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An Exactly Soluble Case of the Triangular Ising Model in a Magnetic Field

A. M. W. Verhagen[1]

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An anisotropic triangular Ising model in which the first- and second-order parameters and the field parameters are functionally related is solved exactly by representing the distribution of the atom patterns in terms of a suitably constructed Markov process. The probabilities of patterns, defined as the probabilities generated by this process, are a mathematically tractable alternative to the classical representation of these probabilities in terms of the partition function. The interaction and field parameters of this Ising model, its magnetization, free energy, and its nearest neighbor correlation functions, are expressed in terms of the parameters of this Markov process. Special cases are worked out in detail and numerical examples are given.

KEY WORDS: Ising models; correlation functions; exclusion patterns; Markov processes; probability generating processes; large atoms; interacting atoms; partition functions; triangular lattice; rectangular lattice; disorder point.

1. INTRODUCTION

The evaluation of the probabilities of atom patterns obeying the Ising model involves a knowledge of the partition function. The partition function of the Ising model has not been found, except for the special case—where the external field parameter B is zero—known as the Onsager solution.[1-3] Here it is shown that an anisotropic triangular Ising model in a field can be solved, provided the interactions and field strength satisfy a certain condition Unfortunately, this condition is temperature dependent. In zero field it implies that the model is at its disorder point.[4,5] The general form of this relation is defined by Eqs. (24), which reduce to (30). Following methods developed by the author in earlier papers,[6] the solution is achieved by constructing a suitable Markov process to represent the probability distribu-

[1] CSIRO Division of Mathematics and Statistics, Canberra City, Australia.

tion of the atom patterns. As a mathematically tractable example of this method, it is proposed to represent a family of generalized Ising distributions of atom patterns on the triangular lattice in terms of a Markov process on the lattice. The parameters of this family of generalized Ising distributions will be expressed in the parameters of the Markov process. The Markov representation thus achieved will be used to find the partial derivatives of the free energy or, equivalently, the coverage (or magnetization) and the first and second correlation functions as well as the free energy of the Ising model itself [cf. (38)].

It is anticipated that by inventing suitable Markov processes involving transition probabilities with respect to more complex atom patterns on the two preceding rows it will be possible to extend the methods developed in this paper to represent more complex Ising models or use these processes to match higher order correlation functions.

2. THE ISING MODEL ON THE TRIANGULAR LATTICE

Consider the triangular lattice, represented in Fig. 1. All sites of the lattice are topologically equivalent; each site has four diagonal neighbors and two horizontal ones. This feature is illustrated in Fig. 2, where sites around the site ξ are labeled 1 or 2 according to whether they are diagonal or horizontal neighbors.

Let the coordinates (i, j) of a site be defined as in Fig. 3, and let the indicator variable $\mu_{i,j}$ for the site (i, j) take the value $+1$ when the site carries an atom and the value -1 when the site (i, j) is empty ($\infty < i < \infty$, $-\infty < j < \infty$). Let $\boldsymbol{\mu}$ represent the collection of all $\mu_{i,j}$ specified for the triangular lattice. The generalized Ising probability of any pattern of atoms on the triangular lattice may then be formally written

$$\mathscr{G}(\boldsymbol{\mu}) = (1/Z)\exp[K_1(\sum \mu_{i,j}\mu_{i+1,j} + \sum \mu_{i,j}\mu_{i,j+1}) + K_2 \sum \mu_{i,j}\mu_{i+1,j+1} + B \sum \mu_{ij}] \tag{1}$$

where the partition function Z is

$$Z = \sum_{\boldsymbol{\mu}} \exp[K_1(\sum \mu_{i,j}\mu_{i+1,j} + \sum \mu_{i,j}\mu_{i,j+1}) + K_2 \sum \mu_{ij}\mu_{i+1,j+1} + B \sum \mu_{ij}] \tag{2}$$

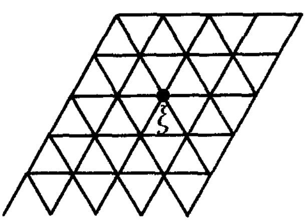


Fig. 1. The anisotropic triangular lattice.

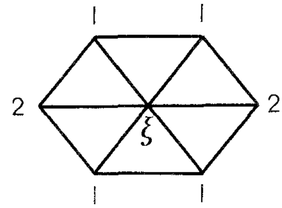


Fig. 2. Diagonal and horizontal neighbor sites around the site ξ.

in which K_1, K_2, and B are expressible in the first two coupling constants and the field by the factor $1/kT$ (cf. Thompson[3]).

Consider the removal of an atom from the site (i, j), which has n_1 diagonal neighbor atoms and n_2 horizontal neighbor atoms. The ratio $\mathscr{R}_{n_1n_2}(K_1, K_2, B)$ of the probabilities of the atom pattern on the lattice with $\mu_{ij} = +1$ and $\mu_{ij} = -1$, i.e., before and after the removal of the atom from the site (i, j), is

$$\begin{aligned}\mathscr{R}_{n_1n_2}(K_1, K_2, B) &= \exp(4n_1K_1 - 8K_2 + 4n_2K_2 - 4K_2 + 2B)\\ &= \exp(2B - 8K_1 - 4K_2)\exp(4K_1n_1)\exp(4K_2n_2) \qquad (3a)\end{aligned}$$

The ratio of the probabilities before and after placing an atom on an empty site $(\bar{i}, \bar{j})$ with $\bar{n}_1$ diagonal neighbor atoms and $\bar{n}_2$ horizontal neighbor atoms is $\mathscr{R}_{\bar{n}_1\bar{n}_2}^{-1}(K_1, K_2, B)$. The effect of one removal from a site (i, j) and one placement of an atom on a site $(\bar{i}, \bar{j})$ in this manner is equivalent to a transfer of an atom from the site (i, j) to the site $(\bar{i}, \bar{j})$. The ratio of the probabilities of the patterns on the lattice before and after such a transfer is

$$\mathscr{T}_{n_1-\bar{n}_1, n_2-\bar{n}_2}(K_1, K_2) = \exp[4K_1(n_1 - \bar{n}_1)]\exp[4K_2(n_2 - \bar{n}_2)] \qquad (3b)$$

As a first step toward finding a Markov representation of the generalized Ising distribution defined by (1), it is proposed to construct a distribution which has the removal ratio (3a) and the transfer ratio (3b) of the generalized

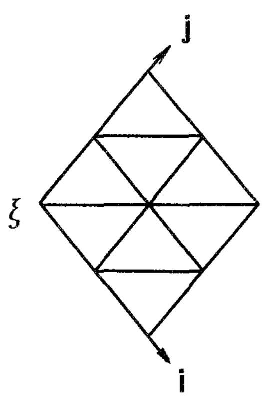


Fig. 3. Coordinates (i, j) for the sites of the triangular lattice.

Ising distribution. This distribution will be called the P distribution to distinguish it from the $\mathscr{G}$ distribution defined by (1).

3. DEFINITION OF THE P DISTRIBUTION OF ATOM PATTERNS ON THE TRIANGULAR LATTICE

Consider the sawtooth arrangement of sites ξ_1, ξ_2,... embedded in the triangular lattice as illustrated in Fig. 4.

Let the superscript $\bullet$ as in $\xi_k^\bullet$ indicate the presence of an atom on the site ξ_k and let the superscript $\circ$ as in ξ_k° indicate that there is no atom on the site ξ_k. Consider the Markov process defined on the sawtooth sites of Fig. 1 by the probabilities

$$\begin{aligned} &\mathrm{Prob}\{\xi_{k+1}^\bullet \mid \xi_k^\bullet\} = a, \qquad &\mathrm{Prob}\{\xi_{k+1}^\circ \mid \xi_k^\bullet\} = 1 - a \\ &\mathrm{Prob}\{\xi_{k+1}^\bullet \mid \xi_k^\circ\} = b, \qquad &\mathrm{Prob}\{\xi_{k+1}^\circ \mid \xi_k^\circ\} = 1 - b \end{aligned} \tag{4}$$

where the vertical bars are read as "given that."

Since under this process the probability that a site carries an atom depends only on whether or not an atom is present on the preceding site, the probability θ that a sawtooth site carries an atom must satisfy

$$\theta = (1 - \theta)b + \theta a \tag{5}$$

which reduces to

$$\theta = b/[(1 - a) + b] \tag{6}$$

This probability is known as the numerical density of the atoms, and is called the coverage of the lattice. It is equal to $\frac{1}{2}(1 + M)$, where M is the magnetization of the lattice.

The sawtooth arrangement of sites illustrated in Fig. 1 may be regarded as consisting of two horizontal rows of sites. The probability distributions of the atom patterns on each row, taken separately, are identical and each depends on the other in the same way. From the distribution of atom patterns on the two rows of sites defined by (4) one may determine the probability distribu-

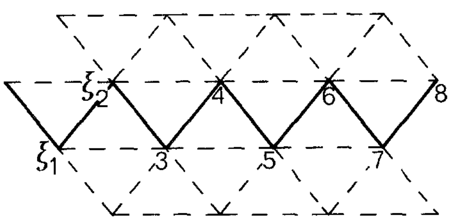
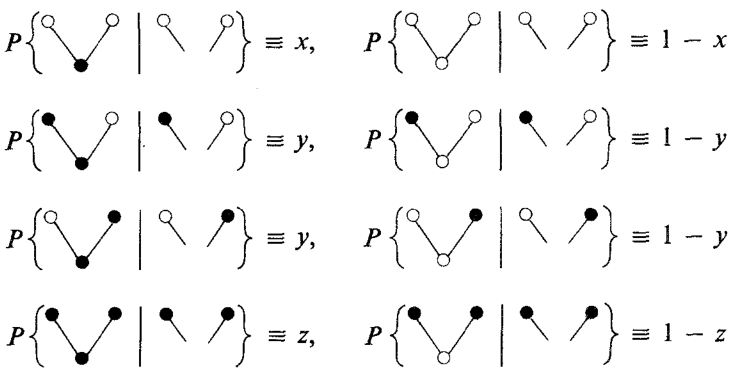


Fig. 4. Sawtooth arrangement of sites ξ_1, ξ_2,... embedded in the triangular lattice.

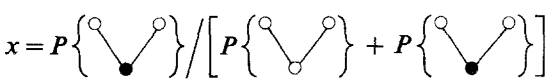
tion of patterns on one row given the pattern on the other. For instance, the pattern on the sites ξ_k and ξ_{k+2} on one row determines the probability of an atom on the site on the other row. The probabilities of interest for the purpose of this paper may be presented and defined as follows:



(7)

where a vertical bar is read as "given that," solid circles represent atoms, and open circles represent empty sites.

The conditional probabilities defined by (7) of patterns on one row given the patterns on the other are readily expressed in terms of the parameters a and b of the Markov process defined by (4). Thus



$$= (1 - \theta)b(1 - a)/\{(1 - \theta)(1 - b)^2 + (1 - \theta)b(1 - a)\} \qquad (8)$$

$$= b(1 - a)/[(1 - b)^2 + b(1 - a)]$$

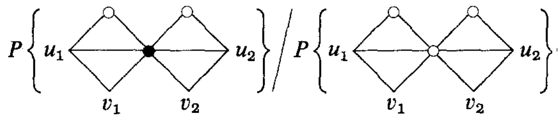
where $1 - \theta$ is the probability that a site is empty and the probabilities of successive atoms and empty sites are defined by (4). Hence

$$x = b(1 - a)/[b(1 - a) + (1 - b)^2], \quad 1 - x = (1 - b)^2/[b(1 - a) + (1 - b)^2]$$
$$y = a/(1 + a - b), \quad 1 - y = (1 - b)/(1 + a - b) \qquad (9)$$
$$z = a^2/[a^2 + (1 - a)b], \quad 1 - z = (1 - a)b/[a^2 + (1 - a)b]$$

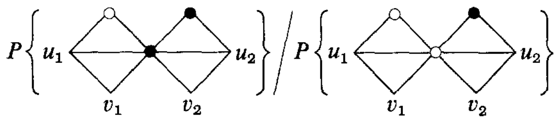
Starting with a pattern on a row of sites, one may generate the probability of patterns on the next row with the aid of the probabilities (9). Repeated application to successive rows generates a probability for any specified pattern on the triangular lattice. The probability distribution of atom patterns defined by this Markovian row-by-row process is stationary and forms a two-parameter family of P distributions.

4. REMOVAL AND TRANSFER RATIOS OF THE P DISTRIBUTIONS

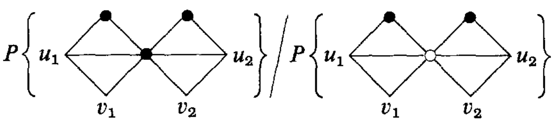
Let u_1, v_1, $\tilde{v}_1$, e, v_2, $\tilde{v}_2$, and u_2 stand for the indicator variables for a site and its neighbors on the first two shells as illustrated in Fig. 5. Then from the row-by-row process defined by (7) it follows that whatever the pattern $(u_1v_1v_2u_2)$, the following hold:



$$= F(u_1, v_1, v_2, u_2)\,\frac{b(1-a)}{(1-b)^2} \tag{10}$$



$$= F(u_1, v_1, v_2, u_2)\,\frac{a}{1-b} \tag{11}$$



$$= F(u_1, v_1, v_2, u_2)\,\frac{a^2}{(1-a)b} \tag{12}$$

where $F(u_1, v_1, v_2, u_2)$ depends only on the pattern $(u_1v_1v_2u_2)$.

The ratios (11)/(10) and (12)/(11) both reduce to $a(1-b)/b(1-a)$ irrespective of the pattern $(u_1v_1v_2u_2)$. Let A_{n_1} stand for the pattern on a site and its diagonal neighbor sites when the central site carries an atom and the number of atoms on these four diagonal neighbor sites is n_1. Similarly, let B_{n_1} stand for the pattern obtained from A_{n_1} by removing the central atom. Then $(u_1A_{n_1}u_2)$ defines a pattern on a site and its diagonal neighbor and $(u_1B_{n_1}u_2)$ represents the pattern obtained from it by removing the central atom. It follows from the invariance of the ratios (11)/(10) and (12)/(11) that

$$\frac{P(u_1A_{n_1}u_2)}{P(u_1B_{n_1}u_2)} = \frac{a(1-b)}{b(1-a)}\,\frac{P(u_1A_{n_1-1}u_2)}{P(u_1B_{n_1-1}u_2)} = \left[\frac{a(1-b)}{b(1-a)}\right]^{n_1}\frac{P(u_1A_0u_2)}{P(u_1B_0u_2)} \tag{13}$$

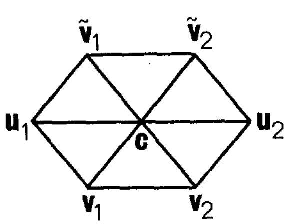


Fig. 5. Indicator variables u_1, v_1, $\tilde{v}_1$, v_2, $\tilde{v}_2$, and u_2 for a site and its six neighbor sites.

The last factor of (13) is a ratio of probabilities of patterns before and after removal and may be expressed as a ratio of probability of simpler patterns by noting that the probability $P(u_1A_0u_2)$ may be written in terms of the pattern (u_1, e, u_2) with $e = 1$. This gives

$$P(u_1A_0u_2) = P(u_1, 1, u_2)(1 - z)^{2u_1}(1 - y)^{2(1-u_1)}(1 - z)^{2u_2}(1 - y)^{2(1-u_2)}$$

$$= P(u_1, 1, u_2)\left(\frac{1 - z}{1 - y}\right)^{2(u_1+u_2)}(1 - y)^4 \tag{14}$$

Similarly,

$$P(u_1B_0u_2) = P(u_1, 0, u_2)\left(\frac{1 - y}{1 - x}\right)^{2(u_1+u_2)}(1 - x)^4 \tag{15}$$

so that the ratio (15)/(14) becomes

$$\frac{P(u_1, A_0, u_2)}{P(u_1, B_0, u_2)} = \left[\frac{(1 - z)(1 - x)}{(1 - y)^2}\right]^{2(u_1+u_2)}\left(\frac{1 - y}{1 - x}\right)^4\frac{P(u_1, 1, u_2)}{P(u_1, 0, u_2)} \tag{16}$$

To reduce the last factor of (16) further it will be convenient to note that from the Markov process defined by (4) it follows that

$$\begin{aligned} P(e = 1, u_1 = 1) &= \theta[a^2 + (1 - a)b] \\ P(e = 1, u_1 = 0) &= \theta[a(1 - a) + (1 - a)(1 - b)] \end{aligned} \tag{17a}$$

and

$$\begin{aligned} P(e = 0, u_1 = 1) &= (1 - \theta)[ba + (1 - b)b] \\ P(e = 0, u_1 = 0) &= (1 - \theta)[b(1 - a) + (1 - b)^2] \end{aligned} \tag{17b}$$

which immediately yields the conditional probability of u_1 given c, as

$$\begin{aligned} P(u_1 = 1|e = 1) &= [a^2 + (1 - a)b] \\ P(u_1 = 0|e = 1) &= [a(1 - a) + (1 - a)(1 - b)] \end{aligned} \tag{18a}$$

and

$$\begin{aligned} P(u_1 = 1|e = 0) &= [ba + (1 - b)b] \\ P(u_1 = 0|e = 0) &= [b(1 - a) + (1 - b)^2] \end{aligned} \tag{18b}$$

It follows by using (18a) and (18b) that

$$P(u_1, 1, u_2) = \theta[a^2 + (1 - a)b]^{u_1+u_2}[a(1 - a) + (1 - a)(1 - b)]^{2-u_1-u_2} \tag{19}$$

and that

$$P(u_1, 0, u_2) = (1 - \theta)[ba + (1 - b)b]^{u_1+u_2}[b(1 - a) + (1 - b)^2]^{2-u_1-u_2} \tag{20}$$

and hence

$$\frac{P(u_1, 1, u_2)}{P(u_1, 0, u_2)} = \frac{\theta}{1-\theta} \frac{[a(1-a) + (1-a)(1-b)]^2}{[b(1-a) + (1-b)^2]^2}$$

$$\times \left[\frac{a^2 + (1-a)b}{a(1-a) + (1-a)(1-b)} \frac{b(1-a) + (1-b)^2}{ba + (1-b)b}\right]^{n_2} \tag{21}$$

where n_2 as before stands for the number of horizontal neighbor atoms.

By substituting (20), the expression (12) reduces to

$$\frac{P(u_1 A_{n_1} u_2)}{P(u_1 B_{n_1} u_2)} = \left\{\frac{\theta}{1-\theta}\left(\frac{1-y}{1-x}\right)^4 \frac{[a(1-a) + (1-a)(1-b)]^2}{[b(1-a) + (1-b)^2]^2}\right\}\left[\frac{a(1-b)}{b(1-a)}\right]^{n_1}$$

$$\times \left\{\frac{(1-z)^2(1-x)^2}{(1-y)^4} \frac{[a^2 + (1-a)b][b(1-a) + (1-b)^2]}{[a(1-a) + (1-a)b][ba + (1-b)b]}\right\}^{n_2}$$

$$\equiv R_{n_1 n_2}(a, b) \tag{22a}$$

Since x, y, and z are expressible in terms of a and b with the aid of formulas (9), the removal ratio $R_{n_1 n_2}(a, b)$ depends only on a, b, n_1 and n_2. When an atom with n_1 diagonal neighbor atoms and n_2 horizontal neighbor atoms is transferred to an empty site with $\tilde{n}_1$ diagonal neighbor atoms and $\tilde{n}_2$ horizontal neighbor atoms, then the transfer ratio, i.e., the ratio of the probabilities of the atom patterns on the lattice before and after the transfer, is $T_{n_1-\tilde{n}_1, n_2-\tilde{n}_2}(a, b)$ and reduces to

$$T_{n_1-\tilde{n}_1, n_2-\tilde{n}_2}(a, b) = \left[\frac{a(1-b)}{b(1-a)}\right]^{n_1-\tilde{n}_1}$$

$$\times \left\{\frac{(1-z)^2(1-x)^2}{(1-y)^4}\right.$$

$$\left.\times \frac{[a^2 + (1-a)b][b(1-a) + (1-b)^2]}{[a(1-a) + (1-a)(1-b)]\,[ba + (1-b)b]}\right\}^{n_2-\tilde{n}_2} \tag{22b}$$

5. THE IDENTITY OF THE FAMILY OF *P* DISTRIBUTIONS AND A FAMILY OF ISING DISTRIBUTIONS ON THE TRIANGULAR LATTICE

The removal ratio $\mathscr{R}_{n_1 n_2}(K_1, K_2, B)$ for the generalized Ising model defined by (3a) and the removal ratio $R_{n_1 n_2}(a, b)$ of the P distribution may be made identical by choosing the parameters K_1, K_2, and B to satisfy the conditions

$$e^{4K_1} = \frac{a(1-a)}{b(1-a)} \tag{23a}$$

$$e^{4K_2} = \frac{(1-z)^2(1-x)^2}{(1-y)^4} \frac{[a^2+(1-a)b][b(1-a)+(1-b)^2]}{[a(1-a)+(1-a)(1-b)][ba+(1-b)b]} \tag{23b}$$

$$e^{2B-8K_1-4K_2} = \frac{\theta}{1-\theta}\frac{(1-y)^4}{(1-x)^4}\frac{[a(1-a)+(1-a)(1-b)]^2}{[b(1-a)+(1-b)^2]^2} \tag{23c}$$

After expressing x, y, and z in terms of a and b using (9) and some reduction, it follows that

$$e^{4K_1} = a(1-b)/b(1-a) \tag{24a}$$

$$e^{4K_2} = b(1-a)(1+a-b)^2/(a^2+b-ab)(1-b+b^2-ab) \tag{24b}$$

$$e^{2B} = a^2(1-b+b^2-ab)/(1-b)^2(a^2+b-ab) \tag{24c}$$

showing that the family of generalized Ising distribution with parameter values K_1, K_2, and B matching a and b as in (24a)–(24c) has removal and placement ratios identical with the P distribution with parameters a and b. Thus the placement of successive atoms on the lattice affects the probability of the patterns under the two distributions equally.

From the definition of transfer ratios in terms of removal and placement ratios it follows that the transfer ratios of the two distributions are also identical when the parameters are matched. For a given pattern with coverage θ any other pattern with coverage θ may be obtained by transfers of atoms. The probability of any pattern obtained in this way may be expressed in the probability of the given pattern by a factor which is the same under the two distributions. Since the sum of the probabilities of all patterns is unity, the probability of the given pattern must be the same under the two distributions. It follows that the probability of each pattern is the same under the two distributions, i.e., the generalized Ising distribution is identical with the P distribution when their parameters are matched by (24a)–(24c). The relations between K_1, K_2, and B defined by (24a)–(24c) may also be obtained explicitly by eliminating a and b. Thus, after rewriting (24a) as

$$b = a/[(1-a)e^{4K_1}+a] \tag{25a}$$

or

$$(1-b) = (1-a)e^{4K_1}/[(1-a)e^{4K_1}+a] \tag{25b}$$

it may be used to simplify (24c) to

$$\frac{1 + [a/(1-b)]e^{-4K_1}}{1 + [(1-b)/a]e^{-4K_1}} = e^{2B} = \frac{1 + Re^{-4K_1}}{1 + (1/R)e^{-4K_1}} \tag{26}$$

where

$$R = \frac{a}{1-b} = (e^{2B+4K_1} - e^{4K_1}) + [(e^{2B} - e^{4K_1})^2 + 4e^{2B}]^{1/2} \tag{27}$$

Using (27) in (25b), we obtain

$$\frac{a}{R} = \frac{(1-a)e^{4K_1}}{(1-a)e^{4K_1} + a} \tag{28}$$

so that

$$a = \frac{(1+R) + [(1-R)^2 + 4Re^{-4K_1}]^{1/2}}{2(1 - e^{-4K_1})} \tag{29}$$

The relation between K_1, K_2, and B, which results by substituting (29) and (25a) in (24b), may conveniently be expressed as[7]

$$e^{4K_2}\cosh^2(2K_1) - 1 = e^{4K_1}(e^{-4K_2} - 1)\sinh^2 B \tag{30}$$

which is readily verified by substituting directly in (30) with (24a)–(24c).

6. CORRELATION FUNCTIONS AND FREE ENERGY

Differentiation of the free energy, defined as[1–3]

$$-\psi/kT \equiv \lim_{N\to\infty} [(\ln Z_N)/N] \tag{31}$$

where Z_N is the partition function for a large, torus-wrapped lattice of N sites, gives[1]

$$(\partial/\partial B)(-\psi/kT) = \langle\mu_{i,j}\rangle \tag{32a}$$

$$(\partial/\partial K_1)(-\psi/kT) = 2\langle\mu_{i,j}\mu_{i,j+1}\rangle \tag{32b}$$

$$(\partial/\partial K_2)(-\psi/kT) = \langle\mu_{i,j}\mu_{i+1,j+1}\rangle \tag{32c}$$

For Ising distributions on the triangular lattice identical with P distributions, expressions (32a)–(32c) may be derived directly from the Markov process (4) defining the P distribution. This gives

$$\langle\mu_{i,j}\rangle = \theta(+1) + (1-\theta)(-1) = -1 + 2\theta = -1 + \frac{2b}{(1-a)+b} \tag{33a}$$

i.e.,

$$\frac{\partial}{\partial B}\left(-\frac{\psi}{kT}\right) = -1 + \frac{2b}{(1-a+b)} \tag{33b}$$

similarly

$$\langle \mu_{i,j}\mu_{i,j+1}\rangle = \theta a(+1) + \theta(1-a)(-1) + (1-\theta)(1-b)(+1) + (1-\theta)(-1)$$

which, by using (5), reduces to

$$\langle \mu_{i,j}\mu_{i,j+1}\rangle = \frac{4ab - 3b + 1 - a}{1 - a + b} = 1 - \frac{4b(1-a)}{(1-a)+b} \tag{34a}$$

i.e.,

$$\frac{\partial}{\partial K_1}\left(-\frac{\psi}{kT}\right) = 2\left[1 - \frac{b(1-a)}{(1-a)+b}\right] \tag{34b}$$

To find $\langle \mu_{i,j}\mu_{i+1,j+1}\rangle$, note that the relative positions of the indicator variates c and u_1 defined in Section 4 are as that of μ_{ij} and $\mu_{i+1,j+1}$. Using the equations (17a) and (17b) developed for c and u_1, it follows that

$$\begin{aligned}\langle \mu_{i,j}\mu_{i+1,j+1}\rangle = {} & \theta[a^2 + (1-a)b](+1) + \theta[a(1-a) + (1-a)(1-b)](-1)\\ & + (1-\theta)[ba + (1-b)b](-1)\\ & + (1-\theta)[b(1-a) + (1-b)^2](+1)\end{aligned} \tag{35a}$$

i.e.,

$$\begin{aligned}\frac{\partial}{\partial K_2}\left(-\frac{\psi}{kT}\right) = {} & \frac{b}{1-a+b}[2a^2 + 2(1-a)b + 2ba + 2(1-b)b - 2]\\ & + [1 - 2ba - 2(1-b)b]\end{aligned} \tag{35b}$$

The derivatives of the free energy with respect to a and b may be written as

$$\frac{\partial}{\partial a}\left(-\frac{\psi}{kT}\right) = \frac{\partial}{\partial B}\left(-\frac{\psi}{kT}\right)\frac{\partial B}{\partial a} + \frac{\partial}{\partial K_1}\left(-\frac{\psi}{kT}\right)\frac{\partial K_1}{\partial a} + \frac{\partial}{\partial K_2}\left(-\frac{\psi}{kT}\right)\frac{\partial K_2}{\partial a} \tag{36}$$

$$\frac{\partial}{\partial B}\left(-\frac{\psi}{kT}\right) = \frac{\partial}{\partial B}\left(-\frac{\psi}{kT}\right)\frac{\partial B}{\partial b} + \frac{\partial}{\partial K_1}\left(-\frac{\psi}{kT}\right)\frac{\partial K_1}{\partial b} + \frac{\partial}{\partial K_2}\left(-\frac{\psi}{kT}\right)\frac{\partial K_2}{\partial b} \tag{37}$$

where the r.h.s. of Eqs. (36) and (37) are expressible in a and b by substituting the partial derivatives of the free energy just derived and the partial derivatives of (24a)–(24c). I am indebted to Baxter[7] for the formula

$$\begin{aligned}-\frac{\psi}{kT} &= -K_2 + \ln\frac{1+a-b}{[a(1-b)]^{1/2}}\\ &= -\frac{1}{4}\ln\frac{b(1-a)(1+a-b)^2}{[a^2 + b(1-b)][(1-b)^2 + b(1-a)]} + \ln\frac{1+a-b}{[a(1-b)]^{1/2}}\end{aligned} \tag{38}$$

which satisfies (36) and (37).

7. THE SPECIAL CASES $a = b, a = 0, a = 1 - b$

7.1. The Special Case $a = b$ (Independence)

When the atoms are independently distributed on the lattice, we have

$$a = b \tag{39}$$

Substitution of (39) in (24a)–(24c) gives

$$e^{4K_1} = 1, \qquad e^{4K_2} = 1, \qquad e^{2B} = a/(1 - a) \tag{40}$$

Since $K_2 = 0$, the subfamily of Ising models represented by (40) is also a subfamily of Ising models, viz., the mathematically trivial family of independent distributions of atoms. Within this subfamily the parameter value $a = \frac{1}{2}$ makes $B = 0$, i.e., yields a trivial member of the one-parameter family of Onsager solutions.

7.2. The Special Case $a = 0$ (Exclusion)

When the atoms are large enough to exclude the presence of other atoms on the first shell of sites around it, we have $K_1 = -\infty$, i.e.,

$$a = 0 \tag{41}$$

Substitution of (41) in (24a)–(24c) and (6) gives

$$e^{4K_1} = 0 \tag{42a}$$

$$e^{4K_2} = (1 - b)^2/[b + (1 - b)^2] \tag{42b}$$

$$e^{2B} = 0, \qquad \text{i.e.,} \quad B = -\infty \tag{42c}$$

$$\theta = b/(1 + b) \tag{43}$$

Of particular interest in this case is the proportion of "free" sites, defined as empty sites with empty diagonal neighbor sites. An empty site with four empty diagonal neighbor sites is just the pattern B_0 defined in Section 4. Thus

$$f = P(B_0) = (1 - \theta)\{(1 - b)[(1 - b)(1 - x) + b(1 - y)]\}^2 \tag{44}$$

When $a = 0$ this reduces to

$$f = \frac{1}{1 + b}\frac{(1 - b)^4}{b + (1 - b)^2} \tag{45}$$

ranging from zero to unity as θ goes from zero to $\frac{1}{2}$.

Table I. Paired Values for e^{4K_1} and e^{4K_2} when $\theta = \frac{1}{2}$

e^{4K_1}	0.1000	0.2500	0.5000	0.7500	1.0000	2.0000	4.0000
e^{4K_2}	0.3306	0.6410	0.8889	0.9796	1.0000	0.8889	0.6400

7.3. The Special Case $a = 1 - b$ ($\theta = \frac{1}{2}$)

When the coverage $\theta = \frac{1}{2}$, it follows from (6) that

$$b = 1 - a \tag{46}$$

Substitution of (46) in (24a)–(24c) gives

$$e^{4K_1} = a^2/(1 - a)^2 \tag{47a}$$

$$e^{4K_2} = 4a^2(1 - a)^2/[a^2 + (1 - a)^2]^2 \tag{47b}$$

$$e^{2B} = 1, \qquad \text{i.e.,} \quad B = 0 \tag{47c}$$

Elimination of the parameter a from Eqs. (47a)–(47c) gives the required relation between K_1 and K_2 explicitly as

$$\tanh K_2 + \tanh^2 K_1 = 0 \tag{48}$$

Equation (40) is just the condition[4,5] that the model is at the disorder point (oscillatory when $b > a$ and monotonic to $a > b$).[4]

The values of e^{4K_2} are tabulated for selected values of e^{4K_1} in Table I, which shows that the second interaction parameter K_2 is closer to zero (i.e., independence) than the first interaction parameter K_1.

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