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1987 J. Phys. A: Math. Gen. 20 5311

(http://iopscience.iop.org/0305-4470/20/15/042)

J. Phys. A: Math. Gen. **20** (1987) 5311-5318. Printed in the UK

A two-dimensional lattice gas model for water

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Received 29 May 1986

Abstract. A water-like lattice gas on the square lattice is introduced. The asymmetry of the hydrogen bond is ignored. Molecules, pictured as having four square-planar oriented bonding arms, may occupy lattice sites in either of two possible orientations, + or ×. The bonding arms of a molecule in the + orientation point toward nearest-neighbour (NN) lattice sites and the bonding arms of a molecule in the × orientation point toward next-nearest-neighbour (NNN) lattice sites. A hydrogen bond, energy $\varepsilon_1 < 0$, occurs between two + oriented molecules on NN lattice sites and a hydrogen bond, energy $\varepsilon_2 < 0$, occurs between two × oriented molecules on NNN lattice sites. Two molecules on NN sites repel with an energy $\gamma > 0$, regardless of their relative orientations. Reflection positivity combined with the Peierls argument is used to prove that phase transitions to both open and close-packed ice phases occur in the model.

1. Introduction

Lattice gas models, in which a lattice site can be either vacant or occupied by a molecule in any one of several orientations, have been used to depict the phase behaviour of water for several years. A two-dimensional triangular lattice gas model that disregarded the asymmetry of the hydrogen bond was proposed by Bell and Lavis (1970). A molecule in this model, pictured as having a trigonal planar shape, was allowed to occupy a lattice site in either of the two orientations in which the three bonding arms pointed toward neighbouring lattice sites. The phase diagram for this model was studied using various approximations (Bell and Lavis 1970, Lavis 1973, 1975, 1976, Young and Lavis 1979, Southern and Lavis 1980).

The phase behaviour of a three-dimensional model that accounts for the asymmetry of the hydrogen bond has also been studied numerically (Bell 1972, Fleming and Gibbs 1974a, b, Bell and Salt 1976, Meijer *et al* 1981, Van Royen and Meijer 1984, Whitehouse *et al* 1984). In this model, tetrahedral molecules are allowed to occupy the sites of a body-centred cubic lattice in any one of twelve possible orientations in which the hydrogen atoms and lone pairs of electrons point toward neighbouring lattice sites. A two-orientation version of this model, in which the asymmetry of the hydrogen bond is ignored, has also been proposed. The phase diagrams for the latter version have been calculated (Meijer *et al* 1982, Lavis and Southern 1984, Van Royen and Meijer 1986).

A two-dimensional model that accounted for the asymmetry of the hydrogen bond was also studied (Lavis and Christou 1979). Molecules in the model occupy the sites of a square lattice in any one of four possible orientations. The two hydrogen atoms of a molecule always reside on adjacent bonding arms and the bonding arms of the molecule point toward next-nearest-neighbour lattice sites.

0305-4470/87/155311+08$02.50

Using the Peierls argument, Heilmann and Huckaby (1979) proved that a phase transition to an open ice phase occurs in the two-orientation version of the water models on the triangular and body-centred cubic lattices. They also proved a phase transition to a close-packed ice phase occurs in the two-orientation water model on the body-centred cubic lattice.

In the present paper, we introduce a two-dimensional square lattice gas model for water in which the asymmetry of the hydrogen bond is ignored. The molecules have four square-planar oriented bonding arms which may point either toward nearest-neighbour (NN) or toward next-nearest-neighbour (NNN) lattice sites. Reflection positivity combined with the Peierls argument (Fröhlich *et al* 1980, Huckaby and Kowalski 1984) is used to prove that phase transitions to both open and close-packed ice-like phases occur in this two-dimensional model. This model is novel because the two close-packed structures are not symmetry related. At closest packing ($\mu \to \infty$), the model is equivalent to an Ising model.

2. The model

Consider a lattice composed of squares:

$$\Lambda = \{(a, b): a, b = 0, 1, \ldots, 2M-1\} \tag{1}$$

with coordinates (x, y) computed modulo $2M$ onto $0 \leqslant x, y < 2M$. Molecules, each with four square-planar oriented bonding arms, can occupy lattice sites in either the + orientation, in which the bonding arms point toward NN sites, or in the × orientation, in which the bonding arms point towards NNN sites.

A hydrogen bond, energy $\varepsilon_1 < 0$, occurs between two + oriented molecules on NN lattice sites and a hydrogen bond, energy $\varepsilon_2 < 0$, occurs between two × oriented molecules on NNN lattice sites. Two molecules on NN sites also interact with a repulsion $\gamma > 0$, whether they form a hydrogen bond or not.

The grand canonical partition function for the model is given as

$$\Xi_\Lambda = \sum_\xi \exp(-H_\Lambda(\xi)/kT) \tag{2}$$

where the Hamiltonian for a configuration ξ can be written as

$$H_\Lambda(\xi) = \sum_r H_{\Lambda,r}(\xi) \tag{3}$$

where $H_{\Lambda,r}$ is the Hamiltonian restricted to a unit square S_r in Λ with a centre at r and lattice sites at each vertex. For this model

$$H_{\Lambda,r}(\xi) = -\mu \sum_i (p_i^+ + p_i^\times)/4 + \varepsilon_1 \sum_{NN} p_i^+ p_j^+/2 + \varepsilon_2 \sum_{NNN} p_i^\times p_j^\times + \gamma \sum_{NN} (p_i^+ + p_i^\times)(p_j^+ + p_j^\times)/2 \tag{4}$$

where μ is the chemical potential, i and j are different vertices of S_r and

$$p_i^C = \begin{cases} 1 & \text{if a molecule in orientation } C \text{ is at site } i \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

The 21 principally different types of configurations on a square region S_r are illustrated in figure 1. The value H_i for each of the 21 configurations on S_r is given

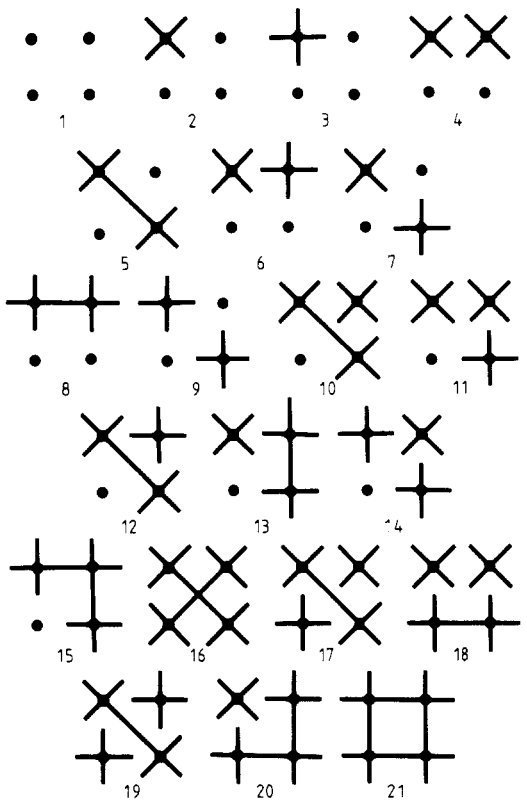

Figure 1. The 21 principal types of configurations about a square region S_r.

Table 1. Values, H_i, of the restricted Hamiltonian $H_{\Lambda,r}$ for each of the 21 possible configurations about a square region S_r as shown in figure 1.

i	H_i
1	0
2, 3	$-\mu/4$
4, 6	$-\mu/2+\gamma/2$
5	$-\mu/2+\varepsilon_2$
7, 9	$-\mu/2$
8	$-\mu/2+\varepsilon_1/2+\gamma/2$
10, 12	$-3\mu/4+\varepsilon_2+\gamma$
11, 14	$-3\mu/4+\gamma$
13	$-3\mu/4+\varepsilon_1/2+\gamma$
15	$-3\mu/4+\varepsilon_1+\gamma$
16	$-\mu+2\varepsilon_2+2\gamma$
17, 19	$-\mu+\varepsilon_2+2\gamma$
18	$-\mu+\varepsilon_1/2+2\gamma$
20	$-\mu+\varepsilon_1+2\gamma$
21	$-\mu+2\varepsilon_1+2\gamma$

in table 1. If a configuration on S_r has a minimum value, H_0, of the restricted Hamiltonian $H_{\Lambda,r}$, S_r will be called a 'ground-state square'. If S_r is not a ground-state square, then it will be called an 'excited-state square'.

Letting $\Delta = \varepsilon_2 - \varepsilon_1$, a consideration of table 1 shows that ground-state squares can have a configuration $i = 5$, corresponding to an open ice structure, only if $\Delta < \gamma$. Consequently, we shall henceforth consider only the case $\Delta < \gamma$.

If $\Delta < \gamma$, a consideration of table 1 shows that ground-state squares have a configuration $i = 1$ if $\mu < 2\varepsilon_2$, $i = 5$ if $2\varepsilon_2 < \mu < 2(\varepsilon_1 + 2\gamma - |\Delta|)$, $i = 16$ if $\Delta < 0$ and $\mu > 2(\varepsilon_1 + 2\gamma - |\Delta|)$ and $i = 21$ if $\Delta > 0$ and $\mu > 2(\varepsilon_1 + 2\gamma - |\Delta|)$.

If $\mu < 2\varepsilon_2$, the ground state is non-degenerate and corresponds to the completely vacant lattice. If $2\varepsilon_2 < \mu < 2(\varepsilon_1 + 2\gamma - |\Delta|)$, the ground state is twofold degenerate, corresponding to the two symmetry-related open ice structures in which one sublattice is vacant and the other is occupied by molecules in the × orientation, each molecule being hydrogen bonded to four other NNN molecules. If $\Delta < 0$ and $\mu > 2(\varepsilon_1 + 2\gamma - |\Delta|)$, the ground state corresponds to the close-packed ice structure consisting of two interlocking open ice structures. If $\Delta > 0$ and $\mu > 2(\varepsilon_1 + 2\gamma - |\Delta|)$, the ground state corresponds to the close-packed ice structure in which every site is occupied by a molecule in the + orientation, each molecule being hydrogen bonded to four other NN molecules.

In §§ 3-5, reflection positivity combined with the Peierls argument (Fröhlich *et al* 1980) will be used to prove the existence of phase transitions to both open and close-packed ice phases in the model.

3. Reflection positivity

Reflection positivity has been used to prove the existence of ordered phases in a large number of lattice models (Fröhlich *et al* 1980). The development given below in § 3 and 4 closely follows that given by Huckaby and Kowalski (1984).

For a square region Λ as defined in equation (1), reflection lines $R_a^{\pm}$ for $0 \leq a \leq M-1$ are defined as $R_a^- = \{(a, y): y \in \mathbb{R}\}$ and $R_a^+ = R_{a+M}^-$. Reflection lines $R_b^{\pm}$ are defined in a similar way. The lines $R_a^{\pm}$ divide Λ into three disjoint regions:

$$\begin{aligned} \Lambda_a^+ &= \Lambda \cap \{(x, y): M + a < x < 2M + a, y \in \mathbb{R}\} \\ \Lambda_a^- &= \Lambda \cap \{(x, y): a < x < M + a, y \in \mathbb{R}\} \\ \Lambda_a^0 &= \Lambda \cap (R_a^- \cup R_a^+). \end{aligned} \tag{6}$$

There is a natural involution

$$\theta_a : (x, y) \to (2a - x, y) \tag{7}$$

which reflects the coordinates through the reflection lines $R_a^{\pm}$. If C_a^+ is the set of allowed molecular configurations on Λ_a^+, and similarly for C_a^- and C_a^0, then $\theta_a C_a^{\pm} = C_a^{\mp}$ and $\theta_a C_a^0 = C_a^0$, the latter transformation being invariant.

For any function $f: C \to \mathbb{C}$, $\theta_a f$ is defined as

$$(\theta_a f)(\xi) = f[\theta_a(\xi)] \qquad \forall \xi \in C. \tag{8}$$

The configuration ξ is denoted as a triple $\xi = (\xi_a^-, \xi_a^0, \xi_a^+)$ where $\xi_a^{\pm} \in C_a^{\pm}$ and $\xi_a^0 \in C_a^0$. Let $F_a^+ = \{f: f(\xi) = f(\xi_a^0, \xi_a^+) \forall \xi \in C\}$. Then $\theta_a f(\xi) = f(\xi_a^0, \xi_a^-)$ if $f \in F_a^+$. A set of functions F_a^- is defined in an analogous way. It can be shown that (Heilmann and Lieb 1979)

$$\sum_{\xi \in C} \bar{f}(\xi) \theta_a f(\xi) \geq 0 \qquad \text{if } f \in F_a^+ \cup F_a^-. \tag{9}$$

The Hamiltonian for the model can be written as

$$H_\Lambda(\xi) = H_a^+(\xi) + \theta_a H_a^+(\xi) = H_a^-(\xi) + \theta_a H_a^-(\xi) \tag{10}$$

where $H_a^\pm \in F_a^\pm$ are given as

$$\begin{aligned} H_a^+(\xi) &= H_a(\xi_a^0, \xi_a^+) - H_a(\xi_a^0)/2 \\ H_a^-(\xi) &= H_a(\xi_a^-, \xi_a^0) - H_a(\xi_a^0)/2. \end{aligned} \tag{11}$$

Since the average value of a function $f: C \to \mathbb{C}$ is given as

$$\langle f \rangle = \Xi_\Lambda^{-1} \sum_{\xi \in C} f(\xi) \exp(-H_\Lambda(\xi)/kT) \tag{12}$$

then equations (10) and (12) give

$$\langle \bar{f} \theta_a f \rangle = \Xi_\Lambda^{-1} \sum_{\xi \in C} \overline{G^\pm(\xi)} \theta_a G^\pm(\xi) \tag{13}$$

where $G^\pm(\xi) = f(\xi) \exp(-H_a^\pm(\xi)/kT)$. If $f \in F_a^+ \cup F_a^-$, then equations (9) and (13) give

$$\langle \bar{f} \theta_a f \rangle \geqslant 0 \qquad \forall f \in F_a^+ \cup F_a^-. \tag{14}$$

It then follows by a standard Cauchy-Schwarz proof that

$$|\langle fg \rangle|^2 \leqslant \langle \bar{f} \theta_a f \rangle \langle \bar{g} \theta_a g \rangle \qquad \forall f \in F_a^+, g \in F_a^-. \tag{15}$$

This inequality will be used in § 4 to obtain an upper bound to the probability that a square region S_r is an excited-state square.

4. A bound on the probability of excited-state squares

Reflection positivity will now be used to obtain an upper bound on the probability of the occurrence of a set of excited-state squares. Let Q be the projection onto configurations in which $S_r \in \mathcal{S}$, where $\mathcal{S}$ is a known subset of the possible types of excited-state squares, i.e.

$$Q_r(\xi) = \begin{cases} 1 & \text{if } S_r \in \mathcal{S} \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

Let L be any non-empty set of squares. Define

$$Q(L) = \prod_{r \in L} Q_r(\xi). \tag{17}$$

The probability P_L that L is a set of excited-state squares in $\mathcal{S}$ is then bounded as $P_L \leqslant g^{|L|}$, where

$$g = \max_L \langle Q(L) \rangle^{1/|L|}. \tag{18}$$

Here $|L|$ indicates the number of squares in L.

Since $L = L_a^- \cup L_a^+$, where $L_a^\pm = L \cap (\Lambda_a^\pm \cup \Lambda_a^0)$, then $Q(L) = Q^+(L) Q^-(L)$, where $Q^\pm(L) = Q(L_a^\pm)$. Since $Q^+ \in F_a^+$ and $Q^- \in F_a^-$, equation (15) gives

$$\langle Q \rangle^2 \leqslant \langle Q^+ \theta_a Q^+ \rangle \langle Q^- \theta_a Q^- \rangle. \tag{19}$$

Let

$$f(Q) = \begin{cases} \langle Q \rangle^{1/|L|} & \text{if } |L| \neq 0 \\ 1 & \text{if } |L| = 0. \end{cases} \tag{20}$$

Then equation (19) becomes

$$f(Q) \leqslant f(Q^+\theta_a Q^+)^{|L_a^+|/|L|} f(Q^-\theta_a Q^-)^{|L_a^-|/|L|}. \tag{21}$$

If some L_m maximises $f(Q)$, then L_m also maximises $f(Q^+\theta_a Q^+)$ (proof by contradiction). Hence if $r \in L_m$, then $\theta_a r \in L_m$ as well. However, since this is true for all θ defined as a reflection through any pair of lines $R_a^\pm$, $R_b^\pm$, then L_m contains all the squares in Λ. Hence $|L_m| = 4M^2$.

Let H_0 be the value of the Hamiltonian restricted to a ground-state square. Let H_* be the smallest value of the Hamiltonian for an excited-state square in $\mathscr{S}$. Then

$$g \leqslant \{3^{4M^2}[\exp(-H_*/kT)]^{4M^2}\Xi_\Lambda^{-1}\}^{1/4M^2} \tag{22}$$

where the factor 3^{4M^2} is the maximum number of configurations in the model. Since $4M^2H_0$ is the Hamiltonian for a ground-state configuration, then $\Xi_\Lambda > \exp(-4M^2H_0/kT)$. Thus

$$g \leqslant 3\exp(-\alpha/kT) \tag{23}$$

where $\alpha = H_* - H_0$. This bound will be used in § 5 to aid in proving the existence of multiple equilibrium states in the model.

5. Phase transitions to open and close-packed ice phases

We shall use the notion (Fröhlich 1978) that a phase transition occurs if the number of equilibrium states is not constant in temperature. Since the present model has finite short-range interactions, the equilibrium state is unique at sufficiently high temperatures (Dobrushin 1968). If it can be shown that multiple equilibrium states are associated with both the open and close-packed ice phases at low temperatures, then the existence of a phase transition to each of these phases will have been established.

To establish the existence of multiple equilibrium states, we shall prove that long-range order occurs at low temperatures in both the open and close-packed ice phases. Let

$$P_r^m = \begin{cases} 1 & \text{if } S_r \text{ belongs to a ground-state configuration } m \text{ on } \Lambda \\ 0 & \text{otherwise.} \end{cases} \tag{24}$$

Long-range order is said to occur if, for two configurations m and n,

$$\lim_{|\Lambda|\to\infty} |\Lambda|^{-2} \sum_{r,r'\in\Lambda} (\langle P_r^m P_{r'}^n\rangle - \langle P_r^m\rangle\langle P_{r'}^n\rangle) \neq 0. \tag{25}$$

We shall first show that $\langle P_r^m P_{r'}^n\rangle \to 0$ as $T \to 0$, if m is a ground-state configuration on Λ, and n does not belong to configuration m at $S_{r'}$. We then show that, for a suitable choice of n, $\langle P_r^m\rangle\langle P_{r'}^n\rangle$ is finite as $T \to 0$, independent of r', proving the existence of long-range order at low temperature.

We shall now define what we shall mean by a contour in a configuration. If an excited-state square and a ground-state square share an edge, then that edge is said to be a 'contour segment'. Two contour segments are connected if they share a common vertex and also divide the four squares at that vertex into two sets, one of which contains only ground-state squares. This prevents the branching of contours.

If S_r is a ground-state square belonging to a ground-state configuration m, and $S_{r'}$, $r' \neq r$ arbitrary, is not a ground-state square belonging to m, then either r or r' is surrounded by a closed contour γ of length $|\gamma|$, which borders ground-state squares on the side containing r.

An examination of figure 1 shows that ground-state squares belonging to different ground states cannot share a common vertex. Thus an excited-state square can have at most two contour segments as edges. The contour γ thus borders a fixed set of $N \geqslant |\gamma|/2$ excited-state squares.

There are less than $3^{|\gamma|}$ contours of length $|\gamma|$ which begin at a certain site. All of the contours surrounding either r or r' can start at either one of the $|\gamma|/2$ sites in a straight line from S_r or at one of the $|\gamma|/2$ sites in a straight line from $S_{r'}$. (Contours that are not homotopic to a point have a vanishing probability in the thermodynamic limit and are not considered in the above argument.)

Hence, if m is a ground-state configuration, and n does not belong to configuration m at $S_{r'}$, then

$$\langle P_r^m P_{r'}^n \rangle \leqslant \sum_{|\gamma| \geqslant 4} |\gamma| 3^{|\gamma|} g^{|\gamma|/2}. \tag{26}$$

For the case of open ice, we let m and n correspond to the two structures composed only of squares of type $i = 5$. As indicated in § 2, if $2\varepsilon_2 < \mu < 2(\varepsilon_1 + 2\gamma - |\Delta|)$, these two structures are the two ground-state configurations. Let the set $\mathcal{S}$ of § 4 contain all possible types of excited-state squares. Equation (26) then ensures $\langle P_r^m P_{r'}^n \rangle \to 0$ as $T \to 0$.

At sufficiently low temperatures, $\langle P_r^m \rangle + \langle P_r^n \rangle > 1 - g$. By symmetry, $\langle P_r^m \rangle = \langle P_r^n \rangle$. Hence $\langle P_r^m \rangle \langle P_{r'}^n \rangle > \frac{1}{4} - g/2$. Hence, at sufficiently low temperature there are multiple equilibrium states corresponding to open ice if $2\varepsilon_2 < \mu < 2(\varepsilon_1 + 2\gamma - |\Delta|)$.

For the case of close-packed ice, we shall use an argument given by Fröhlich *et al* (1980). Let m correspond to the structure composed entirely of squares of type $i = 16$ and let n correspond to the structure composed entirely of squares of type $i = 21$. If $\mu > 2(\varepsilon_1 + 2\gamma - |\Delta|)$, m is the ground-state structure if $\Delta < 0$ and n is the ground-state structure if $\Delta > 0$.

Let $\mathcal{S}$ (see § 4) be the set of all excited-state squares, except those of type $i = 16$ or $i = 21$. Let H_* be the minimum value of the restricted Hamiltonian for a square in $\mathcal{S}$. A consideration of table 1 ensures that if $\mu > 4\gamma$, $H_* - H_0 = \max(-\varepsilon_1, -\varepsilon_2)$. Let $\Delta \in [-a, a]$ where $a > 0$. Since only squares in $\mathcal{S}$ can share an edge with a ground-state square, then $\langle P_r^m P_{r'}^n \rangle \to 0$ as $T \to 0$, uniformly on $[-a, a]$. Also, if configuration l does not correspond to configuration m or n at S_r, $\langle P_r^l \rangle \to 0$ as $T \to 0$, uniformly on $[-a, a]$.

If we now let $\mathcal{S}$ be the set of *all* excited-state squares, then by the development of § 4, if $\Delta = -a$, $\langle P_r^n \rangle \to 0$ as $T \to 0$. If $\Delta = a$, $\langle P_r^m \rangle \to 0$ as $T \to 0$. We now vary Δ from $-a$ to a for a fixed low temperature. Either $\langle P_r^n \rangle$ varies continuously, in which case there is a range of Δ for which $\langle P_r^n \rangle > \frac{1}{3}$ and $\langle P_r^m \rangle > \frac{1}{3}$, or else $\langle P_r^n \rangle$ varies discontinuously, in which case there is at least one value of Δ for which $\langle P_r^n \rangle > \frac{1}{3}$ and $\langle P_r^m \rangle > \frac{1}{3}$. Hence, there are multiple equilibrium states corresponding to close-packed ice.

In the limit of closest packing ($\mu \to \infty$), p_i^C of equation (5) can be written as $p_i^+ = (1 + S_i)/2$, $p_i^\times = (1 - S_i)/2$, where $S_i = +1$ ($S_i = -1$) if site i is occupied by a molecule in the + (×) orientation. The Hamiltonian then becomes the Ising Hamiltonian

$$H_\Lambda(\xi) = K + (\varepsilon_1/4) \sum_{\text{NN}} S_i S_j + (\varepsilon_2/4) \sum_{\text{NNN}} S_i S_j - \Delta \sum_{i \in \Lambda} S_i \tag{27}$$

where K is a constant. The Lee-Yang circle theorem (Lee and Yang 1952) ensures there are no phase transitions if $\Delta \neq 0$. If $\Delta = 0$, the Peierls argument proves there are multiple equilibrium states at low temperature, establishing the existence of a phase transition at $\Delta = 0$ in the limit $\mu \to \infty$.

Acknowledgments

DAH gratefully acknowledges conversations with R B Griffiths, J M Kowalski, J L Lebowitz and A Pękalski. This research was supported by The Robert A Welch Foundation, grant P 446.

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