

## LETTER TO THE EDITOR

# The triangular antiferromagnet with infinite nearest-neighbour coupling

G Einevoll and P C Hemmer

Institutt for Fysikk, NTH, Universitetet i Trondheim, N-7034 Trondheim, Norway

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**Abstract.** We show how the exact interface free energy  $F$  for the Ising antiferromagnet on the triangular lattice with infinite first-neighbour and finite second-neighbour interactions can be determined analytically. From considerations of the angular dependence of the interface free energy we conclude that the transition is not second order. An upper bound for the transition temperature is given.

The Ising antiferromagnet with nearest-neighbour isotropic interactions  $J_1$  on the triangular lattice is the prototypical example of a fully frustrated spin system. The large number of ground states corresponds to a finite zero-temperature entropy per spin. By addition of next-nearest neighbour interactions  $J_2$  a phase transition at finite temperatures can occur, and Slotte and Hemmer (1984) attempted to localise the phase transition through a carefully chosen solid-on-solid set-up. Their numerical results, which include also anisotropic next-nearest-neighbour antiferromagnetic interactions, are summarised in figure 1. The fact that the curves are linear for  $J_2 \ll J_1$  shows that in the limit  $J_1 \rightarrow \infty$  the calculated critical temperature stays finite:

$$\lim_{J_1 \rightarrow \infty} kT_c(J_1, J_2) = (\text{const})J_2. \quad (1)$$

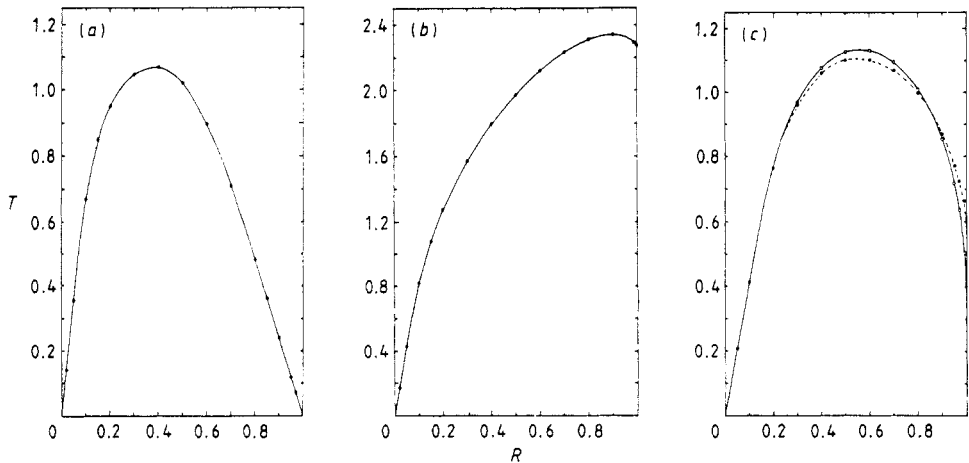
In this Letter we show that it is possible to evaluate the solid-on-solid interface free energy analytically for the limiting case  $J_1 \rightarrow \infty$ . While analytic results are always preferable to numerical values, our motivation has in this case a different origin. A recent study by Shi and Wortis (1988) on the shape of rock-salt crystals contains a conjecture for the *exact* solution of the  $J_1 \rightarrow \infty$  model with next-nearest-neighbour antiferromagnetic interactions. The numerical value for  $T_c$  of their conjecture ( $kT_c/J_2 = 7.11 \dots$ ) is very close to the extrapolated Slotte–Hemmer numerical value ( $kT_c/J_2 \approx 7.12$ ). As will be demonstrated in the first part of this Letter, our present analytic re-evaluation of the latter shows complete agreement with the Shi–Wortis conjecture! In the second part of the Letter, however, we show through an exact evaluation of the interface free energy that the assumption underlying both the previous calculations, namely that the transition is second order, is not correct.

At criticality the interface free energy  $F$  vanishes, i.e. the interface partition function  $Z = \exp(-F/kT)$  equals unity. The partition function is in this case the sum over height

differences  $r_i = (x_i, y_i)$  between nearest-neighbour solid-on-solid columns with the corresponding energy

$$E = \sum_i \{2J_1[\theta(y_i + \frac{1}{2}) + \theta(x_i - \frac{1}{2}) + |x_i + y_i| + |x_{i+1} + y_i|] + 4J_{22} + 2J_{23}(|y_i + x_{i+1} + y_{i+1}| + |x_i + y_i + x_{i+1} - 1|) - 2J_{21}(|y_i + x_{i+1} + y_{i+1} + 1| + |x_i + y_i + x_{i+1}|)\}. \quad (2)$$

Here  $\theta(n)$  is the usual signum function, and  $J_{21}$ ,  $J_{22}$ ,  $J_{23}$  are the antiferromagnetic exchange constants between next-nearest neighbours in the three lattice directions. We refer the reader to Slotte and Hemmer (1984) for details of the solid-on-solid set-up, and the derivation of equation (2), which is their equation (5). (Note that a misprinted sign is corrected in our equation for  $E$ ).



**Figure 1.** The transition temperature, according to Slotte and Hemmer (1984), for the antiferromagnetic triangular lattice with first- and second-neighbour interactions,  $J_1$  and  $J_2$ , with  $R = J_2/(J_1 + J_2)$ . The temperature is given in units of  $(J_1 + J_2)/k$ . (a) Isotropic second-neighbour interactions, (b) second-neighbour interactions acting in two lattice directions, (c) second-neighbour interactions acting in merely one lattice direction (two alternative solid-on-solid set-ups).

The partition function is evaluated by the usual transfer matrix technique, and the transition is located by equating the maximum eigenvalue  $\lambda$  of the transfer matrix to unity:

$$\lambda = 1. \quad (3)$$

The transfer matrix must be chosen with care. The obvious choice which is suggested by equation (2) is not expedient for taking the limit  $J_1 \rightarrow \infty$  since matrix elements diverge, and the symmetrised version used by Slotte and Hemmer for their numerical work suffers from the same difficulty. The following choice, however, is tailored to the limiting process  $J_1 \rightarrow \infty$ . With  $K_1 = J_1/kT$  and  $K_{2i} = J_{2i}/kT$  we set

$$\begin{aligned} \mathbf{T}(r, r') = \exp\{ & -K_1[\frac{1}{2}\theta(x - \frac{1}{2}) + \frac{3}{2}\theta(x' - \frac{1}{2}) + \frac{3}{2}\theta(y + \frac{1}{2}) \\ & + \frac{1}{2}\theta(y' + \frac{1}{2}) + |x + y| + |x' + y'| + 2|x' + y|] \\ & - 4K_{22} - 2K_{23}(|y + x' + y'| + |x + y + x' - 1|) \\ & + 2K_{21}(|y + x' + y' + 1| + |x + y + x'|)\} \end{aligned} \quad (4)$$

and check that

$$\exp(-E/kT) = \prod_i \mathbf{T}(r_i, r_{i+1}).$$

Now we can take  $J_1 \rightarrow \infty$ . Apart from diagonal elements, only five non-diagonal elements remain finite in this limit, and they involve the matrix indices  $r_1 = (0, -1)$ ,  $r_2 = (0, 0)$  or  $r_3 = (1, -1)$ . Thus the eigenvalue problem reduces to finding the maximum eigenvalue of a  $3 \times 3$  matrix. The explicit form follows from equation (4). With

$$T_{ij} = \mathbf{T}(r_i, r_j) \quad i, j = 1, 2 \text{ or } 3 \quad (5)$$

we find that  $T_{23}$  vanishes as  $\exp(-2K_1)$  in the  $J_1 \rightarrow \infty$  limit and that the other eight elements are independent of  $J_1$ .

Taking first *isotropic* second-neighbour interactions ( $K_{21} = K_{22} = K_{23} = K_2$ ), we have, with  $x = \exp(-4K_2)$

$$\mathbf{T} = \begin{pmatrix} x^2 & x^2 & x^2 \\ x^2 & x & 0 \\ x^2 & x^2 & x \end{pmatrix}. \quad (6)$$

The critical condition that the maximum eigenvalue equals unity, gives the following equation:

$$x^6 - 2x^5 + 3x^4 - 2x^3 + 2x - 1 = 0. \quad (7)$$

Factorising the left-hand side as  $(x^3 - x^2 + 1)(x^3 - x^2 + 2x - 1)$  all roots are easily found. The positive zero of the second factor can be written

$$K_{2c} = \frac{1}{2} \ln[(\frac{1}{2} + \sqrt{\frac{23}{108}})^{1/3} + (\frac{1}{2} - \sqrt{\frac{23}{108}})^{1/3}]. \quad (8)$$

One has to check that this is the relevant root of (7). The numerical value corresponds to

$$kT_c = J_2/K_{2c} = (7.112\ 386. \dots)J_2. \quad (9)$$

This is identical to the value conjectured by Shi and Wortis to be the exact transition temperature.

The models with *anisotropic* second-neighbour interactions are easily discussed in the same way. With  $J_{21} = 0$ ,  $J_{22} = J_{23} = J_2$  (next-nearest-neighbour interactions in two lattice directions) we get, with  $y = \exp(-K_2)$

$$\mathbf{T} = \begin{pmatrix} y^{12} & y^{10} & y^8 \\ y^8 & y^6 & 0 \\ y^{10} & y^8 & y^6 \end{pmatrix}. \quad (10)$$

The maximum eigenvalue is unity for  $y^6 = \frac{1}{2}$ , or

$$kT_c = 6J_2/\ln 2 = (8.656\ 17. \dots)J_2. \quad (11)$$

Second-neighbour interactions in one direction correspond to  $J_{21} = J_{23} = 0$ , or to  $J_{21} = J_{22} = 0$ , which gives

$$\mathbf{T} = \begin{pmatrix} y^4 & y^4 & y^4 \\ y^4 & y^4 & 0 \\ y^4 & y^4 & y^4 \end{pmatrix} \quad \text{or} \quad \mathbf{T} = \begin{pmatrix} y^8 & y^6 & y^4 \\ y^4 & y^2 & 0 \\ y^6 & y^4 & y^2 \end{pmatrix} \quad (12)$$

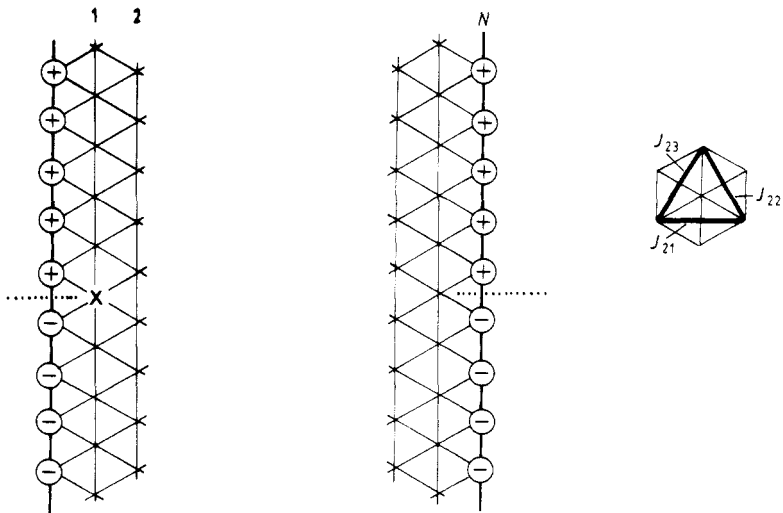
respectively. In both cases the principal eigenvalue equals unity for

$$kT_c = 2J_2 / \ln[\frac{1}{2}(\sqrt{5}) + \frac{1}{2}] = (4.15617 \dots)J_2. \quad (13)$$

The results (11) and (13) are in good agreement with the corresponding extrapolated values from the Slotte–Hemmer calculation.

We will now turn to a more fundamental determination of the  $J_1 = \infty$  interface free energy. The bulk ground state consists of parallel alternating lines of up-spins and down-spins, such that the weakest second-neighbour interaction (here  $J_{21}$ ) acts orthogonal to the direction of these lines. Thus the ground state is doubly degenerate. Forcing the spins at the boundary of the upper half of a rectangular domain to belong to one phase, the boundary spins in the lower half to belong to the other phase, an interface must necessarily be present (figure 2).

The spin configurations that can occur in the interior of the domain are severely restricted when  $J_1 = \infty$ . All but one of the spins in the layer adjacent to the left-hand boundary are uniquely determined, taking negative values in the upper half and positive values in the lower half of the domain. One spin (marked  $\times$  in figure 2) can be either up or down. The effect of this spin being positive is that the interface effectively moves upwards, and we associate an auxiliary variable  $\sigma_1 = 1$  with this upward deflection of the boundary. For a given value of the spin in question, only one spin in the next column



**Figure 2.** The boundary condition which produces the separation of the two phases. Here  $N$  is an even integer. The directions of the second-neighbour interactions are also shown. In column 1 only the spin at  $\times$  is not determined by the boundary condition (when  $J_1 = \infty$ ).

can be oriented freely, etc. In this way the spin configurations allowed by the  $J_1 = \infty$  condition correspond to a unique boundary which can be described by a sequence  $(\sigma_1, \sigma_2 \dots \sigma_N)$ , such that  $\sigma_i = 1$  ( $-1$ ) when the boundary is deflected up (down) at the  $i$ th column.

The second-neighbour interaction gives different weights to these boundary configurations, and it is easy to find the energy associated with a boundary  $(\sigma_1 \dots \sigma_N)$ :

$$E(\sigma_1, \dots, \sigma_N) = \sum_{i=1}^N [-J_{21} \sigma_i \sigma_{i-1} + (J_{22} - J_{23}) \sigma_i - J_{21} + 3J_{22} + 3J_{23}]. \quad (14)$$

To match the right-hand-side boundary condition of figure 2 we must have ( $N$  even)

$$\sum_{i=1}^N \sigma_i = 0. \quad (15)$$

Consequently

$$E = - \sum_{i=1}^N (J_{21} \sigma_i \sigma_{i-1} + J_{21} - 3J_{22} - 3J_{23}). \quad (16)$$

Thus we are led to a one-dimensional Ising model, and its free energy is easily determined. The similarity with the Shi-Wortis calculation has now become evident. The calculation is a solid-on-solid one, but in this case not by assumption. Since  $J_1 = \infty$ , bubbles and overhangs are simply too costly in energy to be present.

In the  $N \rightarrow \infty$  limit the restriction of zero magnetisation has effectively no further influence since (16), without any restriction, yields zero average magnetisation. We find

$$-F_i/NkT = K_{21} - 3K_{22} - 3K_{23} + \ln(2 \cosh K_{21}).$$

This interface free energy vanishes when

$$\exp(3K_{22} + 3K_{23}) = 1 + \exp(2K_{21}). \quad (17)$$

For the isotropic case this is equivalent to the critical condition above, i.e. the Shi-Wortis conjecture.

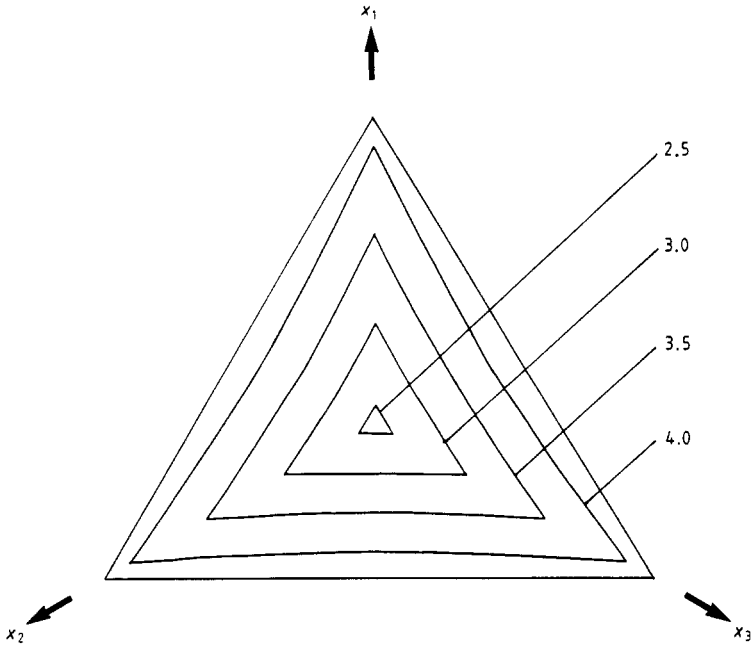
One might believe that this constitutes a verification of the Shi-Wortis conjecture, but this is not so. The reason is the following: the interface free energy depends in general both on the temperature and on the macroscopic orientation of the interface. By the set-up in figure 2 only a horizontal interface is considered. Other directions may be studied by forcing the boundary spins on the right-hand side differently, i.e. replacing (15) by

$$N^{-1} \sum_{i=1}^N \sigma_i = m \equiv (\sqrt{3}) \tan \vartheta \quad (18)$$

where  $\vartheta$  is the angle relative to the horizontal direction in figure 2.

The direction with the minimum interface free energy  $F_m$  (at a given  $T$ ) is the direction which is selected by the *unrestricted* Ising model.  $F_m$  is determined by the maximum eigenvalue of the transfer matrix corresponding to the energy expression (14) in the usual way. We find

$$F_m = -NkT \ln[\exp(2K_{21} - 3K_{22} - 3K_{23})\{\cosh(K_{22} - K_{23}) + [\sinh^2(K_{22} - K_{23}) + \exp(-4K_{21})]^{1/2}\}]. \quad (19)$$



**Figure 3.** The dimensionless temperature  $kT_0/(J_{21} + J_{22} + J_{23})$  as a function of the exchange interactions. Four isotherms are shown. In the diagram each interaction variable  $x_i = J_{21}/(J_{21} + J_{22} + J_{23})$  ranges from zero to unity.

This minimal free energy is positive below a temperature  $T_0$ , determined through the condition  $F_m = 0$ , or

$$2 \exp(-3K_{22} - 3K_{23}) \sinh(2K_{21}) + \exp(3K_{22} + 3K_{23} - 2K_{21}) = 2 \cosh(K_{22} - K_{23}). \quad (20)$$

In the three special cases, considered in the first part, the corresponding values of  $T_0$  are identical to the temperatures (9), (11) and (13), respectively. One can show, more generally, for arbitrary interactions that the  $J_1 = \infty$  Slotte–Hemmer free energy vanishes at a temperature given by (20). Figure 3 shows  $T_0$  as a function of the interaction parameters.

For other directions  $F$  will exceed  $F_m$ . As an example we see from (17) that when  $J_{21} = J_{22} = 0$  the interface free energy in the horizontal direction vanishes at  $kT = 3J_{23}/\ln 2 = 4.328 \dots J_{23}$ , slightly higher than the temperature (13) at which  $F_m$  vanishes. Moreover, when the directions  $\vartheta = \pm\pi/6$  is reached (all  $\sigma_i = +1$  or  $-1$ )  $F$  does not decay at all with increasing temperature.

The main conclusion is that since the interface free energy for different directions does not vanish at the same temperature, the transition is *not* second order. The temperature  $T_0$  is then merely an upper bound for the transition temperature. One may consider the Monte Carlo calculations by Glosli and Plischke (1983) as evidence that the isotropic model has a first-order transition, at least for finite  $J_1$ . (For the isotropic case considered by these authors, with  $J_1 = 10J_2$ , the transition temperature is roughly 10% below the Slotte–Hemmer value.) While both the Shi–Wortis approach and the Slotte–

Hemmer set-up yield the exact minimum interface free energy, the nature of the transition precludes an identification of the transition temperature.

**References**

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