of the equation

$$(1-kx-x)^{k+1} = x(1-kx)^k. \tag{18}$$

Comparing formulae (17) and (18) firstly with formulae (12) and (11), and then with formulae (14) and (15), one can state that the residual entropy of the (J_1, J_k) chain in a zero field is equal to the residual entropy of the antiferromagnetic Ising chain with interaction of range $(k-1)$ in its maximum critical field, whereas the residual entropy of the (J_1, J_k) chain in the critical field (8) is equal to the residual entropy of the antiferromagnetic Ising chain with interaction of range $(2k-1)$ in its maximum critical field. The entropy equalities stay valid even if there appeared non-zero intermediate antiferromagnetic interactions $\{J_2, J_3, \ldots, J_{k-1}\}$ in the case of the (J_1, J_k) chain, or similarly if the intermediate antiferromagnetic interactions, i.e. $\{J_2, J_3, \ldots, J_{k-2}\}$ and $\{J_2, J_3, \ldots, J_{2k-2}\}$, were set equal to zero in the case of the antiferromagnetic Ising chains. The first part of the preceding statement stems from the results obtained in the work of Nagase *et al* (1976), who studied the Ising chain with $J_1 > 0$ and $J_j < 0$ $(k > j > 2)$, while the second part follows from the fact that the ground state degeneracy of an Ising antiferromagnet, *in its maximum critical field* (16), does not depend on the hierarchy within the sequence $\{J_1, J_2, \ldots, J_j, \ldots, J_k\}$ and hence some (or all) of the elements $\{J_2, J_3, \ldots, J_{k-1}\}$ may vanish (Hajduković and Milošević 1982).

Results presented in this letter are of a methodological interest within the theoretical foundations of the third law of thermodynamics (see e.g. Aizenmann and Lieb 1981). However, they also imply that the peculiarities associated with the ANNNI-like systems (which have brought about many fascinating experimental and theoretical pursuits; see e.g. Rossat-Mignod *et al* (1980), Fisher and Selke (1981), Pokrovsky and Uimin (1982)) can be expected in an anisotropic system composed of the antiferromagnetic Ising chains. Such a system, according to the obtained results, may also exhibit a multiphase point, determined by the corresponding critical field and depicted as an origin of an infinite number of distinct, spatially modulated, layered magnetic phases (Fisher and Selke 1981). The new multiphase point should have an additional peculiarity, interesting from the experimental point of view. Namely, it can be switched off, or turned on, by varying the magnetic field in the vicinity of its critical value.

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References

Aizenmann M and Lieb H E 1981 *J. Stat. Phys.* **24** 279–97
Domb C 1960 *Adv. Phys.* **9** 149–244
Fisher M E and Selke W 1981 *Phil. Trans. R. Soc.* **302** 1–44
Hajduković D and Milošević 1982 *J. Phys. A: Math. Gen.* **15** 3561–9
Nagase M, Nakamura T and Igarashi J 1976 *Prog. Theor. Phys.* **56** 1396–410
Pokrovsky V L and Uimin G 1982 *J. Phys. C: Solid State Phys.* **15** L353–6
Redner S 1981 *J. Stat. Phys.* **25** 15–23
Rossat-Mignod J, Burlet P, Quezel S and Vogt O 1980 *Physica* **102B** 237–48