Study of Ising model on the rectangular-triangular lattice

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Abstract. The Ising model is studied on a new type of lattice which is named the rectangular-triangular lattice. The critical temperature for the ferromagnetic lattice is calculated exactly and it is shown that the antiferromagnetic lattice does not order at any temperature. Ground state properties are investigated and some features of frustration on the antiferromagnetic Ising lattice outlined.

1. Introduction

Critical phenomena in two dimensions are usually studied on well-known planar lattices like the square (rectangular), triangular, honeycomb and kagomé lattices. A variety of methods exist (Temperley 1972) to calculate the partition function and associated thermodynamic properties of the Ising model on such lattices. Also, there exist several transformations like the dual, star-triangle and decoration-iteration transformations which connect pairs of partition functions of two-dimensional (2-d) Ising lattices (Syozi 1972). Using these transformations, one can calculate the critical temperature of Ising lattices exactly.

The 2-d planar lattices can be broadly divided into two categories: loose-packed like square and honeycomb lattices and close-packed like triangular and kagomé lattices. A loose-packed lattice has plaquettes of even number of bonds only and can be divided into two non-overlapping sublattices α and β such that every nearest neighbour spin of a spin in α belongs to the β sublattice. There is complete symmetry between the effects of ferromagnetic (FM) and antiferromagnetic (AFM) interactions and the critical temperatures in both the cases coincide. For close-packed lattices this symmetry is no longer present. Such lattices contain plaquettes of odd number of bonds and for the AFM Ising model, the minimum energy requirements for all the bonds in a plaquette cannot be simultaneously satisfied. This leads to the so-called 'frustration effect' (Toulouse 1977)—the frustrated assembly of spins has many configurations of lowest energy so that the entropy per site is finite at absolute zero.

Frustration plays a key role in spin glass phenomena. Theoretical studies in this connection have to deal with the difficult problem of taking averages over the probability distribution of frustrated cells. On the other hand as Toulouse (1977) has

remarked, the phenomenon of frustration should be studied in its own right. Simple model systems are required for such studies. Close-packed lattices with AFM Ising interactions between spins are good candidates. Wannier (1950) showed that because of the large degeneracy of the ground state, the triangular lattice, a fully frustrated lattice, does not fit into an AFM arrangement and is disordered at all temperatures. Kano and Naya (1953) proved the same for the kagomé lattice. Villain (1977) considered a square lattice Ising model in which frustration is produced in every plaquette by making one bond in it antiferromagnetic and the rest ferromagnetic. The first and the last of the above models are fully frustrated models. Simple model systems have also been studied (Longa and Olés 1980) in which frustration is distributed periodically.

In this paper, we study a 2-d planar lattice which we call the rectangular-triangular (RT) lattice, which like the triangular and kagomé lattices does not fit into an AFM arrangement and is frustrated. In §2, we calculate the exact critical temperature of the FM Ising RT lattice and show that the AFM model is disordered at all temperatures, i.e., does not have a critical temperature. In §3, the ground state energies of both the FM and AFM lattices have been calculated. Also, an approximate lower bound to the AFM ground state entropy per site has been estimated as a rough measure of the ground state disorder.

2. Calculation of critical temperature

The RT lattice is drawn in figure 1a and its dual lattice the pentagonal-hexagonal (PH) lattice is drawn in figure 1a (dotted line) and also in figure 1b (solid line). We now study the Ising model on such lattices. The edges of the RT and PH lattices can be grouped into four classes for each lattice—class j consists of edges parallel to the edges marked K_j (for RT lattice) in figure 1a or L_j (for PH lattice) in figure 1b. The K_j's and L_j's are Ising interaction strengths in which the usual Boltzmann factor $1/k_BT$ has been absorbed. The critical condition of the RT lattice is determined in the usual manner (Baxter 1982). The partition function of the PH lattice with $5N$ sites can be written as

$$Z^{PH}_{5N}\{L\} = \exp\{N(3L_1 + 2L_2 + 2L_3 + L_4)\}$$
$$\sum_P \exp(-2L_1r_1 - 2L_2r_2 - 2L_3r_3 - 2L_4r_4), \qquad (1)$$

where the P summation is over all polygon configurations on the RT lattice, r_j being the number of lines on edges of type j. The dual of PH lattice of $5N$ sites is the RT lattice with

(a)   (b)
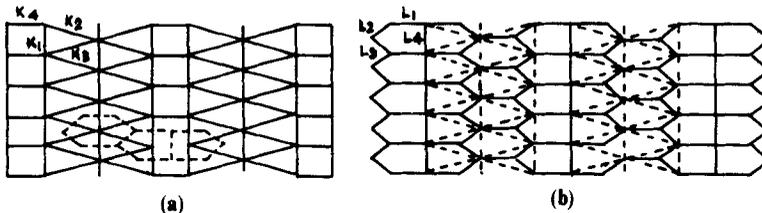
Figure 1. **a.** Rectangular-triangular (RT) lattice (solid line). **b.** Its dual pentagonal-hexagonal (PH) lattice (solid line).

3N sites. Its partition function can be written as

$$Z_{3N}^{RT}\{K\} = 2^{3N} (\cosh^3 K_1 \cosh^2 K_2 \cosh^2 K_3 \cosh K_4)^N$$

$$\sum_P v_1^{r_1} v_2^{r_2} v_3^{r_3} v_4^{r_4}, \tag{2}$$

where $v_j = \tanh K_j$, $j = 1, 2, 3, 4$ and P denotes summation over all polygon configurations on the RT lattice itself. If we define

$$\tanh K_j = \exp(-2L_j), j = 1, 2, 3, 4, \tag{3}$$

then from (1) and (2)

$$Z_{5N}^{PH}\{L\} = (S_1)^{3N/2} (2S_2 S_3)^N (S_4)^{N/2} Z_{3N}^{RT}\{K\} \tag{4}$$

where

$$S_j = \tfrac{1}{2} \exp(2L_j) \frac{1}{\cosh^2 K_j},$$

$$= \sinh 2L_j = \frac{1}{\sinh^2 K_j}. \tag{5}$$

From (3) it is clear that the coupling constants K_j's and L_j's are reciprocally related, i.e., if K_j's are large and positive L_j's are small and vice versa. The coupling constants, we recall, contain the Boltzmann factor $1/k_B T$, so in (4) we have a mapping which connects a low (high) temperature Ising model on a RT lattice to a high (low) temperature model on the PH lattice. Equation (4) represents what is known as the duality relation. This relation by itself cannot give us information on the location of the critical temperature.

In the next step, we use the well-known star-triangle transformation (Syozi 1972, the solid lines are replaced by dotted lines as in figure 1b) to connect the partition function of the PH lattice of coupling constants L_j's ($j = 1, 2, 3, 4$) to that of the RT lattice of coupling constants K_j^*'s ($j = 1, 2, 3, 4$). The coupling constant L_4 remains unchanged in the transformation. There are N such bonds of strength L_4. Also, there are N bonds of strength L_1 which are unaffected by the star-triangle transformation. We combine the results of this transformation and the duality transformation given by (5) to get the self-duality relation for the RT Ising lattice

$$Z_{3N}^{RT}\{K\} (S_1)^{3N/2} (2S_2 S_3)^N (S_4)^{N/2} R^{-2N} = Z_{3N}^{RT}\{K^*\}, \tag{6}$$

where

$$R^2 = \frac{2}{k^2 \sinh 2K_1^* \sinh 2K_2^* \sinh 2K_3^*} \tag{7}$$

$\sinh 2K_j^* \sinh 2L_j = k^{-1}, j = 1, 2, 3$ or using (5) $k \sinh 2K_j^* = \sinh 2K_j, j = 1, 2, 3$, each of the L_j type of bonds is $2N$ in number. Since $L_4 = K_1^*$, $\sinh 2K_1^* \sinh 2K_4 = 1$. For $N L_1$ type of bonds,

$$L_1 = K_4^*, \sinh 2K_4^* \sinh 2K_1 = 1. \tag{8}$$

Also,

$$k = \frac{(1 - v_1^{*2})(1 - v_2^{*2})(1 - v_3^{*2})}{4[(1 + v_1^* v_2^* v_3^*)(v_1^* + v_2^* v_3^*)(v_2^* + v_3^* v_1^*)(v_3^* + v_1^* v_2^*)]^{1/2}}, \tag{9}$$

where $v_j^* = \tanh K_j^*$ and

$$\frac{1}{k} = \frac{(1 - v_1^2)(1 - v_2^2)(1 - v_3^2)}{4[(1 + v_1 v_2 v_3)(v_1 + v_2 v_3)(v_2 + v_3 v_1)(v_3 + v_1 v_2)]^{1/2}}$$

$$v_j = \tanh K_j. \tag{10}$$

The star-triangle relation connects the partition function of Ising model on the PH lattice at high (low) temperature to that on the RT lattice at high (low) temperature (see Baxter 1982). So, the self-duality relation (6) obtained after duality and star-triangle transformations, connect the partition function of Ising model on the RT lattice at high temperature to that on the RT lattice at low temperature. From (7)–(10) it is easy to check that if we want a volume in the parameter space (K_1, K_2, K_3, K_4) to be self-dual, i.e., to map into itself, then one must also obey the condition that in (6) we put

$$(S_1)^{3N/2}(2S_2S_3)^N S_4^{N/2} R^{-2N} = 1. \tag{11}$$

If there is only one critical volume in (K_1, K_2, K_3, K_4) space then this must be the self-dual volume, hence the condition of criticality is given by (11).

We focus attention on the isotropic RT lattice with $K_1 = K_2 = K_3 = K_4 = K$. In this limit, (11) reduces to the equation for the critical point K_c given by

$$\sinh^4 2K_c \, (\exp(4K_c) + 3)(\exp(4K_c) - 1) - 4 = 0. \tag{12}$$

The value of $K_c = \cdot 3228 \ldots$. For AFM Ising model K is negative which does not give any solution for K_c. This corresponds to the fact that the AFM RT lattice does not order even at absolute zero.

3. Ground state properties

We now focus attention on the isotropic RT lattice. Two-thirds of the lattice sites have coordination number 5 and the rest have coordination number 6. So the average coordination number of the RT lattice is 16/3. For the FM Ising lattice the ground state energy is $-8/3 \, NJ$ where N is the number of lattice sites and J the coupling strength. For the AFM Ising lattice, the best one can do is to have two interactions of the right kind and the third 'broken' or unsatisfied in triangular plaquettes and to keep the horizontal bonds unbroken in rectangular plaquettes. In this case, the ground state energy is half that of the FM lattice. For triangular and kagomé lattices, the AFM ground state energies are 1/3rd of their FM equivalents.

Figure 2a shows an arrangement of spins for the AFM RT lattice which gives rise to minimum energy. Each column consists of alternating spins with no broken bonds in rectangular plaquettes. Also, in the region of triangular plaquettes, rows of positive spins are alternated with rows of negative spins. One can, however, think of configurations of higher weight, e.g., keeping all the bonds in rectangular plaquettes unbroken. For example, treating the columns of such plaquettes as single columns one can lay down these columns and the single columns in between independently, the

(a)   (b)
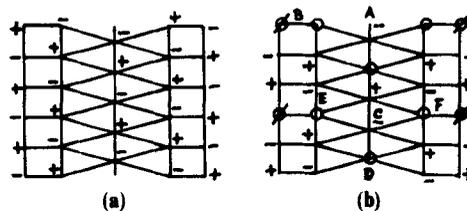
Figure 2. **a.** A simple arrangement of spins with minimum energy. **b.** Another arrangement of minimum energy having finite entropy per lattice site.

configuration of each column being that of alternating spins. Figure 2b shows a spin arrangement of still greater weight and also of finite entropy per lattice site ($N \to \infty$ limit is assumed, where N is the total number of lattice sites). We can reverse any one of the encircled spins along columns marked A without change in energy. Such spins are $N/9$ in number since the number of A columns is $N/3$ and every third spin in an A column is an encircled spin. Encircled spins which are nearest neighbours along B lines are assigned opposite signs (this is indicated through the symbols 0 and ϕ) and are to be flipped simultaneously so that minimum energy configuration is retained. A new set of $N/9$ free spins is obtained thereby. There is still a large amount of 'contingent freedom' (Wannier 1950). It may happen that three neighbouring encircled spins (like D, E, F in figure 2b) forming a triangle centred around a spin on column A have equal signs of one particular kind. By the arguments of fluctuation theory such arrangements will occur at one out of eight positions since a collection of three spins has eight possible configurations and all of them are equally probable. The central spin may then be reversed without change in energy. The central spins being on column A give rise to a number of $(N/72) + (N/72)$ free spins. For example, if the central spin C is surrounded by encircled spins of negative sign, then C may be flipped without change in energy and there are $(2 \times N)/(8 \times 9)$ such spins. So effectively there is a total number of $(N/9 + N/9 + 2 \times N/72) = N/4$ free spins and the weight of the ground state configuration is $2^{N/4}$. The weightage may be put to higher values by considering more involved contingencies. Thus the zero point entropy per lattice site is given by

$$S(0) > \tfrac{1}{4} R \ln 2, \; NR = k_B, \text{ the Boltzmann constant.} \tag{13}$$

Hence the ground state of the AFM RT lattice is disordered and possesses a finite entropy per lattice site. Also as discussed in §2, the AFM RT lattice does not order at any temperature. This behaviour of the RT lattice is similar to that of the AFM triangular and kagomé lattices. In this connection we note that the PH lattice, the AFM dual lattice of the RT lattice, is also a frustrated lattice.

4. Concluding remarks

We have studied a new type of lattice called the RT lattice which along with its dual, the PH lattice, are frustrated lattices for AFM Ising interactions. They are new additions to the growing list of frustration models though a full analysis of frustration on these lattices, e.g., exact calculation of ground state entropy and correlations is yet to be carried out. Apart from the study of frustration, the two lattices which are two ordinary planar lattices can be made use of for usual studies made on 2-d planar lattices. Examples include several thermal (magnetic order → disorder transitions) and geometrical (e.g., percolation) critical phenomena. In §2, we have already calculated the exact critical temperature for the FM Ising model on the RT lattice. A richer variety of phase diagram is expected if one studies Ising model with competing interactions, i.e., with both FM and AFM interactions present.

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