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Zeros of the Partition Function Using Theorems of Ruelle

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Theorems of Ruelle which provide a technique for finding regions of the relevant complex planes free of zeros of the partition function are used to study certain Ising spin systems. Of particular interest is the antiferromagnetic triangle lattice system with $h \neq 0$ and systems having three-body interactions.

KEY WORDS: Partition function; zeros; ferromagnet; antiferromagnet.

1. INTRODUCTION

Interest in the location of the partition function's zeros (hereafter pfz's) began in 1952 with the publication by Lee and Yang[1,2] of two seminal papers on phase transitions. Since that time there have been a number of important results concerned with this subject. In particular Ruelle,[3,4] using the idea of "contractions" introduced by Asano,[5] developed a method which enables one to find regions of the complex z plane free of pfz's. Here $z = \exp(2\beta h)$ and h is the external magnetic field.

We shall use Ruelle's methods to analyze Ising spin systems on the triangle lattice and other lattices having a triangular structure associated with them, e.g., the Kagomé and Union Jack lattices. Interest in systems of this type dates back to 1950 with Houtappel[6] and Wannier[7] and continues today especially regarding the systems with antiferromagnetic pair interactions; see, for example, Lin and Wu,[8] and also Doczi-Reger and Hemmer,[9] with references therein. Also interest exists in cases having three-body interactions present; see, for example, Baxter and Wu,[10] Wood

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and Pegg,[11] Liu and Stanley,[12] and references therein. Both pair interaction and three-body interaction systems will be considered and in both cases ferromagnetic and antiferromagnetic interactions will be considered.

The purpose of the paper is twofold. First, new uses of the Ruelle theorems are shown, e.g., on systems with many-body interactions. Second, rigorous statements are obtained concerning the location of the pfz's for systems on lattices having triangular structure and from these results statements regarding the nonexistence of phase transitions for these lattices.

In Section 2 the pertinent theorems of Ruelle are presented. Then in Section 3 these theorems are used to acquire results on pfz's for Kagomé, triangle, and Union Jack lattices having only pair interactions, while in Section 4 these same lattices having only three-body interactions are studied.

2. GENERAL RUELLE THEOREMS

For completeness we now state the theorems of Ruelle[4] that we will need in the following sections. Runnels and Hubbard[13] have also restated some of these theorems and in addition have pointed out some important features regarding their use.

Let Λ be a finite set of lattice sites and let P be the partition function for Λ with some given interaction between these sites. A site i is either occupied or unoccupied (in spin language $S_i = \pm 1$). Assuming that we have a different activity at each site then we have

$$P = \sum_{X \subseteq \Lambda} e^{-\beta U(X)} \prod_{x \in X} z_x \tag{2.1}$$

The main theorem of Ruelle is as follows.

Theorem 2.1. Let Λ' and Λ'' be two finite sets of lattice sites and P' and P'' be the partition functions for the two sets of sites. It is assumed that there exist closed subsets M'_x of the complex plane such that $0 \notin M'_x$ and $P' \neq 0$ when

$$z'_x \notin M'_x \tag{2.2}$$

for all $x \in \Lambda'$. Similar assumptions hold for P''. Define

$$P = \sum_{X \subseteq \Lambda' \cup \Lambda''} e^{-\beta U'(X \cap \Lambda') - \beta U''(X \cap \Lambda'')} \prod_{x \in X} z_x \tag{2.3}$$

Then $P \neq 0$ when

$$z_x \notin \begin{cases} M'_x, & x \in \Lambda' \backslash \Lambda'' \\ M''_x, & x \in \Lambda'' \backslash \Lambda' \\ -M'_x M''_x, & x \in \Lambda' \cap \Lambda'' \end{cases} \tag{2.4}$$

where

$$-M_x'M_x'' = \{ -z_x'z_x'' : z_x' \in M_x' \text{ and } z_x'' \in M_x'' \} \tag{2.5}$$

We use the terminology of Runnels and Hubbard and call the product defined by (2.5) the "set product." The major difficulty with the use of this theorem as now stated is that the z_i's are independent of each other, whereas we normally are interested in the case where all the z_i's are equal to one another. The regions M_x are much more difficult to find when z_i's need not be equal to one another. Ruelle's next theorem allows us to set all z_i's equal in special cases and then find regions free of zeros.

Theorem 2.2. Let $Q(z)$ be a polynomial of degree n with complex coefficients and $P(z_1, \ldots, z_n)$ a polynomial which is symmetric in its arguments, of degree 1 in each, and such that

$$P(z, z, \ldots, z) = Q(z) \tag{2.6}$$

If the roots of Q are all contained in a closed circular region M, and $z_i \notin M, \ldots, z_n \notin M$, then $P(z_1, \ldots, z_n) \neq 0$.

A circular region is the inside or outside of a circle or a half-plane. All the systems considered in the following two sections have the symmetry required by Theorem 2.2.

3. PAIR INTERACTION SYSTEMS

In this section we restrict ourselves to the case where only pair interactions occur between the spins. Interactions occur between every pair of spins of each elementary triangle of the lattice. We define $+2J$ to be the interaction energy between two unaligned spins and zero to be the interaction energy beteeen two aligned spins. First the case of ferromagnetic systems, i.e., $J > 0$, will be considered and then the more complicated and more interesting antiferromagnetic systems follow.

Proposition 3.1. There are no pfz's on the positive real z axis, i.e., the free energy is an analytic function of h, if

for the Kagomé lattice, $$0 \leqslant 2\beta J < \frac{1}{2}\log(3) = 0.549 \tag{3.1}$$

for the triangle lattice, $$0 \leqslant 2\beta J < \frac{1}{2}\log\left(\frac{3}{2}\right) = 0.203 \tag{3.2}$$

for the Union Jack lattice,[2] $$0 \leqslant 2\beta J < \frac{1}{2}\log\left(\frac{3}{\sqrt{2}+1}\right) = 0.109 \tag{3.3}$$

[2] There have been two different types of lattices described as "Union Jack" lattices. See, for example, Domb[14] or Temperley[22] for one type and Hintermann and Merlini[15] for the other type. Our Union Jack lattice shown in Fig. 1c is the type of Hintermann and Merlini.[15]

Proof. The partition function for the triangle subgroup with $a \equiv \exp(2\beta J)$ and $y_i = \exp(\beta h_i)$ for $i = 1, 2$, or 3 is

$$P(y_1, y_2, y_3) = y_1 y_2 y_3 + \frac{1}{a^2}\left(y_1 y_2 \frac{1}{y_3} + y_1 \frac{1}{y_2} y_3 + \frac{1}{y_1} y_2 y_3\right) + \frac{1}{a^2}\left(y_1 \frac{1}{y_2 y_3} + \frac{1}{y_1} y_2 \frac{1}{y_3} + \frac{1}{y_1 y_2} y_3\right) + \frac{1}{y_1 y_2 y_3} \quad (3.4)$$

multiplying by $y_1 y_2 y_3$ we have

$$y_1 y_2 y_3 P(z_1, z_2, z_3) = z_1 z_2 z_3 + \frac{1}{a^2}(z_1 z_2 + z_1 z_3 + z_2 z_3) + \frac{1}{a^2}(z_1 + z_2 + z_3) + 1 \quad (3.5)$$

where $z_i = (y_i)^2$. The right-hand side of (3.5) fulfills the conditions of Theorem 2.2 and therefore we need only find a closed circular region M containing all the zeros of the following:

$$Q(z) = z^3 + \frac{3}{a^2} z^2 + \frac{3}{a^2} z + 1 = (z + 1)\left[z^2 + \left(\frac{3}{a^2} - 1\right)z + 1\right] \quad (3.6)$$

In the case of a lattice where each site is in four triangle subgroups as it is for the Union Jack lattice (see Figs. 1c and 1f) we want this closed circular

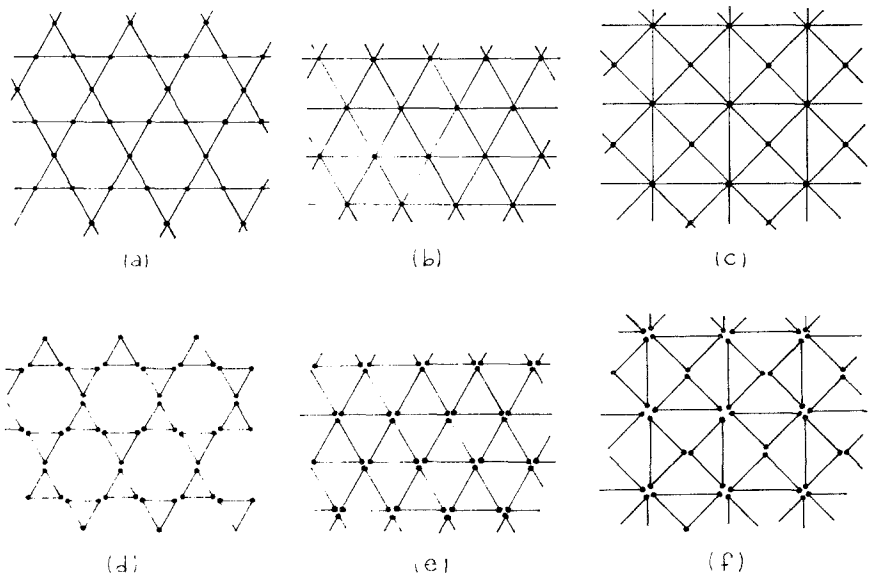


Fig. 1. Parts (a), (b), and (c) are, respectively, the Kagomé, triangle, and Union Jack lattices; (d), (e), and (f) are respectively the Kagomé, triangle, and Union Jack lattices decomposed into their triangle subgroups for systems with pair interactions.

region to be contained in the angular region

$$\frac{3\pi}{4} < \arg z < \frac{5\pi}{4} \tag{3.7}$$

This is because to build up the Union Jack lattice from our triangle subgroups we will need to use Theorem 2.1 a maximum of three times per site. Some sites require only contraction since they belong to only two triangle subgroups but it is those sites belonging to four triangle subgroups which set the limits of the theorem. These sites will be included in three contractions resulting in three set products of the form of Eq. (2.5). After these three set products the region of (3.7) becomes $0 < \arg z < 2\pi$.

Since the zeros of (3.6) lie on the unit circle in the z plane the requirement of the above paragraph results in needing to find the value of a when the zeros of (3.6) are $z = -1$ and $-(1 \pm i)/\sqrt{2}$. This occurs when $a = [3/(\sqrt{2} + 1)]^{1/2}$. For all a's in the interval $1 \leqslant a < [3/\sqrt{2} + 1)]^{1/2}$ the zeros then fall in the region defined by (3.7) and the result (3.3) follows.

Similar analysis results in the bounds (3.1) and (3.2) though in these cases we need only require that M is contained in the regions $\pi/2 \leqslant \arg Z < 3\pi/2$ and $2\pi/3 < \arg Z < 4\pi/3$, respectively. ■

Remarks. (a) The result for the triangle lattice was given in Ruelle.[4]

(b) It is of interest to compare these bounds to the exact values of the critical temperature found by duality and similar transformations. See the review article by Syozi[16] where it is shown that

for the Kagomé lattice,	$2\beta_c J = 0.929$	(3.9)
for the triangle lattice,	$2\beta_c J = 0.549$	(3.9)
for the Union Jack lattice,	$2\beta_c J = 0.509$	(3.10)

One sees from this comparison that as the number of contractions and therefore set products increases the worse the bound on the critical temperature given by the pfz's approach becomes.

For lattices with antiferromagnetic pair interactions, replacing the ferromagnetic interactions just considered, $J \leqslant 0$ and therefore $a \leqslant 1$, the situation is both more interesting and complex. We will consider these systems in two parts. First results similar to those for the ferromagnetic system are found, that is, results giving an upper bound on the critical temperature for *all* values of h. For ferromagnetic systems one knows there is no phase transition for $h \neq 0$ but this is not the case for antiferromagnetic systems. So in our second part we look explicitly at bounds on the critical temperature as a function of h.

Again the triangle subgroup fulfills the condition of Theorem 2 and we need only to find a closed circular region M which is contained in the appropriate angular segment. Of course now for the antiferromagnetic case

the zeros are no longer on the unit circle in the z plane but on the negative real axis.

Proposition 3.2. There are no pfz's on the positive real z axis, i.e., the free energy is an analytic function of h if

$$\text{for the Kagomé lattice,} \qquad -\infty < 2\beta J \leqslant 0 \tag{3.11}$$

$$\text{for the triangle lattice,} \qquad -0.255 = \frac{1}{2}\log\left[\frac{3(2-\sqrt{3})}{10-5\sqrt{3}}\right] < 2\beta J \leqslant 0 \tag{3.12}$$

$$\text{for the Union Jack lattice,} \qquad -0.122 = \frac{1}{2}\log\left[\frac{3(\sqrt{2}-1)}{3-\sqrt{2}}\right] < 2\beta J \leqslant 0 \tag{3.13}$$

Proof. Again we start with the Union Jack lattice. The closed circular region M must be contained in the angular region of (3.7) for the same reasons as stated in the proof of Proposition 3.1. For $a^2 = [3(\sqrt{2}-1)]/[3-\sqrt{2}]$ the zeros are $z = -1$ and $-\sqrt{2} \pm 1$. The two lines with $\arg z = 3\pi/4$ and $\arg z = 5\pi/4$ are tangent to the circle whose center is at $z = -\sqrt{2}$ and whose radius is 1.0. Therefore the circle lies in the proper angular sector and the result, (3.13), follows. The other two lattices are analyzed in a similar manner. ■

Remarks. (a) The results of Proposition 3.2 for the Kagomé lattice can also be proven using a theorem of Heilmann.[17]

(b) The Kagomé and triangle lattices with antiferromagnetic pair interactions have been shown to have no phase transition at $h = 0$. The pfz approach above duplicates this result for the Kagomé lattice but not for the triangle lattice. This once again shows that the larger the number of contractions necessary to build up the lattice, the less accurate the bound.

For nonzero values of h the triangle lattice with antiferromagnetic pair interactions is still of interest today. It was first conjectured by Domb[14] that for $h \neq 0$ a phase transition may exist and that the phase diagram has the form sketched in Fig. 2. A review of some of the initial approximate solutions is given by Burley.[18] Recent results can be found in Lin and Wu,[8] Doczi-Reger and Hemmer,[9] and also Kinzel and Schick.[19] We know of no rigorous results on this system for $h \neq 0$. We now use Ruelle's pfz method to find regions in the h–T plane where the free energy is analytic. Before we state the results we will need the following lemma.

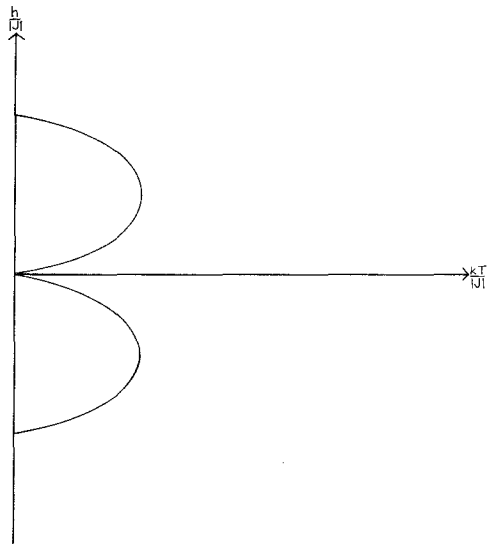


Fig. 2. Conjectured phase diagram for the triangle lattice with nearest-neighbor antiferromagnetic interactions.

Lemma 3.3. For a region M which is a half-plane of the z plane which crosses the negative real z axis at a point b as shown in Fig. 3, the nth set product of the region does not contain the following interval of the real z plane:

$$0 \leqslant z < \left[\frac{|b|}{\cos(\pi/(n+1))} \right]^{n+1} \tag{3.14}$$

Proof. See Appendix A.

Remark. In the use of Ruelle's theorems by Runnels and Hubbard[13] for hard-core lattice gas systems, similar half-plane regions were used. In their determination of the zero-free region of the real z axis they were forced to use two assumptions in taking the set product. The above does away with a need for these assumptions and eliminates some lengthy use of Lagrange multipliers.

Proposition 3.4. For the triangle lattice one has that for values of J, β, and h such that

$$z < \left| \left(1 - \frac{3}{a^2}\right) + \left[\left(\frac{3}{a^2} - 1 \right) - 4 \right]^{1/2} \right|^3 \tag{3.15}$$

the free energy is an analytic function.

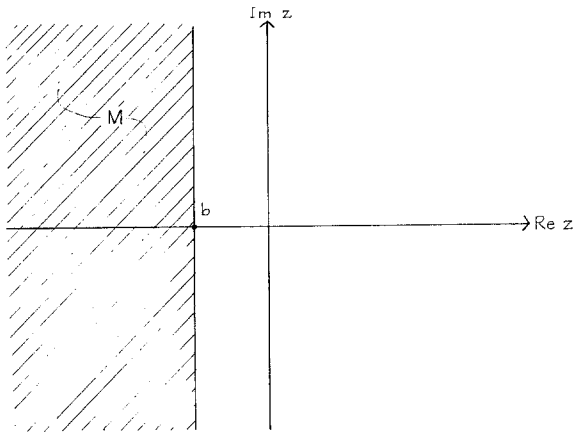


Fig. 3. The half-plane M containing the zeros of the triangle subgroup partition function.

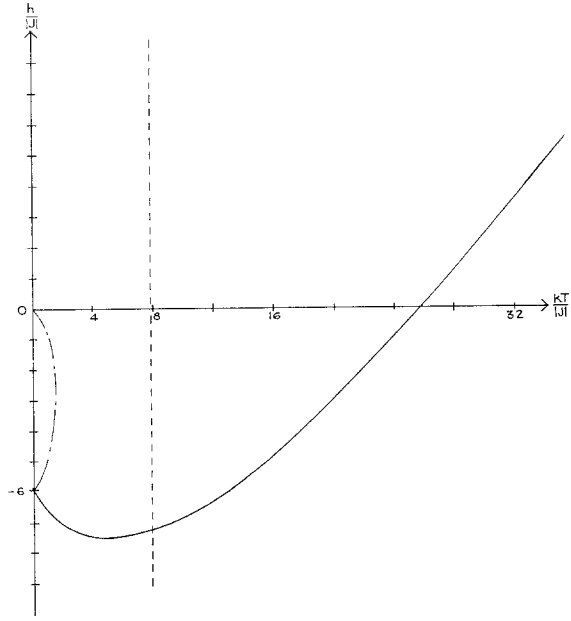


Fig. 4. The solid line denotes the boundary of the zero-free region of the $h-T$ plane given by (3.15), the dotted line gives the zero-free region given by (3.12), and the dot–dash line represents Monte Carlo results for the phase diagram.[19] All are for the triangle lattice with nearest-neighbor antiferromagnetic interactions.

Proof. We decompose the triangle lattice as before into triangle subgroups and the partition function we need is again Eq. (3.6). We want to find a region M containing the zeros of (3.6) of the form of M in Fig. 3. The edge of the half-plane will cross the negative real z axis at the value of the maximum zero. This value is denoted as b in Fig. 3 and is given by

$$b = \frac{1}{2}\left[\left(1 - \frac{3}{a^2}\right) + \left[\left(\frac{3}{a^2} - 1\right) - 4\right]^{1/2}\right] \tag{3.16}$$

Since two contractions on each site are necessary to build up the triangle lattice from our subgroup we must have two set products, i.e., $n = 2$, and by Lemma 3.3 the result follows. ■

Remarks. (a) The zero-free regions of the h–T plane given by Proposition 3.4 and that given by Proposition 3.2, are shown in Fig. 4.

(b) The zero-free region of Fig. 4 can be extended to include the reflection of this region about the kT/J axis because of the symmetry of the Hamiltonian.

4. THREE-BODY INTERACTION SYSTEMS

We now consider the Union Jack, triangle, and Kagomé lattices where only three-body interactions between the three sites of the triangle subgroups are present along with the interactions with the external magnetic field. The author knows of no prior use of the Ruelle theorems to study systems with many-body interactions. The initial theorems were not restricted to pair interactions but the analysis itself may be much more complicated than with pair interaction cases. The particular cases considered here are only slightly more complicated because we retain the symmetry of the partition function necessary to use Theorem 2.2.

We take as the Hamiltonian for each elementary triangular group of the lattice

$$H(s_1, s_2, s_3) = -J' s_1 s_2 s_3 - \sum_{i=1}^{3} h_i s_i \tag{4.1}$$

Proposition 4.1. There are no pfz's on the positive real z axis if

for the Kagomé lattice, $$-\infty < \beta J < \infty \tag{4.2}$$

for the triangle lattice, $$\log\left(\frac{54}{55}\right) < \beta J < \log\left(\frac{55}{54}\right) \tag{4.3}$$

for the Union Jack lattice, $$\log\left(\frac{129}{130}\right) < \beta J < \log\left(\frac{130}{129}\right) \tag{4.4}$$

given the Hamiltonian Eq. (4.1) on each elementary triangle of the lattice.

Proof. The partition function for the triangle subgroups with Hamiltonian (4.1) is

$$P(y_1, y_2, y_3) = wy_1y_2y_3 + \frac{1}{w}\left(y_1y_2\frac{1}{y_3} + y_1\frac{1}{y_2}y_3 + \frac{1}{y_1}y_2y_3\right) + w\left(y_1\frac{1}{y_2y_3} + \frac{1}{y_1}y_2\frac{1}{y_3} + \frac{1}{y_1y_2}y_3\right) + \frac{1}{w}\frac{1}{y_1y_2y_3} \tag{4.5}$$

with $w = \exp(\beta J')$ and $y_i = \exp(\beta h_i)$. As with the pair interaction case the partition function rewritten in terms of $z_i = \exp(2\beta h_i)$ satisfies the symmetry requirements of Theorem 2.2 and therefore we need only find a closed circular region M containing all the zeros of

$$Q(z) = wz^3 + \frac{3}{w}z^2 + 3wz + \frac{1}{w} \tag{4.6}$$

For both positive and negative values of J there is one zero of (4.6) which lies on the negative real z axis. The other two are complex conjugates of one another and lie on circles centered at $\pm i(1/\sqrt{3})$ with radius $2/\sqrt{3}$. All three zeros move in the z plane as a function of βJ, whereas in Section 3 one zero remained fixed at $z = -1$. Therefore (4.6) does not reduce itself to a quadratic equation as (3.6) did. We have thus used the computer to find the zeros of (4.6).

Again as in the pair interaction case we need the closed circular region M to be contained in the appropriate angular region of the z plane. However, these angular regions are not the same as needed for the pair interaction systems because the number of contractions necessary to build up the desired lattice is not the same, except for the Kagomé lattice. For the triangle lattice we now need five contractions per site (see Fig. 5a), and some sites in the Union Jack lattice require seven contractions per site (see Fig. 5b). Since for the Kagomé lattice we only need the zeros to be in the left half-plane we have no phase transition for all finite βJ. The bounds on βJ given for the other two lattices are sufficient to guarantee that M is small enough to be contained in the proper angular regions. As stated above the zeros were found using a computer and then it was proven that the three zeros of Eq. (4.6) with βJ values as given in the proposition could be contained in a circular region M which itself could be contained in the appropriate angular region. ■

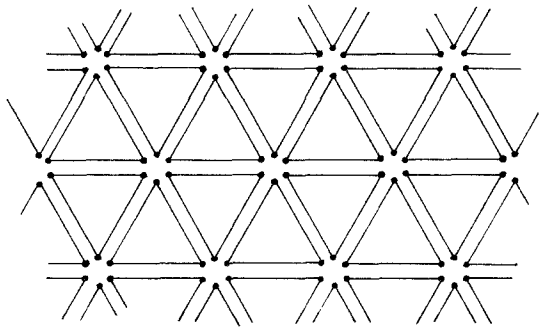
Remarks. (a) Any lattice which can be decomposed into three site subgroups with the three sites interacting via a three-body interaction can be treated by this method. This would include the triangulated dice lattices considered by Wu,[20] and by Liu and Stanley.[12] These lattices require an

even greater number of contractions than those systems considered in Proposition 4.1 and once again the bounds become less accurate.

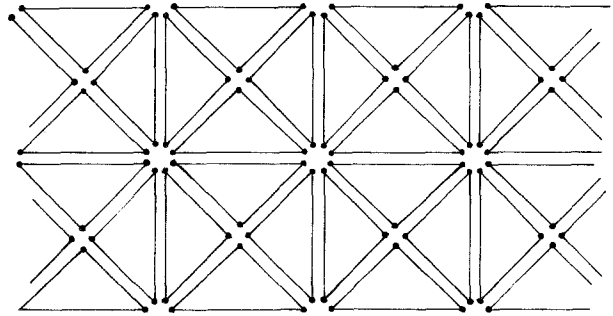
Considering cases where less contractions are necessary one can use the decompositions shown in Figs. 1e and 1f to construct triangle and Union Jack lattices with three-body interactions amongst only alternating triangles of the lattice.

(b) Bounds on the region of the $h-T$ plane where no phase transition occurs could also be found by the same basic methods as used in Section 3.

(c) Finally it should be pointed out that systems with interactions other than three-body interaction systems can be decomposed into elementary subgroups and if they have the symmetry required by Theorem 2.2 can be



(a)



(b)

Fig. 5. Part (a) is the triangle lattice decomposed into triangle subgroups for systems with three-body interactions; (b) is the Union Jack lattice decomposed for the similar situation.

easily studied using the pfz approach. For example, a four-body interaction amongst the four sites of a square subgroup has the required symmetry. Such a subgroup can be used to construct the "three-dimensional" Ising models with four spin interactions studied by Suzuki.[21]

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APPENDIX A

Proof of Lemma 3.3. For notational simplicity we prove the lemma for two set products. The extension to n set-products follows immediately from the same method. For one set product we choose any $z_1 \in M$ and $z_2 \in M$ and form $-z_1 z_2$. For two set products we choose an additional $z_3 \in M$ and take the product $z_1 z_2 z_3$. The proof now consists of two parts.

(A) We are only interested in the region of the positive real z axis that is not covered by the product $z_1 z_2 z_3$. Clearly the interval $0 < z < |b|^3$ is not covered by the product, but as we move further out along the z axis we will reach a minimum value of z which is covered. Call this minimum value $z_{\min} = C$ and assume $z_1' z_2' z_3' = C$. We first show that z_1', z_2', and z_3' are all located on the edge of M. In polar form $z_j = r_j \exp(i\phi_j)$ for $j = 1$, 2, and 3. For $z_1' z_2' z_3'$ we must have $\phi_1 + \phi_2 + \phi_3 = 2\pi$ or 4π and $r_1 r_2 r_3 = C$. Now if z_1', z_2', and z_3' are not all on the edge of M then we could proceed inward along a radial line keeping $\phi_1 + \phi_2 + \phi_3 = 2\pi$ or 4π but reducing the value of r_j for any j where z_j' is not on the edge. But then C is not the minimum. Hence for the minimum we must have all the z_j' on the edge of M.

(B) We now must show, given part (A), that $\phi_1 = \phi_2 = \phi_3$ and thus $\phi_j = 2\pi/3$ for all j or $4\pi/3$ for all j. Since M crosses the negative z axis at b and all r_j are on the edge of M, then $r_j = |b|/\cos\theta_j$ where $\theta_j = \pi - \phi_j$. The condition on $\phi_1 + \phi_2 + \phi_3$ becomes $\theta_1 + \theta_2 + \theta_3 = \pm\pi$. The product $z_1 z_2 z_3$ becomes $|b^3|/\cos(\theta_1)\cos(\theta_2)\cos(\theta_3)$ and thus for this to be a minimum the product of the cosines must be a maximum. The product can be written as $-\cos(\theta_k)\cos(\theta_i)\cos(\theta_k + \theta_i)$ for $k = 1$, 2, or 3 and $i = 1$, 2, or 3 but $k \neq i$. Since we want the maximum we take partial derivatives and set them equal to zero obtaining the following condition:

$$\tan\theta_k = -\tan 2\theta_i \tag{A1}$$

Therefore it follows that $\theta_k + 2\theta_i = n\pi$. The restriction on the θ_j that $-\pi/2 < \theta_j < \pi/2$ constrains the n to the values 0 and ± 1. The restriction

that $\theta_1 + \theta_2 + \theta_3 = \pm\pi$ eliminates the possibility of $n = 0$. It also shows that $\theta_k + 2\theta_i = \pi$ only when $\theta_1 + \theta_2 + \theta_3 = \pi$ or $\theta_k + 2\theta_i = -\pi$ only when $\theta_1 + \theta_2 + \theta_3 = -\pi$. From this one obtains $\theta_1 = \theta_2 = \theta_3$. ■

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