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Abstract. It is shown that the zero-field Ising model is equivalent to a polymer model in which a bond of a polymer chain can assume one *gauche* and one *trans* state. The Ising model is defined on a lattice graph G of degree $d = 4$, whereas the polymer model is defined on a covering lattice digraph D^c of out-degree $d^* = 2$. As an example, a polymer model, defined on the Manhattan square lattice, is shown to be equivalent to the zero-field Ising model on the square lattice. The polymer model can be used to discuss the melting transition in polymers.

1. Introduction

Nagle (1973, 1974) used several two-dimensional lattice models to discuss the theory of the melting transition in polymers. The models chosen there were all isomorphic to exactly solvable dimer and six-vertex models. This work was motivated by a number of equivalences between different counting problems on the square and other lattices, derived mainly from the study of the various vertex models (Rys 1963, Wu 1967, Lieb and Wu 1972). In particular it has been pointed out (Lieb and Wu 1972) that, on the square lattice, there is a one-to-one correspondence between six-vertex (ice) configurations and the configurations of non-intersecting polygons that cover all lattice points. Such polygonal configurations will be referred to here as close-packed configurations of polygons. Assigning an energy $\epsilon > 0$ (flex-energy) to certain steps of the polygons of such configurations, Nagle (1974) showed that the derived polygon (polymer) model is isomorphic to the well known F model (Rys 1963), solved by Lieb (1967).

In Nagle's polymeric F model the close-packed configurations of polygons on the square lattice represent the configurations of a polydisperse system (polymer molecules of the system do not have the same chain length) of cyclic polymers constrained to the square lattice at maximum density (undiluted polymer system). Since in this representation the polygons are non-intersecting, the excluded volume constraint, that any two polymer segments cannot occupy the same lattice point, is taken into account correctly. An intramolecular interaction of rotational isomeric type (Volkenstein 1958) may be introduced by assigning different energies to topologically distinct arrangements of successive lines (or steps) of a polygon. On the square lattice, Nagle specified two *gauche* states (preceding step at a 90° angle) and one *trans* state (preceding step at zero angle) for each step of a polygon (bond of a polymer).

In the usual lattice model of melting transition in polymers (Flory 1956, Gordon 1965), one employs a diamond lattice for the packing of the polymer chains and

postulates that the lowest conformational free energy of a polymer chain corresponds to the 'all-planar' *trans* conformation whereby any three successive bonds of the chain are coplanar. A state of higher energy will be generated if a bond is bent out of the planar form. Thus, a conformational energy of a bond depends on the orientation of the preceding two bonds, whereas in the polymeric F model and in the model to be presented in this paper the energy of a bond depends only on the preceding bond. However, in both cases crystallisation in polymers is considered to be brought about as a result of chain 'inflexibility', i.e., as a result of the energetic preference for the *trans* over the *gauche* state.

In this paper, we present a polymer model which can be transformed to the zero-field Ising model on a lattice graph G of degree $d = 4$. The polymer model involves another lattice digraph D^c which can be obtained from G. The transformation takes place in several steps as follows.

Step 1. Consider a lattice graph G of degree $d = 4$.

Step 2. Obtain a lattice digraph D by assigning a direction to each line of G in such a way that there will be two lines directed away from each point.

Step 3. Obtain the covering digraph D^c (for definitions see § 2).

Step 4. Define a polymer model on D^c as follows. (i) Let the configurations of the polymer system be represented by the close-packed configurations of co-oriented polygons on D^c. (ii) Since there will be two lines directed away from each point, a bond of a polymer (polygon) can assume only two states; depending upon the preceding bond, define one of these two states as the *gauche* state and the other as the *trans* state of the bond.

Step 5. Prove that the polymer model on D^c is equivalent to the zero-field Ising model on G (see § 3).

We point out that the lattice digraph D of step 2 is not unique, and therefore the Ising model on G is equivalent to many polymer models defined on D^c for the various choices of D.

An example is given in § 4, where we show that a polymer model, defined on the Manhattan square lattice with the same rotational isomeric interaction as in Nagle's polymeric F model, is equivalent to the zero-field Ising model on the square lattice (Onsager 1944).

We shall begin by setting out a number of essential definitions.

2. Graph-theoretical preliminaries

A *graph* $G \equiv G(P; E)$ is a set P (the point set) of points and a set E (the edge set) of lines or edges joining certain pairs of distinct points. If two points $p \in P$ and $p' \in P$ are joined by an edge $e \in E$, then p and p' are *adjacent* or *neighbours*, and e is said to be *incident* with p and p'. Two edges are said to be *adjacent* if they have a point in common. The *degree* of a point is the number of edges incident with that point. A graph is *regular* if all its points have the same degree (to be denoted d). A lattice graph is a regular graph whose points are joined with edges in some repetitive way. An *n-cycle* or *n-polygon* is an alternating cyclic sequence of $n > 2$ distinct edges (the steps) and n distinct points of the form $|p_1, e_1, p_2, e_2, \ldots, p_n, e_n| \equiv |p_2, e_2, \ldots, p_n, e_n, p_1, \varepsilon_1| \equiv, \ldots, \equiv |p_n, e_n, p_1, e_1, \ldots, p_{n-1}, e_{n-1}|$, in which each point p_i is incident with the preceding $(e_{i-1}; e_{-1} \equiv e_n)$ and the succeeding edge (e_i). If n is odd (even) the n-cycle is an odd (even) cycle. A *subgraph* of G is a graph obtained from G by deleting subsets of its

points and edges. A *spanning* subgraph is a subgraph that contains all points of G. A *close-packed configuration of polygons* of G is a regular spanning subgraph of G of degree 2.

A *digraph* is a graph in which every edge is assigned a direction, from one point p (the initial point) to the other point p' (the final point). The edges of a digraph are called *arcs*. An arc will be denoted by $a \equiv (p, p')$, where (p, p') must be considered as an ordered pair of points. A digraph will be denoted by $D \equiv D(P; A)$, where P is the point set and A is the arc set of D. The *out-degree* (*in-degree*) of a point p is the number of arcs of D having p as their initial (final) point. A digraph is *closed* if every point has the same out-degree as its in-degree. A closed digraph is regular if every point has the same out-degree d^* as every other point; we call such a digraph a *closed digraph of out-degree* d^*. Two adjacent arcs of the form (p, p') and (p', p'') are *consecutive* or *co-oriented*, whereas two arcs of the form (p, p') and (p'', p') are called *antidirected*. If D is one of the possible digraphs which may obtained from a graph G, then G is said to be the graph of D (as an alternative the notation $G(D)$ could be used; however, when no confusion can arise, the reference to D will be omitted). A *circuit* or *co-oriented polygon* is an oriented cycle of the form

$$|p_1, (p_1, p_2), p_2, (p_2, p_3), p_3, (p_3, p_4), \ldots, (p_{n-1}, p_n), p_n, (p_n, p_1)|$$
$$\equiv |p_1 \to p_2 \to p_3 \to, \ldots, \to p_n \to|.$$

An *anticycle* is an even oriented cycle of the form

$$|p_1, (p_1, p_2), p_2, (p_3, p_2), p_3, (p_3, p_4), \ldots, (p_{n-1}, p_n), p_n, (p_1, p_n)|$$
$$\equiv |p_1 \to p_2 \leftarrow p_3 \to, \ldots, \leftarrow p_{n-1} \to p_n \leftarrow|.$$

A *close-packed configuration of co-oriented polygons* of D is a closed spanning subgraph of D of out-degree 1.

The *covering digraph* (often called *line graph*) D^c of a digraph D is defined as follows. (i) To every arc (p, p') of D there corresponds a point $p\{(p, p')\}$ of D^c, and (ii) two points of D^c of the form $p\{(p, p')\}$ and $p\{(p', p'')\}$ are joined by an arc of the form $(p\{(p, p')\}, p\{(p', p'')\})$. If D^c is the covering digraph of D, then D is said to be the *underlying digraph* of D^c and G (the graph of D) is said to be the *underlying graph* of D^c (note that $G \equiv G(D) \neq G(D^c)$). Not every digraph D has an underlying digraph; whenever the underlying digraph of D exists it will be denoted by D^u (thus, by definition, $(D^c)^u \equiv D$). For an example see figures 1(*a*) and (*b*). There are many characterisations of covering digraphs (Berge 1973). However, since, for the application we have in mind, we shall be concerned only with closed digraphs of out-degree $d^* = 2$, we proceed to obtain a necessary and sufficient condition for such a digraph to be the covering digraph of some other digraph. Henceforth, we deal only with closed digraphs of out-degree $d^* = 2$, which will simply be referred to as *digraphs*.

If the points and the arcs of a digraph D can be partitioned to a set of arc-disjoint anticycles $h_1, h_2, \ldots, h_m$ in such a way that every point p of D belongs to two anticycles, one out-going from p and one in-coming to p, then we say that D has an *anticycle partition*. If every h_i is an *n*-anticycle we say that D has an *n*-anticycle partition.

Theorem 1. The underlying digraph D^u of a digraph D exists *if and only if* D has a four-anticycle partition.
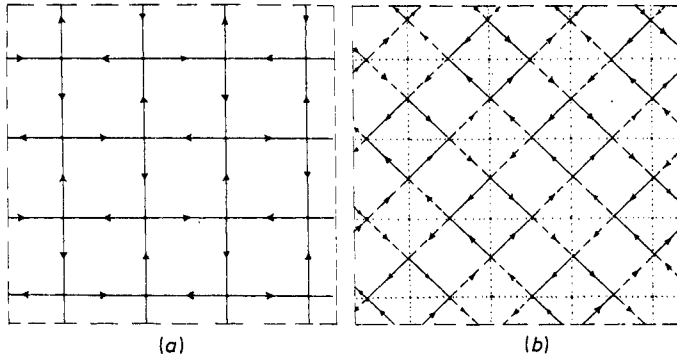
Figure 1. (*a*) A (square) lattice digraph D of out-degree $d^* = 2$. (*b*) The covering lattice digraph D^c of D is shown by oriented lines. The four-anticycle partition of D^c is illustrated by full and broken arcs. Either all the arcs of a four-anticycle are full arcs or they are all broken arcs. The underlying graph G (square lattice) is shown by dotted lines. Opposite sides are to be identified.

Proof. If D^u exists (so that $(D^u)^c \equiv D$), let the points of D^u be denoted by p, p', p_i and p_i'. Consider an arc (p, p') of D^u and its adjacent arcs (p_1', p'), (p', p_2'), (p', p_3'), (p, p_1), (p_2, p), (p_3, p). By definition the following arcs are arcs of $(D^u)^c$: $(p\{(p, p')\}, p\{(p', p_2')\})$, $(p\{(p_1', p')\}, p\{(p', p_2')\})$, $(p\{(p_1', p')\}, p\{(p', p_3')\})$, $(p\{(p, p')\}, p\{(p', p_3')\})$; $(p\{(p_3, p)\}, p\{(p, p')\})$, $(p\{(p_2, p)\}, p\{(p, p')\})$, $(p\{(p_2, p)\}, p\{(p, p_1)\})$, $(p\{(p_3, p)\}, p\{(p, p_1)\})$. The first four arcs form a four-anticycle out-going from the point $p\{(p, p')\}$ of $(D^u)^c$, namely the four-anticycle

$$\lvert p\{(p, p')\} \rightarrow p\{(p', p_2')\} \leftarrow p\{(p_1', p')\} \rightarrow p\{(p', p_3')\} \leftarrow \rvert.$$

The other four arcs form a four-anticycle in-coming to $p\{(p, p')\}$, namely the four-anticycle

$$\lvert p\{(p_3, p)\} \rightarrow p\{(p, p')\} \leftarrow p\{(p_2, p)\} \rightarrow p\{(p, p_1)\} \leftarrow \rvert.$$

Therefore, every point $p\{(p, p')\}$ of D belongs to two four-anticycles and since $d^* = 2$ every arc of D belongs to one and only one four-anticycle, i.e., D has a four-anticycle partition. In figure 1(*b*) the arcs of a covering digraph have been distinguished as full and broken arcs in order to illustrate the four-anticycle partition.

Conversely, suppose that D has a four-anticycle partition and let the points of D be denoted by p and p'. Construct a digraph D' as follows. (i) With every four-anticycle h_i of D associate a point $p\{h_i\}$ of D', and (ii) with every point p of D whose out-going four-anticycle is h_j and whose in-coming four-anticycle is h_i associate an arc $(p\{h_i\}, p\{h_j\})$ of D'. From the definitions of D' and $(D')^c$, one can see that there is a one-to-one correspondence between the points of $(D')^c$ and the points of D. Identify the points of $(D')^c$ with the points of D; thus $p\{(p\{h_i\}, p\{h_j\})\} \equiv p$, where p is the common point of h_i and h_j. Let p' be one of the two points to which h_j is in-coming and h_k the four-anticycle that is out-going from p', i.e., $p' \equiv p\{(p\{h_j\}, p\{h_k\})\}$. The arc (p, p') is an arc of $(D')^c$ because the arcs $(p\{h_i\}, p\{h_j\})$ and $(p\{h_j\}, p\{h_k\})$ are consecutive arcs of D'. The arc (p, p') is also an arc of D because h_j is a four-anticycle of D out-going from p and in-coming to p'. There is a one-to-one correspondence between the arcs of D and the arcs of $(D')^c$. Therefore, $(D')^c = D$ and $D' = D^u$.

Corollary 1. The number of close-packed configurations of co-oriented polygons on a covering digraph D^c is 2^N, where N is the number of points of the underlying graph $G(D)$.

Proof. With every four-anticycle we can associate two pairs of non-adjacent arcs (see figure 2) which will be called the *dimer states* of the four-anticycle. By specifying the dimer state for every four-anticycle of D^c we obtain a closed spanning subgraph of D^c of out-degree 1, i.e., we obtain a close-packed configuration of co-oriented polygons on D^c (see figure 3, § 4). By considering all the possible combinations of the dimer states of the four-anticycles of D^c we obtain all the possible close-packed configurations of co-oriented polygons on D^c. Since the number of four-anticycles of D^c equals the number of points of G, we have the desired result.

Figure 2. A four-anticycle and its two dimer states (A and B).

3. Equivalence of a polymer model on D^c and the Ising model on G

We consider the Ising model on a lattice graph G of degree $d = 4$. Every point p_j $(j = 1, 2, \ldots, N)$ of G can assume two spin states which are described by the spin variable s_j $(s_j = \pm 1)$. A spin configuration $\{s\}$ on G is obtained by specifying the values of all the variables s_j. There are 2^N spin configurations on G. We also consider the covering digraph D^c of any digraph D of G. D^c has a four-anticycle partition $h_1, h_2, \ldots, h_N$. Think of the two dimer states of a four-anticycle h_j of D^c as the two spin states of the point $p_j \equiv p\{h_j\}$ of G. Thus, by this representation we can state (see corollary 1) the following proposition.

Proposition 1. There is a one-to-one correspondence between spin configurations on G and close-packed configurations of co-oriented polygons (polymers) on D^c.

Suppose that the two dimer states $(s_j = \pm 1)$ of any four-anticycle h_j are such that the two dimers of the $s_j = +1$ dimer state are both of type A (say horizontal), whereas the two dimers of the $s_j = -1$ dimer state are both of some other kind B (say vertical). For a point p of D^c whose out-going four-anticycle is h_j and whose in-coming four-anticycle is h_i, assume that $s_i = +1$. Then, the arc (bond) out-going from p can be in two states with respect to its preceding arc, i.e., either we have an A–A state $(s_i = +1, s_j = +1)$ or an A–B state $(s_i = +1, s_j = -1)$. Similarly, if $s_i = -1$ we have the states B–B $(s_i = -1, s_j = -1)$ and B–A $(s_i = -1, s_j = +1)$. We define the A–B (or B–A) state as the *gauche* state and the A–A (or B–B) state as the *trans* state of the arc of D^c out-going from any point p. If the dimer states of the four-anticycles of D^c are (topologically) incomparable, then the distinction between type-A and -B dimer states is arbitrary. As a result, the topology of a *trans* (*gauche*) state of an arc may not be the same for all arcs of D^c. However, if all four-anticycles of D^c are of the same 'form' (see figure 1(b)), then the concept *trans* and *gauche* are well defined.

Proposition 2. There is a one-to-one correspondence between arcs in *gauche* states of a given close-packed configuration of co-oriented polygons on D^c and pairs of neighbouring spins in opposite spin states of the corresponding spin configuration on the underlying graph G.

4. Application to a lattice graph

Propositions 1 and 2 establish the equivalence of the zero-field Ising model on G and the polymer (polygon) model on D^c in which *gauche* and *trans* states of a polymer bond are defined to depend upon the preceding bond. We proceed to illustrate this by an example. Consider the lattice digraph shown in figure 3. Following Kasteleyn (1963), we call this digraph 'the Manhattan square lattice (MSL)'. The MSL is the covering digraph of the digraph shown in figure 1(*a*). The underlying graph of the MSL is the square lattice (SL) shown in figures 1(*b*) and 3 by dotted (unoriented) lines. Note that we have used diagonal periodic boundary conditions on the MSL in order to obtain ordinary boundary conditions on the underlying SL.
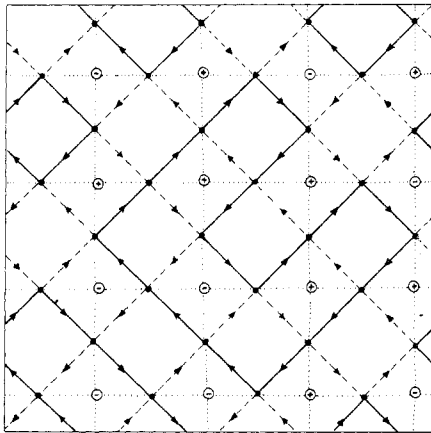

Figure 3. Full circles and oriented lines (full or broken) show the Manhattan square lattice (MSL). Open circles and dotted lines show the underlying square lattice (SL), plus and minus signs in the open circles specify a spin configuration on this lattice. A plus sign corresponds to two arcs of the MSL that form a dimer state of the associated four-anticycle, one arc pointing upwards to the right at 45° and one arc pointing downwards to the left at 45°. A minus sign corresponds to the dimer state formed by two arcs, one pointing upwards to the left at 45° and one downwards to the right at 45°. The dimers of a dimer state are shown as full arcs. Full arcs show the close-packed configuration of co-oriented polygons on the MSL corresponding to the spin configuration on the underlying SL.

We define a polymer model on the MSL as follows.

(i) The configurations of the polymer system are represented by the close-packed configurations of co-oriented polygons on the MSL.

(ii) We specify rotational isomerism: an arc (bond) of a co-oriented polygon (polymer) is on a *gauche* state (energy $\epsilon > 0$) if it is at an angle of 90° to its preceding arc and it is on a *trans* state if it is at zero angle (collinear) with its preceding arc. Since $d^* = 2$ for every bond there are two states, one *gauche* and one *trans* state.

Let the variable describing the spin state of the jth point in the kth row of the SL be denoted $s_{j,k}$ $(s_{j,k} = \pm 1; j = 1, 2, \ldots, n; k = 1, 2, \ldots, m; n = n^*; m = \frac{1}{2}m^*; N = nm; N^* = n^*m^*)$ where m and n are the numbers of rows and columns of the SL, and m^* and n^* the numbers of rows and columns of the MSL. To match the energies we note that, if $E^{\mathrm{I}}_{\{s\}}(J)$ is the energy of a spin configuration $\{s\}$ on G—for an Ising ferromagnet with an interaction energy $J > 0$ between neighbouring spins—then

$$E^{\mathrm{I}}_{\{s\}}(J) = -J \sum_{j=1}^{n} \sum_{k=1}^{m} (s_{j,k}s_{j+1,k} + s_{j,k}s_{j,k+1}). \tag{1}$$

The energy of a close-packed configuration of co-oriented polygons on D^c, $E^*_{\{s\}}(\epsilon)$, corresponding to a spin configuration $\{s\}$ on G, is given by

$$E^*_{\{s\}}(\epsilon) = \frac{1}{2}\epsilon \sum_{j=1}^{n} \sum_{k=1}^{m} [(1 - s_{j,k}s_{j+1,k}) + (1 - s_{j,k}s_{j,k+1})]$$

$$= mn\epsilon + E^{\mathrm{I}}_{\{s\}}(\tfrac{1}{2}\epsilon). \tag{2}$$

The corresponding partition functions are therefore related by

$$Z^*_{m^*,n^*}(\epsilon, T) = \exp(-mn\epsilon/kT)Z^{\mathrm{I}}_{m,n}(\tfrac{1}{2}\epsilon, T) \tag{3}$$

where

$$Z^{\mathrm{I}}_{m,n}(J, T) = \sum_{\{s\}} \exp(-E^{\mathrm{I}}_{\{s\}}(J)/kT). \tag{4}$$

Clearly, the model has the same transition features as the zero-field Ising model on the square lattice, with the well known logarithmic singularity of the specific heat. The critical temperature, T_c, is located by $\sinh(\epsilon/kT_c) = 1$. However, we shall not discuss transition features here since there is a vast literature on the subject.

5. Concluding remarks

It has been shown that the zero-field Ising model on a lattice graph G of degree $d = 4$ is equivalent to a polymer model defined on a covering digraph D^c. The transformation is not restricted to two-dimensional, or planar, lattice graphs; it can be applied just as well to three-dimensional lattice graphs, the only restriction being that the lattice digraph—on which the polymer model is defined—is a covering digraph of out-degree $d^* = 2$. The present paper offers a new and interesting interpretation of the Ising model. Furthermore, it suggests that even a polymer system with one *trans* and only one *gauche* rotation for each bond may exhibit sensible phase transition behaviour. This is in contrast with the behaviour of the 'dimer model B to a polymer chain' presented by Nagle (1973, 1974), which also has one *gauche* rotation, but the model remains 'frozen' in its ground state.

We also suggest that transition features of a polymer model depend on the number of *gauche* rotations assumed by the bonds of the polymer chains. To support this we compare the polymer model on the MSL and Nagle's polymeric F model on the SL. Both these models are isotropic (neither lattice direction is preferred) and they have the same rotational isomeric interaction. However, in the former a bond can assume only one *gauche* rotation, whereas in the latter a bond can assume two such rotations. These two models have very different behaviour: the F model undergoes an infinite-order

transition with a finite and continuous specific heat at T_c, whereas the Ising model has a logarithmically diverging specific heat at T_c. This dramatic change in behaviour must be related to the loss of the second *gauche* rotation.

The order–disorder model, termed 'polymer model' in this paper, may be appropriate to describe the melting transition in polymers (Flory 1956, Nagle 1974, Malakis 1976) or transitions in polymeric systems such as biological membranes (Nagle 1973). The polymer melting model was originally introduced by Flory (1956), who used an approximate method (known as the Flory–Huggins approximation) in order to obtain an expression for the partition function. This approximation has been examined critically by Nagle (1974), Gordon *et al* (1976) and Malakis (1976).

Nagle's polymeric *F* model and the model in this paper are, as far as we are aware, the only isotropic polymer models which can be solved without resorting to any kind of approximation. Of course, they are not ideal polymer models, their main defect being the existence of short cyclic polymers, at least above T_c. Also, it should be pointed out that the main simplification rendering both these models 'exactly' solvable is that one does not fix the chain length of the polymer chains, but rather allows the chain length to vary with temperature.

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