CHAPTER 37

Combinatorics in Statistical Physics

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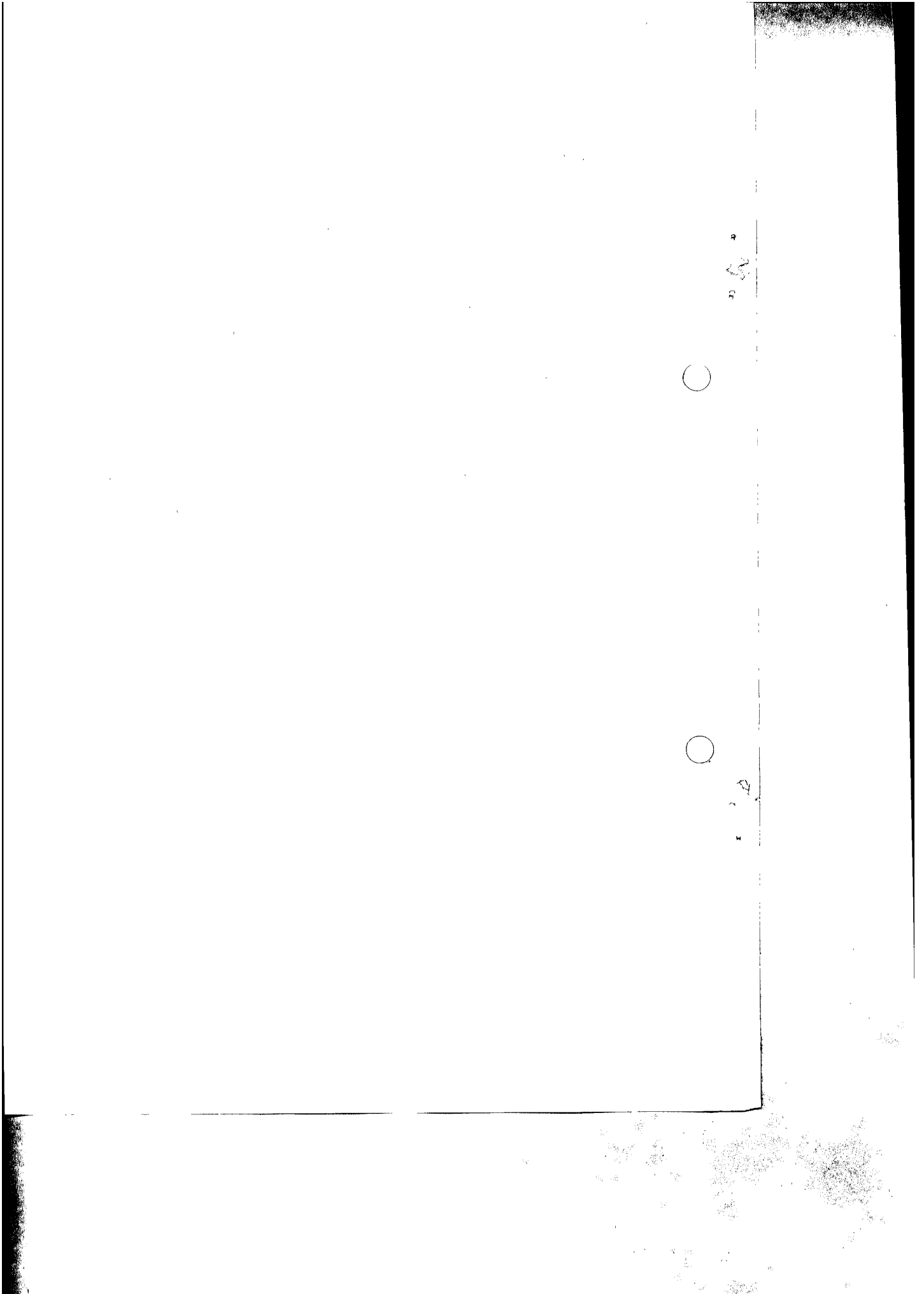*Merton College and Mathematical Institute, University of Oxford, Oxford OX1 4JD, UK*

Contents

1. Introduction

Combinatorics and physics interact in various ways. It is impossible to survey here all the connections. We concentrate in this chapter on statistical physics since several of the most basic problems in this area have a combinatorial flavour.

Sections 2 and 3 of this chapter are concerned with two of the most fundamental areas, namely the study of the Ising model and the theory of percolation processes. Both of these areas of research are huge, but they share the common property that some of the most primitive and easily stated problems are, after more than thirty years of research, still largely unanswered.

In section 4 we present, among other models, some of the classical enumeration problems of statistical physics; again there are many open questions and very few exact results.

Sections 5 and 6 are concerned with two of the (relatively few) "techniques" which have been developed to deal with the sort of problems we are discussing. Transfer matrices and subadditive function theory are basic tools in this area of mathematical physics. This is illustrated by a simplified version of the dimer problem, it amounts to counting the number of ways of placing dominoes on a rectangular chessboard.

Finally we illustrate in Section 7 the application of ideas from combinatorial optimization to statistical physics by showing how the problem of finding the ground states of a spin glass model may be reduced to a very basic, though difficult (NP-hard) problem in discrete optimization.

2. The Ising model

The density of water varies as a function of temperature, and generally as a continuous function. Of course the variation is not continuous in the neighbourhood of the boiling point, nor at the freezing point. Although we are accustomed to such behaviour, it is paradoxical. The forces acting between the individual molecules vary continuously as the temperature varies. Why then should there be a change of state at certain temperatures? Statistical physics is devoted to the attempt to understand this behaviour.

As is customary in science and mathematics, the study begins by setting up a grossly simplified model. We assume that the system consists of a finite number of particles, and that the system is at any instant in one of a number of states. The behaviour of the system is governed by its Hamiltonian H, which is a function of the state. Its value $H(\sigma)$ is equal to the energy of the system in state σ. Examples of Hamiltonians will be given later in this section and also in section 7. The *partition function* of the system is defined to be

$$Z = Z(T) = \sum_{\sigma} \exp[-H(\sigma)/(kT)] \,. \tag{2.1}$$

Here T is the temperature of the system and k is Boltzmann's constant. If the

system consists of N particles, we sometimes write Z_N in place of Z. It is taken as an axiom that all large-scale properties of the system are determined by Z. (Sometimes an attempt is made to disguise the fact that this is an axiom, and not a theorem. Also a system can have more than one partition function; the one we have just defined is the *canonical* partition function.)

In stochastic versions of the problem it is assumed that in the stationary state the probability that the system is in the state σ is given by

$$Z^{-1} \exp[-H(\sigma)/(kT)]$$

and that the *free energy* of the system is

$$F = -kT \log Z .$$

The latter is a particularly important parameter of the system, and explains the fact that one deals with $\log Z$ as often as with Z. We are interested in the behaviour of Z for systems with a large number of particles, as the temperature T ranges over the positive reals. The value of Z depends on the number of particles N in the system as well as on the temperature. In all cases of interest to us, $\log Z$ is a linear function of N when all other parameters are fixed. The number of particles in any realistic physical system is, for all mathematical purposes, infinite. Hence we are led to study

$$\lim_{N \to \infty} \frac{1}{N} \log Z_N(T)$$

as a function of T. Following Baxter (1982, p. 14), we say that a model has been solved if its free energy is known. The phase transitions of the model correspond to the points, called *critical points*, at which the free energy is not an analytic function.

We now consider a typical and important system, the *Ising model*. We are given a graph $G = (V, E)$ embedded in $\mathbb{R}^2$ or $\mathbb{R}^3$. There is an atom placed at each vertex. Each atom has a spin associated to it, this spin takes only two values. The energy of the system is understood to be the sum of the energies due to the interaction of each pair of atoms. The contribution due to a pair of atoms will be assumed to depend only on whether they are adjacent in G or not. The interaction is completely determined by whether the given pair have the same spin, or not.

The state of the system can be represented by a function σ from $V(G)$ into the set $\{-1, 1\}$ and the Hamiltonian $H(\sigma)$ will be a sum over the edge set E of G. Writing σ_i for the state of atom i, we find that the partition function of this system at temperature T is

$$Z(G) = \sum_\sigma \exp\left[-\sum_{ij \in E} \beta \sigma_i \sigma_i \right]. \tag{2.2}$$

The constant $\beta = J/(kT)$ will vary inversely with the temperature and is proportional to the interaction J.

The graphs in which physicists are interested are usually infinite. However, they are usually the limit, in a natural sense, of a sequence of finite graphs. This will be made clearer by the examples which follow. The most important cases of the Ising model are when G is either the 2-dimensional square lattice, or the 3-dimensional cubic lattice. The solution of the 2-dimensional Ising problem on the square lattice was a major achievement of Onsager in 1944. (For an account of this, and any other historical remarks in this section, see Thompson 1972.) The 3-dimensional model is still unsolved.

There are some important extensions of the Ising model. We assumed implicitly that each of the two states available to an individual atom was equally likely. However, if there is an external magnetic field acting then one of the two states becomes more probable. The 2-dimensional Ising model has only been solved under the assumption that there is no external field. (The presence of an external field in any model is a major complication.) Another possibility is that the interactions between a pair of adjacent atoms may not be independent of the edge. (This is certainly a physically reasonable possibility.) Thus on the square lattice, the interactions arIsing from the horizontal edges may differ from the interactions on the vertical edges. Allowing for this does not usually cause problems; on the contrary it can even be useful, as we will see.

A question which may well have arisen by now is, what does all this have to do with combinatorics? To explain this, we study the basic Ising model on the square lattice. Let G_n denote the Cartesian product $P_n \times P_n$ of two paths with n vertices. Thus G_n has n^2 vertices and, for large n, may be viewed as an approximation to the infinite square lattice. By expanding the exponential in (2.2) and since $\sigma_i \sigma_j$ takes only the values $+1$ and -1, we have

$$\exp(\beta \sigma_i \sigma_j) = \cosh(\beta) + \sigma_i \sigma_j \sinh(\beta) = \cosh(\beta)(1 + \sigma_i \sigma_j \tanh(\beta)),$$

whence the partition function for G_n at temperature T can be expressed as

$$Z(G_n) = \sum_\sigma (\cosh(\beta))^{|E(G_n)|} \prod_{ij \in E(G_n)} (1 + \sigma_i \sigma_j \tanh(\beta)) .$$

With some ingenuity (see, e.g., section 6.1 of Thompson 1972 or Biggs 1977, p. 2) this may be rewritten as

$$Z(G_n) = 2^{|V(G_n)|} (\cosh(\beta))^{|E(G_n)|} \sum_{l \geqslant 0} N(l)(\tanh(\beta))^l , \qquad (2.3)$$

where $N(l)$ is the number of spanning subgraphs of G_n with l edges and all vertices having even valency. (These are called the Eulerian subgraphs of G_n.) This shows that determining the partition function for the Ising model is equivalent to the purely combinatorial problem of enumerating the Eulerian subgraphs of G_n.

It should be noted that (2.3) is valid with any graph G in place of G_n. In particular if we replace G_n by P_n then we obtain

$$Z(P_n) = 2^n (\cosh(\beta))^{n-1} .$$

From this we can deduce that

$$\lim_{n \to \infty} (Z(P_n))^{1/n} = 2 \cosh(\beta) .$$

Since $\cosh(\beta)$ is an analytic function, it follows that the Ising model on the infinite path does not have a critical point. As we noted earlier in this section, Onsager showed that the Ising model on the infinite square lattice does have a phase transition. (See chapter 5 of Thompson 1972.)

A short introduction to the Ising problem will be found in Cipra (1987).

Partition functions and rank polynomials

We now show how Fortuin and Kasteleyn (1972) demonstrated that the Ising and other physical problems could be related to the Whitney rank polynomial or Tutte polynomial (see chapter 9 by Welsh).

Let G be a graph, which now may have loops and multiple edges. Any subset S of $E(G)$ forms a spanning subgraph of G, with the same vertex set as G, and edge set S. The *rank* of S is defined to be $|V(G)|$, less the number of connected components in the subgraph formed by S. We will denote it by $r(S)$. The *rank polynomial* of a graph G is defined to be

$$R(G; x, y) = \sum_{S \subseteq E(G)} x^{r(E)-r(S)} y^{|S|-r(S)} .$$

The rank polynomial has some interesting properties. If G is the disjoint union of graphs G_1 and G_2 then

$$R(G; x, y) = R(G_1; x, y)R(G_2; x, y) . \tag{2.4}$$

If $e \in E(G)$, let $G \backslash e$ be the graph obtained by deleting e from G, and let G/e be the graph obtained by contracting e (i.e., by deleting e and then identifying its end points). Then, if e is not a cut-edge or a loop, one can show that

$$R(G; x, y) = \sum_{S \subseteq E(G), e \in S} x^{r(S)} y^{|S|-r(S)} + \sum_{S \subseteq E(G), e \notin S} x^{r(S)} y^{|S|-r(S)}$$

$$= R(G/e; x, y) + R(G \backslash e; x, y) . \tag{2.5}$$

In the remaining cases we have

$$R(G; x, y) = \begin{cases} (1 + x)R(G/e; x, y) , & \text{if } e \text{ is a cut-edge} , \\ (1 + y)R(G \backslash e; x, y) , & \text{if } e \text{ is a loop} . \end{cases}$$

Now consider the partition function for the Ising model on a graph G, which can be written in the form

$$Z(G) = \sum_{\sigma} \prod_{ij \in E(G)} \lambda^{\sigma_i \sigma_j} ,$$

where $\lambda = \exp \beta$. The product $\sigma_i \sigma_j$ is either 1 or -1. Define E_σ^+ to be the set of edges ij of G such that $\sigma_i \sigma_j = 1$ and let E_σ^- be the remaining edges of G. Let

$m = |E(G)|$. Then we have

$$Z(G) = \sum_\sigma \lambda^{|E_\sigma^+| - |E_\sigma^-|} = \sum_\sigma \lambda^{m - 2|E_\sigma^-|} .$$

If $e = ij$ is a fixed edge in $E(G)$, not a loop or a cut-edge, it follows that

$$Z(G) = \sum_{\sigma_i = \sigma_j} \lambda^{m - 2|E_\sigma^-|} + \sum_{\sigma_i \neq \sigma_j} \lambda^{m - 2|E_\sigma^-|}$$

$$= \lambda Z(G/e) + \lambda^{-1}(Z(G \backslash e) - Z(G/e))$$

$$= (\lambda - \lambda^{-1})Z(G/e) + \lambda^{-1}Z(G \backslash e) . \qquad (2.6)$$

We can now use the following theorem of Oxley and Welsh (1979).

Theorem 2.7. *Let f be a real-valued function defined on graphs which satisfies the recursion*

$$f(G) = af(G/e) + bf(G \backslash e)$$

when e is an edge of G and not a loop or cut-edge, and

$$f(G) = \begin{cases} (1 + x)f(G/e) , & \text{if } e \text{ is a cut-edge} , \\ (1 + y)f(G \backslash e) , & \text{if } e \text{ is a loop} , \end{cases}$$

where $1 + x$ and $1 + y$ are the values taken by f on a cut-edge and loop respectively. Then if G has n vertices, m edges and c components, we have

$$f(G) = b^{m - n + c} a^{n - c} R\left(G; \frac{1 + x}{a} - 1, \frac{1 + y}{b} - 1\right) .$$

It follows that the partition function for the Ising model on a graph G is determined by its rank polynomial. From (2.6) we see that we can apply the previous theorem with $Z(G)$ in place of $f(G)$. Then

$$a = \lambda - \lambda^{-1} , \qquad b = \lambda^{-1}$$

and

$$1 + x = \lambda + \lambda^{-1} , \qquad 1 + y = \lambda^{-1} .$$

Theorem (2.7) now yields that

$$Z(G) = \lambda^{-m}(\lambda^2 - 1)^{n - c} R\left(G; \frac{2}{\lambda^2 - 1}, \lambda^2 - 1\right) .$$

A natural extension of the Ising model is to allow the spins to take more than two values. More precisely, if we allow the spin at each vertex to take values from the set $\{1, 2, \ldots, q\}$ and then define the partition function Z by $Z = \sum_\sigma \exp[\sum_{ij \in E} \beta\delta(\sigma_i, \sigma_j)]$ where δ is the usual delta function, we have what is known as the *q-state Potts model*.

Using a similar argument to that just given it is easy to see that again Z satisfies

a contraction–deletion recurrence formula. Hence for any graph G, Z is an evaluation of the rank polynomial of G; though along a different curve in the xy-plane, namely $xy = q$. For a proof of this and for details of the way in which the percolation and ice models to be discussed below can be represented in terms of the rank polynomial see Welsh (1990) or the original paper of Fortuin and Kasteleyn (1972).

For excellent rigorous mathematical treatments of these topics we refer to the monographs of Ruelle (1969) or Thompson (1972).

3. Percolation processes

As its name suggests, percolation theory is concerned with flow in random media. Its origin in the work of Broadbent and Hammersley (1957) was as a model for molecules penetrating a porous solid, electrons migrating over an atomic lattice, solute diffusing through a solvent, or a disease infecting a community.

As an example of percolation in the wider sense consider the following problem in communication theory.

Example (*Random graphs and reliability*). Let N be the network shown in fig. 3.1(a). Suppose each directed edge has probability p of being reliable, that is, allowing a message to pass. Suppose further that the reliability of each edge is independent of the reliability of any other edge. What is the probability that there is a path from A to B consisting only of reliable edges?

Denoting this event by $A \sim B$, simple calculation shows that it is just the probability that not all the routes from A to B are unreliable. Since the routes have no edge in common we are dealing with independent random variables and we have

$$\Pr[A \sim B] = 1 - (1 - p^2)^3 .$$

However, if we try the same problem for the network N', of fig. 3.1(b) the problem becomes much more complicated. This is due solely to the *dependence* in N' of the events "the route $ACDB$ is reliable" and "the route ACB is reliable".

This problem illustrates the intrinsic difficulty of percolation problems – stochastic dependence occurs in all but the most trivial cases and makes computation
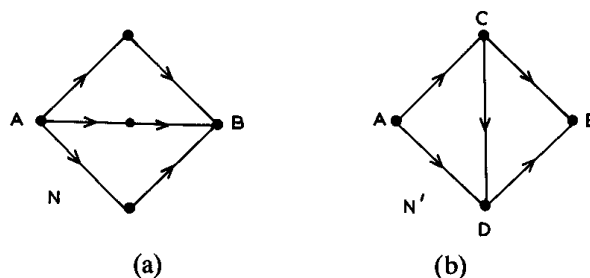

(a)   (b)

Figure 3.1.

very difficult. Indeed, even with the speed of modern computing machines it is still impractical to determine the reliability of moderate-sized networks. In the language of computational complexity the problem is #P-hard (see chapter 29 by Shmoys and Tardos).

In *classical percolation theory* we are concerned with the probability of infinite clusters in a "regular crystal lattice". The definition of what exactly is meant by a "regular crystal lattice" is rather difficult to formulate precisely – it varies from author to author. For the purposes of this chapter it can be regarded as typified by the regular lattices shown in fig. 3.2, though of course the physically most interesting cases are when the lattice is 3-dimensional.

Bond percolation

Suppose now that we fix attention on the 2-dimensional square lattice, and suppose that there is a supply of fluid at the origin and that each edge of $\mathscr{L}_2$ allows fluid to pass along it with probability p, independently for each edge. Let $P_n(p)$ be the probability that fluid spreads to at least n vertices. Thus

$$P_1(p) = 1 ,$$

$$P_2(p) = 1 - (1 - p)^4 ,$$

and in theory $P_N(p)$ can be calculated for any integer N. However, the reader will rapidly find it prohibitively time consuming. The case $N = 7$ is a fair piece of work! Obviously,

$$P_N(p) \geqslant P_{N+1}(p)$$

and hence the limit

$$P(p) = \lim_{N \to \infty} P_N(p)$$

exists and represents the probability that fluid spreads an infinite distance from the origin.

Very little has been rigorously proved about $P(p)$. For example, even though $P_j(p)$ is a polynomial in p and hence we would expect $P(p)$ to be a continuous function of p, this has not yet been proved. It is clear that there exists a *critical*
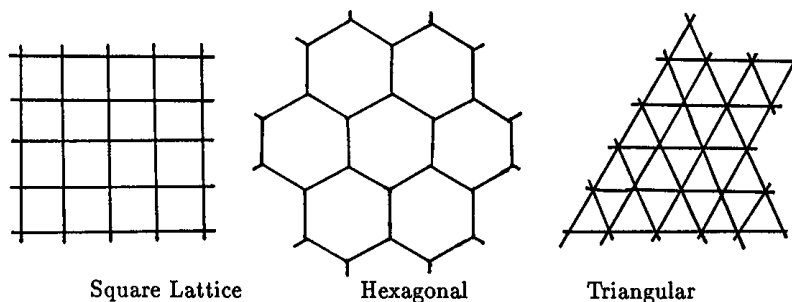

Square Lattice   Hexagonal   Triangular

Figure 3.2.

probability p_c such that

$$p < p_c \Rightarrow P(p) = 0 \quad \text{and} \quad p > p_c \Rightarrow P(p) > 0 .$$

However, determining the value of this critical probability is, as we will see, a very difficult problem. Monte Carlo simulations suggest that for all well-known lattices the behaviour of $P(p)$ has roughly the same S-shaped form as shown in fig. 3.3.

Atom or site percolation

In atom percolation, instead of each edge being randomly blocked with probability $1 - p$ or open with probability p, each vertex is blocked independently with probability $1 - p$ or open with probability p. Again we are interested in the probability of fluid spreading locally or an infinite distance.

Exactly analogous results hold for atom percolation as for bond percolation though of course the numerical values of the critical probabilities p_c and percolation probabilities $P(p)$ differ. In one sense atom percolation is the more important since any bond percolation problem on a lattice $\mathcal{L}$ can be turned into an atom percolation problem on a related lattice $\mathcal{L}$, namely the *line graph* of $\mathcal{L}$.

One of the few relatively easy results which has been proved is the following due to Fisher (1961) and Hammersley (1961a). For any regular lattice, if $P^A(p), P^B(p)$ represent respectively the atom and bond percolation probabilities on the lattice then

$$P^A(p) \leqslant P^B(p) , \quad 0 \leqslant p \leqslant 1 .$$

Clearly this implies that for any lattice the critical probability for atom percolation is at least as big as the critical probability for bond percolation.

The cluster problem

An alternative approach to percolation theory is the study of the distribution of white and black clusters when the edges (or vertices) of a graph are independently painted white with probability p and black with probability $q = 1 - p$.
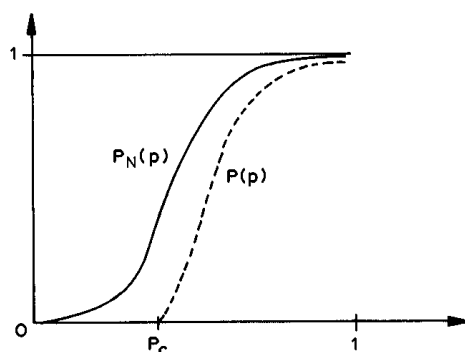

Figure 3.3.

Again we shall concentrate on the edge problem for the square lattice. A white *cluster* is a maximal connected subset of white edges of the lattice. The two main quantities of physical interest are:

(a) the average number of white clusters;

(b) the average number of vertices in a white cluster.

To be more precise let $\mathcal{L}_m$ denote a square section of the square lattice containing m^2 vertices and hence $2(m-1)^2$ edges. If ω denotes a particular black/white painting of $\mathcal{L}_m$ then let $c_m(\omega)$ denote the number of white clusters and let its average value over all paintings ω be denoted by $K_m(p)$.

Similarly if we let the distinct clusters under ω be labelled $A_1, \ldots, A_{c(\omega)}$, we define

$$S_m(p) = \left\langle \left[\frac{|V(A_1)| + \cdots + |V(A_{c(\omega)})|}{c_m(\omega)} \right] \right\rangle,$$

where $|V(A_i)|$ denotes the number of vertices ion A_i, and $\langle \cdot \rangle$ denotes the expectation over all black and white paintings. Thus $S_m(p)$ is the average number of vertices in a white cluster.

Note that if isolated points are not counted as clusters then the expected number of clusters in this sense is given by $K_m(p) - m^2 q^4$ where $q = 1 - p$. This is because the probability that a particular vertex forms an isolated cluster is just the probability that the four edges incident with it are painted black, that is q^4. Thus the average number of isolated points amongst the white clusters is $m^2 q^4$.

The average number of black clusters is obviously $K_m(1-p)$ and the average number of vertices in a black cluster is obviously $S_m(1-p)$. Little more is known theoretically about either of these functions, other than that

$$K_m(p) \sim m^2 \lambda(p) \quad \text{as } m \to \infty,$$

where λ is an undetermined function of p.

Roughly speaking the quantities $K_m(p)$ and $S_m(p)$ are reciprocal, though theoretically all that has been proved is that

$$S_m(p) \geq m^2 / K_m(p).$$

For p greater than the critical probability p_c we have a positive probability of an infinite white cluster in $\mathcal{L}_\infty$. Hence, a fortiori, as $p \to p_c$ the average size of a cluster tends to ∞. Numerical evidence suggests that, as p approaches p_c from below, there exist constants C and γ such that as $m \to \infty$, $S_m(p) \to S(p)$ where

$$S(p) \sim C(p_c - p)^{-\gamma},$$

where, moreover, γ is an invariant depending only on the dimensionality of the lattice.

One of the most interesting theoretical results on the cluster problem is the following theorem of Harris (1960).

Theorem 3.1. *For the cluster problem on the infinite square lattice, if p is strictly greater than the critical probability then, with probability one, the set of white edges contains only one infinite component.*

Extensions of this to higher dimensions can be found in Grimmett (1989).

Determining the critical probability

The problem of finding critical probabilities for particular lattices, first posed in 1957, has received great attention, but is still proving to be a remarkably difficult problem. A vast amount of numerical estimation (based on Monte Carlo methods, Padé approximations and the like) has been carried out, so good numerical estimates exist for most of the 2- and 3-dimensional lattices.

Theoretically much less is known. A landmark in the study of critical probabilities was the paper by Sykes and Essam (1964) which, though unrigorous, gave convincing arguments for believing that for bond percolation on a planar lattice the critical probabilities were related by

$$p_c(\mathscr{L}) + p_c(\mathscr{L}^*) = 1 , \qquad (3.2)$$

where $\mathscr{L}^*$ is the planar dual of $\mathscr{L}$.

An obvious consequence of this is the following.

Theorem 3.3. *For bond percolation on the square lattice, the critical probability is* $\frac{1}{2}$.

This result was finally proved by Kesten (1980) by a series of ingenious arguments which have led to a rigorous proof by Wierman (1981) of the following result, again first shown unrigorously by Sykes and Essam (1964).

Theorem 3.4. *For bond percolation on the 2-dimensional triangular lattice (T) and the hexagonal lattice (H),*

$$p_c(T) = 2 \sin(\pi/18) ,$$
$$p_c(H) = 1 - 2 \sin(\pi/18) .$$

However, all of these arguments are very much restricted to 2 dimensions. A fundamental and very difficult problem is the following.

Problem 3.5. Determine the critical probability of bond or site percolation on the 3-dimensional cubic lattice.

Even for 2-dimensional planar lattices there are many open problems. For example: the following is known from Toth (1985) and Zuev (1987).

Theorem 3.6. *The critical probability of site percolation on the square lattice is between* 0.5095 *and* 0.68189.

However, this is a very wide range and we pose the following.

Problem 3.7. What is the critical probability for site percolation on the square lattice?

First passage percolation

This originated in the paper of Hammersley and Welsh (1965) as a model for a "time dependent" percolation process. It contains ordinary percolation as a special case and in its most general sense can be regarded as a randomized version of the shortest route problem in graphs.

Consider the square lattice in which each edge, is, independently, assigned a non-negative random length drawn from a known probability distribution F.

Let t_n be the random first passage (shortest) path length from the origin to $(n, 0)$ in this lattice and let $\tau(n)$ be its expected value over all possible *states* (that is distribution of lengths). The fundamental observations are that for $m, n \in \mathbb{Z}$

$$\tau(m + n) \leq \tau(m) + (n) \tag{3.8}$$

so that by the theory of subadditive functions

$$\lim_{n \to \infty} \frac{\tau(n)}{n} = \inf_n \frac{\tau(n)}{n} = \mu \tag{3.9}$$

exists.

The *time constant* μ depends only on the distribution F and is, like the critical probability of ordinary percolation, a not very well-understood lattice invariant. For example when the lengths are uniformly distributed in $[0, 1]$ it is known from Monte Carlo studies that $\mu \simeq 0.323$, but its exact evaluation seems a hopelessly intractable problem.

Apart from its intrinsic interest, first passage percolation led Hammersley and Welsh (1965) to set up a theory of subadditive stochastic processes which are now a fundamental tool in probability and probabilistic combinatorics, see for example Kingman (1973).

Correlated percolation

In an ideal world one would like to be able to remove the restriction that the random component associated with an edge in each of the above models was independent of all other edges. This is the subject of correlated percolation which is now a topic of considerable interest in the physical literature but for which (understandably) there are very few theoretical results.

For comprehensive rigorous accounts of what is now a huge area of research in

statistical physics we refer to the monographs of Smythe and Wierman (1978), Kesten (1982) and Grimmett (1989).

4. Enumeration and related problems

Several fundamental problems in statistical physics and related areas of the natural sciences reduce to enumerating structures of different types. In this section we discuss a few of the most studied and basic problems of this nature.

Animals or polyominoes

Consider the 2-dimensional square lattice $\mathscr{L}_2$ with origin 0. An *animal* or *polyomino* of n cells is a connected subgraph of $\mathscr{L}_2$ containing 0 and having n vertices. Let $a(n)$ denote the number of distinct animals having n cells. Then clearly $a(1) = 1$, $a(2) = 4$ and counting the 3-celled animal types illustrated in fig. 4.1, we see $a(3) = 18$.

The fundamental problem which is now at least 30 years old is to determine the form of $a(n)$ for the different lattices. However, as with percolation theory, rigorous exact results about animals are pretty scarce.

First we will point out the connection between animals and percolation theory. Suppose that we could determine $a(n, b)$, the number of animals with n cells and b boundary cells. (As the name suggests a cell is a *boundary* cell of a specific animal A if it is a vertex of $\mathscr{L}$ which is not in A but is adjacent to a vertex of A.) Then from $a(n, b)$ it is not difficult to compute the average cluster size in a percolation model. From this we get good bounds for the critical probability.

Other applications of animals are to growth problems and as models of branched polymers with excluded volume.

Now let us turn to some basic results about $a(n)$ for the square lattice. A straightforward counting argument gives

$$2^n \leq a(n) \leq (6.25)^n . \tag{4.1}$$

It is also easy to prove that, for any positive integers m, n,

$$a(m + n) \geq a(m)a(n) . \tag{4.2}$$

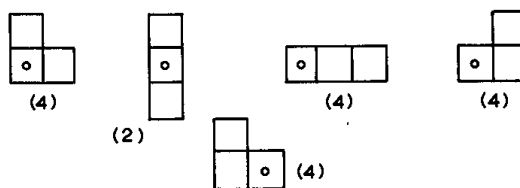Proof: Each animal has a top right corner and a bottom left corner. By "sticking"

Figure 4.1.

the bottom left corner of an n-celled animal to the top right corner of an m-celled animal we obtain an $(m + n)$-celled animal.

By the basic property of subadditive functions, (4.1) and (4.2) give the fundamental result which holds (by analogous argument) for any regular lattice.

Theorem 4.3. *For any lattice $\mathscr{L}$ there exists a constant $a(\mathscr{L})$ such that if $a(n)$ denotes the number of n-celled animals of $\mathscr{L}$ then*

$$\lim_{n \to \infty} a(n)^{1/n} = \sup_{n \geqslant \infty} [a(n)]^{1/n} = a(\mathscr{L}) .$$

Determining the limiting constant $a(\mathscr{L})$ exactly seems to be very difficult and even the best known bounds are not very tight. For example, in the most studied case of the square lattice, concatenation methods coupled with computer counts give the best known lower bound of 3.79 for $a(\mathscr{L}_2)$ while the best upper bound gives $a(\mathscr{L}_2) \leqslant 4.65$. There are reasons for believing that $a(\mathscr{L})$ is just above 4 in the case of this lattice.

For more details on these methods, the corresponding results for other lattices and a discussion of related problems we refer to a recent excellent review of Whittington and Soteros (1990).

Self-avoiding walks and polygons

Another counting problem closely connected with percolation theory and similar in spirit to the animal problem of the previous section is the following. A *self-avoiding walk* of length n on a lattice $\mathscr{L}$ is a path of n edges which has one endpoint at the origin. If $f(n)$ denotes the number of such self-avoiding walks, on the square lattice then clearly $f(1) = 4$, $f(2) = 12$ and in general it is easy to show that

$$2^n \leqslant f(n) \leqslant 4.3^{n-1} . \tag{4.4}$$

Using the submultiplicative property

$$f(m + n) \leqslant f(m)f(n)$$

and a similar bound to (4.4) for a general lattice, leads to the fundamental result.

Theorem 4.5. *For any lattice $\mathscr{L}$, there exists a constant $\mu = \mu(\mathscr{L})$ (known as the connective constant) such that if $f_{\mathscr{L}}(n)$ denotes the number of self-avoiding walks of length n on $\mathscr{L}$ then*

$$\lim_{n \to \infty} f_{\mathscr{L}}(n)^{1/n} = \inf_n [f_{\mathscr{L}}(n)]^{1/n} = \mu(\mathscr{L}) .$$

Determining μ exactly for any lattice except the regular tree has been a much studied problem since it was first posed in 1957. Even good bounds seem to be difficult to obtain. For example, for the 2-dimensional square lattice, the best bounds so far known are $2.57 \leqslant \mu \leqslant 2.73$.

A closely related quantity is $g_{\mathscr{L}}(n)$ which counts the number of self-avoiding polygons of n steps. Clearly $g_{\mathscr{L}}(n) \leq f_{\mathscr{L}}(n)$ but Hammersley (1961b) proved that for any lattice with connective constant $\mu(\mathscr{L})$,

$$\lim_{n \to \infty} g_{\mathscr{L}}(n)^{1/n} = \mu(\mathscr{L}) \, .$$

There are physical reasons (based on renormalisation arguments) and some numerical evidence which support the intriguing conjecture that there exist constants α and β such that

$$f_{\mathscr{L}}(n) \sim n^{\alpha} \mu^{n} \, , \qquad g_{\mathscr{L}}(n) \sim n^{\beta} \mu^{n}$$

and that α, β are dimensional invariants, in other words they only depend on the dimension of the lattice. Since Kesten (1963), there has been a great deal of rigorous mathematical progress notably by Hara and Slade (1992). For more details see Madras and Slade (1993).

The ice problem

As its name suggests the "ice problem" originates in the statistical physics associated with models used to calculate the residual entropy of "square ice". In its most general form an *ice model* specifies a set of allowable configurations at each vertex. All allowable configurations are of equal thermodynamic weight and the problem reduces to calculating the partition function, that is, enumerating the number of allowable configurations.

Probably the most studied ice problem is the following. Given any 4-regular graph G count the number of orientations ω of G which have the property that at each vertex there are exactly two inward and two outward pointing edges.

Another way of looking at this enumeration problem is as follows. Fix an orientation ω_0 of G. To each directed edge of G assign either a $+1$ or a -1 in such a way that the net flow into each vertex of G is zero. In other words, the ice problem on G is exactly the problem of counting nowhere-zero flows mod 3 in G, discussed in chapters 4 (Appendix) and 9. But this is exactly the evaluation of the Tutte polynomial of G at the point $(0, -2)$, or the rank polynomial of G at $(-1, -3)$.

Equivalently, by using the fact that when G is a planar graph, and G^* is its planar dual, $T(G; x, y)$ equals $T(G^*; y, x)$ and from the relation between Tutte polynomials and chromatic polynomials we see the following.

Proposition 4.6. *The ice problem on a 4-regular planar graph G is equivalent to counting 3-colourings of the dual graph.*

A remarkable result of Lieb (1967) is that if $Z(m, n)$ denotes the ice partition function (that is the number of ice orientations) on the $m \times n$ portion of the square lattice, then

$$\lim_{m,n \to \infty} [Z(m, n)]^{1/mn} = (\tfrac{4}{3})^{3/2} \, . \tag{4.7}$$

Percus (1971) gives a very complete and clear account of the different approaches to the ice problem culminating in a proof of (4.7) by the transfer matrix method to be described in section 5.

As far as statistical physics is concerned, the problems of most interest are when G is a 3-dimensional lattice. As far as mathematical solution is concerned, only a few 2-dimensional ice models have been solved, a comprehensive account of these is given in Baxter (1982).

The monomer–dimer problem

Let $p(G, k)$ denote the number of k-matchings in the graph G, with the understanding that $p(G, 0) = 1$. Define the polynomial $Q(G, z)$ by

$$Q(G, z) = \sum_{k \geq 0} p(G, k) z^{n - 2k} .$$

This is a modified form of the matchings polynomial, which is discussed in section 5 of chapter 31 (Godsil). It can also be viewed as the partition function of a physical system.

Consider a collection of sites on the surfaces of a metallic crystal. The surface is exposed to a gas consisting of monomers and dimers, e.g., hydrogen at a high temperature. Each site on the surface is occupied, either by a monomer or by one of the two ends of a dimer. Of course a pair of sites can be occupied by a dimer only if they are neighbours. The state of the system can be represented by a matching in a graph G. This has the crystal sites as its vertices, with two sites adjacent if and only if they can be occupied by the same dimer. Those pairs of sites occupied by dimers determine a matching. Hence the system is completely described by the graph G, the matching and the temperature. (The latter determines the energy gained by filling the crystal sites with monomers and dimers.)

The physical question is whether this system will undergo a phase transition as the temperature varies. In fact it does not, except possibly when there are no monomers. This was proved by Heilmann and Lieb (1972). They showed that all zeros of $Q(G, z)$ have zero real part, and their absolute value is bounded above by $2\sqrt{\Delta - 1}$, where Δ is the maximum valency of a vertex in G. From these facts they eventually deduce the absence of a phase transition. The matchings polynomial has a number of interesting combinatorial properties; see chapter 3 (Pulleyblank).

Hard hexagons

We work on the triangular lattice. Consider a system where some of the vertices of this lattice are covered by hexagons, with each hexagon covering a central vertex and its six neighbours. Two adjacent vertices cannot be both at the centre of a hexagon. We can describe the state σ of the system by assigning a weight 1 to each vertex at the centre of a hexagon, and 0 to the remaining vertices. Thus we may view σ as a 01-vector indexed by the vertices of the lattice. The partition

function is

$$Z = \sum_{\sigma} z^{\sigma_1 + \cdots + \sigma_N} \prod_{ij \in E} (1 - \sigma_i \sigma_j) \, ,$$

where the product is over all edges of the lattice, and the exponent of z is just the number of hexagons. Baxter establishes an invariance property of this partition function using the star–triangle relation. From this he then deduces the free energy. One surprise is an intimate connection with the Rogers–Ramanujan identities. We direct the reader to Andrews (1982) and Andrews et al. (1984) for more information about this relationship.

5. Transfer matrices

Many of the combinatorial problems arIsing in statistical physics can be reduced to enumeration problems, and these in turn can sometimes be solved by the method of *transfer matrices*, which we now discuss.

We begin with the problem of determining the number of ways an $m \times n$ chessboard can be covered with dominoes. Suppose that our board has been covered with dominoes. The given covering can be encoded by assigning one of four states $\{U, D, L, R\}$ to each square of the board. The state of a square determines where the other half of the domino covering the square lies. Thus, if the other half of the domino covering a square is above it, then the square has state U. If it is below we use D, and if it is to the left or the right we use L or R respectively. It should be clear that many assignments of states to squares do not correspond to coverings, but every covering gives rise to a unique assignment of states to squares.

Now we take our coding a step further. View our chessboard as a sequence of n columns. Once a covering is given, the state of the vertices in a given column can be represented by a vector, with states as entries. (Of course, the set of possible vectors for the first and last columns will be a subset of the possible vectors for an interior column.) Thus our covering can now be encoded as a sequence

$$\sigma_1, \ldots, \sigma_n \, ,$$

where σ_i is the state vector for the ith column.

Let Σ be the set of all possible state vectors for a column. Construct a graph $G = G(\Sigma)$ with vertex set Σ, and with two vertices σ and σ' adjacent if there is a covering such that there are consecutive columns with states σ and σ'. The states that can be taken by the first column form a subset, S say, of $V(G)$ and the states available to the last column form a subset F, say. The number of possible coverings of our $m \times n$ chessboard can now be shown to equal the number of walks of length n in G which start at a vertex in S and finish at a vertex in F. (Our terminology here follows that used in section 5 of chapter 31 by Godsil).

If A is the adjacency matrix of G and we denote the characteristic vectors of the sets S and F by $\chi(S)$ and $\chi(F)$ respectively then the required number of walks

is

$$\chi(S)^{\mathrm{T}} A^n \chi(F).$$

Using the theory of the spectral decomposition of a symmetric matrix we may write

$$A^n = \sum_\theta \theta^n Z_\theta,$$

where θ ranges over the distinct eigenvalues of A and Z_θ is the matrix representing orthogonal projection onto the eigenspace associated to θ. Denote the largest eigenvalue of A by θ_1. Then by the Perron–Frobenius theory we know that if G is connected then θ_1 is simple, and for any other eigenvalue θ, we have $|\theta| < \theta_1$. It follows that

$$\frac{\chi(S)^{\mathrm{T}} A^n \chi(F)}{\theta_1^n} \to \chi(S)^{\mathrm{T}} Z_{\theta_1} \chi(F)$$

and hence that

$$(\chi(S)^{\mathrm{T}} A^n \chi(F))^{1/n} \to \theta_1 \tag{5.1}$$

as n tends to infinity.

The number of domino coverings of our chessboard can be expressed as the number of perfect matchings in a graph, H say. The vertices of H are the squares of the chessboard, and two squares are adjacent in H if and only if they are adjacent on the board. Any domino covering gives a perfect matching in the graph. A generalisation of the original problem can now be obtained as follows. Assign a weight to each edge of H and define the weight of a matching to be the product of the weights of the edges it uses. Instead of simply computing the number of perfect matchings in H, we may determine the sum of the weights of all perfect matchings. The weights we use may be variables, in which case the sum will be a polynomial. (For example we might assign a weight α to each edge of H joining two squares in the same column of the board, and a weight β to the remaining edges. The sum will then be a homogeneous polynomial in α and β.)

In particular, the partition function for the Ising problem itself can be expressed in terms of the number of perfect matchings in an edge-weighted planar graph. (See Appendix E in Thompson 1972.) If we then seek to determine this partition function by a transfer matrix argument, we will find it expressed in the form

$$Z = u^{\mathrm{T}} A^n v$$

for a suitable matrix A and vectors u and v. A statistical physicist would then be concerned with properties of the limit

$$(u^{\mathrm{T}} A^n v)^{1/n}$$

as n tends to infinity. From the discussion above of the domino problem, we may

see that this quantity may be expressed as the largest eigenvalue of a symmetric matrix. Alternatively, we could use the generating function

$$\sum_{n \geq 0} \lambda^n u^{\mathrm{T}} A^n v \;;$$

the largest eigenvalue of A is, in general, the reciprocal of the radius of convergence of this power series.

To close this section, we remark that a solution to the chessboard problem will be found in section 4 of Lovász (1979). (However, it uses Pfaffians rather than transfer matrices. Pfaffians are discussed briefly in section 5 of chapter 31 by Godsil.) A more leisurely introduction to the method of transfer matrices may be found in Percus (1971) and Stanley (1986). A number of applications of this method can be found in Baxter (1982).

6. Duality, stars and triangles

In this section we shall illustrate by example a technique which has been frequently used to resolve (combinatorial) problems of physics. The partition function for the Ising model has two interesting invariance properties. First, if G is a plane graph with dual G^* then their rank polynomials are related by

$$R(G; x, y) = R(G^*; y, x) \;.$$

A proof of this will be found in chapter 9 by Welsh. If

$$\lambda = \left(\frac{\mu^2 + 1}{\mu^2 - 1} \right)^{1/2}$$

then

$$R\!\left(G; \frac{2}{\lambda^2 - 1}, \lambda^2 - 1 \right) = R\!\left(G; \mu^2 - 1, \frac{2}{\mu^2 - 1} \right) = R\!\left(G^*; \frac{2}{\mu^2 - 1}, \mu^2 - 1 \right) .$$

Recalling the relation of the rank polynomial to the partition function described in section 2, this leads to a relation between the partition function for the Ising model on the graph G, expressed in terms of λ, and the partition function of G^*, expressed in terms of $[(\mu^2 + 1)/(\mu^2 - 1)]^{1/2}$. If G is the infinite square lattice then G^* is isomorphic to G and the duality relation becomes an invariance condition. Physically this can be viewed as a relation between the values of the partition function at high temperatures and low temperatures. For more details, see Thompson (1972) or Baxter (1982).

For our next invariance property, we need to consider a generalisation of the Ising model, with partition function

$$Z(G) = \sum_{\sigma} \exp\!\left[-\sum_{ij \in E(G)} \beta_{ij} \sigma_i \sigma_j \right] .$$

Recall from section 2 that in the case of uniform interactions $\beta = J/kT$, here we allow all the interactions J to vary to that β also varies.

By way of example, if G is the square lattice we might have $\beta_{ij} = K$ for all horizontal edges and $\beta_{ij} = L$ for all vertical edges. If $e = ij$ and $\lambda_e = \exp \beta_{ij}$ then we find in place of (2.6) that

$$Z(G) = (\lambda_e - \lambda_e^{-1})Z(G/e) + \lambda_e^{-1}Z(G \backslash e) .$$

Consider the star S and triangle T, with weights as indicated in fig. 6.1.

Suppose that in both cases the vertices 1, 2 and 3 are assigned states σ_1, σ_2 and σ_3. Suppose that the vertices 1, 2 and 3 in S are part of some larger graph G. Then $Z(G)$ is a sum over all possible state assignments of its vertices. For a given state, the corresponding term in the sum is the product of a contribution from the edges of S, and one from the edges not in S. The contribution from S is

$$\exp[\sigma_0(L_1\sigma_1 + L_2\sigma_2 + L_3\sigma_3)] .$$

We divide the possible states into pairs, where members of the same pair differ only in the value of σ_0. Thus we may write $Z(G)$ in the form

$$\sum_\sigma 2\cosh(L_1\sigma_1 + L_2\sigma_2 + L_3\sigma_3)f(\sigma) , \tag{6.1}$$

where $f(\sigma)$ is the contribution of the edges not in S, given the values of σ on the vertices of $G \backslash 0$.

Now suppose that we alter G by deleting the vertex 0 and the three edges of S, replacing them with the three edges of T. The new graph, which we denote by G', thus has one less vertex than G. Its partition function can be written in the form

$$\sum_\sigma \exp(K_1\sigma_2\sigma_3 + K_2\sigma_1\sigma_3 + K_3\sigma_1\sigma_2)f(\sigma) . \tag{6.2}$$

Then the surprise is, that given L_1, L_2 and L_3, it is possible to choose K_1, K_2 and K_3 so that

$$2\cosh(L_1\sigma_1 + L_2\sigma_2 + L_3\sigma_3) = R \exp(K_1\sigma_2\sigma_3 + K_2\sigma_1\sigma_3 + K_3\sigma_1\sigma_2)$$
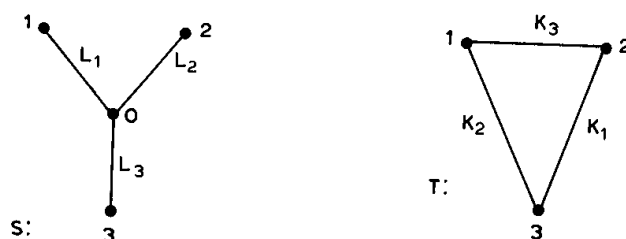

Figure 6.1.

and then $Z(G) = RZ(G')$. To achieve this we need

$$2\cosh(L_1 + L_2 + L_3) = R\exp(K_1 + K_2 + K_3),$$
$$2\cosh(-L_1 + L_2 + L_3) = R\exp(K_1 - K_2 - K_3),$$
$$2\cosh(L_1 - L_2 + L_3) = R\exp(-K_1 + K_2 - K_3),$$
$$2\cosh(L_1 + L_2 - L_3) = R\exp(-K_1 - K_2 + K_3).$$

Denote the four terms on the left by c, c_1, c_2 and c_3 respectively. Then multiplying these four equations together yields that

$$R^4 = cc_1c_2c_3$$

is a necessary condition. Further manipulations yield

$$\sinh(2K_1)\sinh(2L_1) = \sinh(2K_2)\sinh(2L_2) = \sinh(2K_3)\sinh(2L_3) = d^{-1},$$

where

$$d^{-1} = \frac{\sinh(2L_1)\sinh(2L_2)\sinh(2L_3)}{2(cc_1c_2c_3)^{1/2}},$$

as a second necessary condition. If the values of R and K_i are as given by the last three equations then $Z(G) = RZ(G')$. (For help with the missing details, see chapter 6 of Baxter 1982.)

If G is the hexagonal lattice then it can be transformed into a triangular lattice by repeatedly replacing stars by triangles. (The hexagonal lattice is bipartite; replace all the stars centered on vertices in one of the two colour classes.) This gives us a relation between an Ising model on the hexagonal lattice and one on the triangular lattice. We obtain a second, independent, relation by recognising that the hexagonal lattice is the planar dual of the triangular lattice. Composing these relations yields an expression for the partition function of an Ising model at low temperature in terms of a partition function at high temperature, for both the triangular and hexagonal lattices. This is an analogue of the relation obtained for the square lattice above. (Again, see Baxter 1982 for more detail.)

Other applications of this star–triangle transformation, which is really a special instance of planar duality theory have been in percolation theory, to the Potts model and to the six and eight vertex ice model. More details may be found in Temperley (1981).

7. Ground states of spin glasses

We will now turn to a different application of combinatorics in statistical physics and outline how some questions about spin glasses can be answered by employing the mathematical machinery of combinatorial optimization. We concentrate on showing that the problem of determining ground states of spin glasses can be viewed as a so-called maximum cut problem in graphs.

The study of order–disorder phenomena is a flourishing branch in today's physics. One of the most successful attempts to understand disorderly systems has been the study of spin glasses. They occupy a central position in this area. The composition of a spin glass is unremarkable – perhaps a few iron atoms scattered in a lattice of copper atoms – but its magnetic properties are confoundedly complicated and sometimes tantalizingly unpredictable. "Spin" is the quantum-mechanical spin from which magnetic effects arise; "glass" refers to the disorder in the orientations and interactions of the spins. For an introduction to the general theory of spin glass models see Mezard et al. (1987).

Physicists have developed a number of theories to model spin glasses and explain their behaviour. Some of these theories predict contradicting phenomena. These phenomena occur in situations which are hard to realize experimentally. In order to test the theories and guide the design of experiments, researchers have designed computer models to simulate the behaviour of spin glasses and then observe which phenomena occur. Some aspects studied in these models lead to optimization problems. The papers by Toulouse (1977), Bieche et al. (1980), and Barahona et al. (1982) have pioneered the study of spin glasses from an optimization point of view and pointed out the close links of the ground state problem to interesting models in combinatorial optimization.

A spin glass is an alloy of magnetic impurities diluted in a non-magnetic material. Alloys that show spin glass behaviour are, for instance, CuMn; the metallic crystal AuFe; the insulator EuSrS; the amorphous metal GdAl. One characteristic of spin glasses is a peak in magnetic susceptibility at a certain temperature. This peak indicates a phase transition. Another phase transition may take place at very low temperature. However, it is an open question at present whether, or under what conditions on the spin glass, such a phase transition occurs, and what order phenomena show up at low temperature.

We will now present a mathematical model of spin glasses. We assume a given spin glass that contains n magnetic impurities (atoms). Each magnetic atom i has a magnetic orientation (spin) which is represented by a 3-dimensional unit-length vector S_i. Between each pair i, j of magnetic atoms there is an interaction J_{ij} that depends on the non-magnetic material and on the distance r_{ij} between the atoms. Several proposals in the literature model this interaction. One common feature of many of these models is that the absolute value of the interaction decreases rapidly with distance and that small changes of distance may result in a change of the sign of the interaction. One example of such an interaction function which is used frequently is

$$J_{ij} = J(r_{ij}) = A\frac{\cos(Dr_{ij})}{B^3 r_{ij}^3},$$

where A, B, and D are material-dependent constants. In another model some number J is chosen and the interactions have to satisfy

$$J_{ij} \in \{0, +J, -J\}.$$

If atoms i and j have spins S_i and S_j, the energy interaction between i and j is given by

$$H_{ij} = J_{ij} S_i \cdot S_j ,$$

where $S_i \cdot S_j$ denotes the Euclidean inner product. Given a spin configuration or state, σ, the energy of the whole system is given by the Hamiltonian

$$H(\sigma) = -\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} J_{ij} S_i \cdot S_j - h \sum_{i=1}^{n} S_i \cdot F ,$$

where a unit length vector $F \in \mathbb{R}^3$ represents the orientation of an exterior magnetic field and h represents the strength of this field.

The study of this Hamiltonian is a major issue in statistical physics. Its difficulty has led to considering various simplifications. One such simplification is to replace the 3-dimensional vectors S_i and the magnetic field F by 1-dimensional vectors σ_i, respectively f, with values $+1$ or -1 (called "*Ising spin*"), meaning magnetic north pole "up" and magnetic north pole "down". Such a representation is called the *Ising model* of spin glasses, see section 2 of this chapter for a general introduction to this model and some of its properties. There are, in fact, substances which show an up/down behaviour and for which the Ising model seems to be the "correct" model and not just a simplification.

Models that consider interactions between all pairs of impurities were introduced by Sherrington and Kirkpatrick and are called *long range models*. A number of models consider only interactions between "close" impurities (so-called nearest neighbour interactions), and set to zero the interactions between impurities that are far apart. These models, introduced by Edwards and Anderson, are called *short range models*. Many physicists consider short range models more realistic (see Young 1984). Moreover, a number of substances show short range interactions only: next-neighbour and second-next-neighbour, say.

It is customary to make further simplifications and to consider the spins regularly distributed, say on a 2- or 3-dimensional grid (that is square or cubic lattice). In a typical short range model of such a given structure, interactions are non-zero only along edges of the grid, so, for instance, in two-space, an impurity interacts only with (at most) four other impurities, its neighbours in the grid graph. Two grid models of this type have been studied intensively: the *Gaussian model*, where the interactions are chosen from a Gaussian distribution, and the $\pm J$-*model*, where the interactions between impurities take only the values $+J$ or $-J$, J a fixed positive number, according to some probability distribution. In a real spin glass (an alloy), the magnetic impurities are randomly distributed. Note that in the models just introduced, the spins are regularly distributed in a grid, but the interaction values are considered random.

The partition function of the Ising model has been introduced in section 2. For our purposes, it is useful to write it in the following way. Let Ω be the set of all possible configurations of Ising spins on a grid, say. So $|\Omega| = 2^n$, if there are n spins. Then the behaviour of the system at temperature T is believed to be

described by the magnetic partition function

$$Z(T) = \sum_{\sigma \in \Omega} \exp\left(\frac{-H(\sigma)}{kT}\right),$$

where k is the Boltzmann constant. As mentioned in section 2, analytic expressions of the partition function, in general, are not known.

At $0°K$, the spin glass system attains a minimum energy configuration. Such a configuration is called a *ground state*. A ground state can be found by minimizing the Hamiltonian associated with the system. We will now present the reduction of the problem of finding a minimum energy spin configuration in the Ising model to a max-cut problem in graphs.

Suppose we have magnetic impurities $1, 2, \ldots, n$ and an exterior magnetic field, 0. We set $V = \{0, 1, \ldots, n\}$ and consider V as the vertex set of a graph $G = (V, E)$. For a pair i, j of impurities, G contains an edge ij if the interaction J_{ij} between i and j is non-zero. An edge $0i$ links every impurity i, $1 \le i \le n$, to the magnetic field 0. Let us call G the *interaction graph* of the spin system. An Ising spin $\sigma_i \in \{-1, +1\}$ is associated with each impurity. The Ising spin σ_0 of the exterior magnetic field can be set to $+1$ without loss of generality. Let h be the strength of the magnetic field and set $J_{0i} = h$ for $i = 1, \ldots, n$, then we can write the Hamiltonian of this model as a quadratic function in ± 1-variables in the following way:

$$H(\sigma) = -\sum_{\substack{ij \in E \\ i,j > 0}} J_{ij} \sigma_i \sigma_j - h \sum_{i=1}^{n} \sigma_i = -\sum_{ij \in E} J_{ij} \sigma_i \sigma_j.$$

Each spin configuration σ corresponds to a partition of V into V^+ and V^-, where $V^+ = \{i \in V \mid \sigma_i = +1\}$ and $V^- = \{i \in V \mid \sigma_i = -1\}$. So we can write the energy of the state σ in the form

$$H(\sigma) = -\sum_{ij \in E(V^+)} J_{ij} \sigma_i \sigma_j - \sum_{ij \in E(V^-)} J_{ij} \sigma_i \sigma_j - \sum_{ij \in \delta(V^+)} J_{ij} \sigma_i \sigma_j$$

$$= -\sum_{ij \in E(V^+)} J_{ij} - \sum_{ij \in E(V^-)} J_{ij} + \sum_{ij \in \delta(V^+)} J_{ij}.$$

Recall that, for each subset W of V, $E(W) = \{ij \in E \mid i, j \in W\}$ and $\delta(W) = \{ij \in E \mid i \in W, j \in V \setminus W\}$ and that the edge sets of type $\delta(W)$ are called cuts. Setting $C = \sum_{ij \in E} J_{ij}$, we see that

$$H(\sigma) + C = 2 \sum_{ij \in \delta(V^+)} J_{ij},$$

and defining $c_{ij} = -J_{ij}$ for all $ij \in E$, we find that the problem of minimizing H is equivalent to maximizing

$$c(\delta(V^+)) = \sum_{ij \in \delta(V^+)} c_{ij}$$

over all $V^+ \subseteq V$. The problem of finding, given a graph with edge weights, a cut $\delta(W)$ such that the sum of weights of the edges of $\delta(W)$ is as large as possible is known as the *max-cut problem*. Thus finding a ground state in the Ising model of a spin glass is equivalent to finding an optimum solution of the corresponding max-cut problem.

To determine ground states of spin glasses or, equivalently, cuts of maximum weight, physicists have introduced the so-called *simulated annealing method*. This is an algorithmic analogue of standard techniques in the material sciences where, for instance, large (and perfect) crystals are grown by using a careful scheme of cooling and heating the material to temperatures very close below and above the critical temperature where the liquid freezes into an ordered array of atoms, the crystal. This method was formulated as a general heuristic for the solution of arbitrary combinatorial optimization problems, see, for example, Kirkpatrick et al. (1983), and usually turned out to be a reasonable, though slow, approximation algorithm, see Johnson et al. (1989, 1991).

It soon became clear that, by simulated annealing, states of low energy can be reached but that there is no guarantee or proof that a true ground state can be found. Thus more sophisticated combinatorial methods came into play that we briefly want to mention. More detailed and thorough surveys of these aspects with large lists of references are Barahona et al. (1988), Grötschel et al. (1987).

From the complexity point of view (cf. chapter 29 by Shmoys and Tardos) it turned out that the max-cut problem is NP-hard for general graphs, and so the spin glass problem is. But much more restricted spin systems turned out to lead to hard optimization models. For instance, finding a ground state is NP-hard even if the interaction graph of the spin system is a 3-dimensional grid, or a 3-dimensional grid with just two layers, or even a planar grid with an external magnetic field, provided the interactions are taken from $\{-J, 0, J\}$.

On the other hand, if the interaction graph of the spin system is a planar graph and there is no external field then using the duality theory of planar graphs one can transform the associated max-cut problem to a so-called *Chinese postman problem*. This problem can be solved by the algorithm of Edmonds and Johnson (1973) which combines a series of shortest path calculations and an application of the matching algorithm in an ingenious way. Barahona (1983) extended this to graphs not contractible to the complete graph K_5. Using the Edmonds–Johnson algorithm, ground states of large planar spin systems can (and have been frequently) calculated easily.

The most interesting open questions about spin glasses occur, however, in three dimensions or when an external magnetic field is involved. To solve such (NP-hard) instances various enumeration techniques (e.g., the transfer matrix method) have been designed. The most successful approach seems to be the use of cutting plane algorithms (cf. chapter 37) that are based on an intensive study of the so-called *cut polytope*. This approach is called polyhedral combinatorics and is explained in chapter 30. With these linear programming based cutting plane algorithms, spin systems in three dimensions or two dimensions with magnetic field can be treated that have well over thousand spins. Algorithms of this type

terminate with an optimality guarantee, that is, true ground states can be found; and they have further desirable features. But, of course, no polynomial running time guarantee can be given. For more information, see Barahona et al. (1988) and Grötschel et al. (1987), in particular, for a list of open problems in physics that may reach a better level of understanding by a systematic and intensive use of the combinatorial methods outlined above. A collection of papers and surveys on various aspects of spin glasses (including the ones discussed here) is Van Hemmen and Morgenstern (1987).

8. Conclusion

This has been just a glimpse of a fascinating but very difficult area of research. For example there is no mention of the important topic of cluster expansions. Details of this and many other links between combinatorics and physics may be found in the articles of Kasteleyn (1967) and Temperley (1979a). Almost all the problems discussed are probably hard in the sense of computational complexity, except for the very restricted cases. The role of planarity appears to be significant in making a problem easier, see for example Kasteleyn (1961). For more on the complexity of these physical problems see the monograph of Welsh (1993).

As far as solution is concerned, apart from the approach suggested in section 7, the most significant theoretical advance would appear to be the results of Jerrum and Sinclair (1993) that the monomer–dimer problem and the ferromagnetic version of the Ising model have a *fully polynomial randomised approximation scheme*. Put more loosely, this says that there are fast (in the sense of polynomial time) good Monte Carlo methods for these problems. Whether such schemes exist for the other problems discussed in the chapter is an important but as yet unanswered question.

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References

Andrews, G.E.
[1982] *q-Series: Their Development and Application in Analysis, Number Theory, Combinatorics, Physics, and Computer Algebra* (American Mathematical Society, Providence, RI).
Andrews, G.E., J. Baxter and P.J. Forrester
[1984] Eight-vertex SOS model and generalized Rogers–Ramanujan identities, *J. Statist. Phys.* 35, 193–266.
Barahona, F.
[1983] The max cut problem in graphs not contractible to K_5, *Oper. Res. Lett.* 2, 107–111.
Barahona, F., R. Maynard, R. Rammal and J.P. Uhry
[1982] Morphology of ground states of a two dimensional frustration model, *J. Phys. A* 15, L673-L699.

Barahona, F., M. Grötschel, M. Jünger and G. Reinelt
[1988] An application of combinatorial optimization to statistical physics and circuit layout design, *Oper. Res.* **26**, 493–513.

Baxter, R.J.
[1982] *Exactly Solved Models in Statistical Mechanics* (Academic Press, London).

Bieche, I., R. Maynard, R. Rammal and J.P. Uhry
[1980] On the ground states of the frustration model of a spin glass by a matching method of graph theory, *J. Phys. A* **13**, 2553–2576.

Biggs, N.
[1977] *Interaction Models* (Cambridge University Press, Cambridge).

Broadbent, S.R., and J.M. Hammersley
[1957] Percolation processes I. Crystals and mazes, *Proc. Cambridge Philos. Soc.* **53**, 629–641.

Cipra, B.A.
[1987] An introduction to the Ising model, *Amer. Math. Monthly* **94**, 937–959.

Edmonds, J., and E.L. Johnson
[1973] Matching, Euler tours and the Chinese postman, *Math. Programming* **5**, 88–124.

Fisher, M.E.
[1961] Critical probabilities for cluster size and percolation problems, *J. Math. Phys.* **2**, 620–627.

Fortuin, C.M., and P.W. Kasteleyn
[1972] On the random-cluster model. I. Introduction and relation to other models, *Physica* **57**, 536–564.

Grimmett, G.R.
[1989] *Percolation* (Springer, New York).

Grötschel, M., M. Jünger and G. Reinelt
[1987] Calculating exact ground states of spin glasses, a polyhedral approach, in: *Heidelberg Colloquium on Spin Glasses*, eds. J.L. van Hemmen and I. Morgenstern (Springer, Berlin) pp. 325–353.

Hammersley, J.M.
[1961a] Comparison of atom and bond percolation processes, *J. Math. Phys.* **2**, 728–733.
[1961b] The number of polygons on a lattice, *Proc. Cambridge Philos. Soc.* **57**, 516–523.

Hammersley, J.M., and D.J.A. Welsh
[1965] *First Passage Percolation, Subadditive Processes, Stochastic Networks and Generalised Renewal Theory, Bernoulli–Bayes–Laplace Anniversary Volume* (Springer, Berlin) pp. 61–110.

Hara, T., and G. Slade
[1992] The face expansion for self avoiding walk in five or more dimensions, *Rev. Math. Phys.* **4**, 235–327.

Harris, T.E.
[1960] A lower bound for the critical probability in a certain percolation process, *Proc. Cambridge Philos. Soc.* **56**, 13–20.

Heilmann, C.J., and E.H. Lieb
[1972] Theory of monomer–dimer systems, *Comm. Math. Phys.* **28**, 190–232.

Jerrum, M.R., and A.J. Sinclair
[1993] Polynomial-time approximation algorithms for the Ising model, *SIAM J. Comput.* **22**, 1087–1116.

Johnson, D.S., C.R. Aragon, L.A. McGeoch and C. Schevon
[1989] Optimisation by simulated annealing: an experimental evaluation. I. Graph partitioning, *Oper. Res.* **37**, 865–892.
[1991] Optimisation by simulated annealing: an experimental evaluation. II. Graph colouring and number partitioning, *Oper. Res.* **39**, 378–406.

Kasteleyn, P.W.
[1961] The statistics of dimers on a lattice, *Physica* **27**, 1209–1225.
[1967] Graph theory and crystal physics, in: *Graph Theory and Theoretical Physics*, ed. F. Harary (Academic Press, London) pp. 43–110.

Kesten, H.
[1963] On the number of self avoiding walks, *J. Math. Phys.* **4**, 960–969.

[1980]   The critical probability of bond percolation on the square lattice equals $\frac{1}{2}$, *Comm. Math. Phys.* **74**, 41–59.

[1982]   *Percolation Theory for Mathematicians* (Birkhäuser, Boston).

Kingman, J.F.C.

[1973]   Subadditive ergodic theory, *Ann. Probab.* **1**, 833–909.

Kirkpatrick, S., C.D. Gelatt and M.P. Vecchi

[1983]   Optimization by simulated annealing, *Science* **220**, 671–680.

Lieb, E.H.

[1967]   Residual entropy of square ice, *Phys. Rev.* **162**, 162–171.

Lovász, L.

[1979]   *Combinatorial Problems and Exercises* (North-Holland, Amsterdam). 2nd Edition: 1993.

Madras, N., and G. Slade

[1993]   *The Self Avoiding Walk* (Birkhäuser, Boston).

Mezard, M., G. Parisi and M.A. Virasoro

[1987]   *Spin Glass Theory and Beyond* (World Scientific, Singapore).

Oxley, J.G., and D.J.A. Welsh

[1979]   The Tutte polynomial and percolation, in: *Graph Theory and Related Topics*, eds. J.A. Bondy and U.S.R. Murty (Academic Press, London) pp. 329–339.

Percus, J.K.

[1971]   *Combinatorial Methods* (Springer, New York).

Ruelle, D.

[1969]   *Statistical Mechanics* (Benjamin, New York).

Smythe, R.T., and J.C. Wierman

[1978]   First passage percolation on the square lattice, *Lecture Notes in Mathematics*, Vol. 671 (Springer, Berlin).

Stanley, R.P.

[1986]   *Enumerative Combinatorics*, Volume I (Wadsworth and Brooks/Cole, Monterey, CA).

Sykes, M.F., and J.W. Essam

[1964]   Exact critical percolation for size and bond problems in two dimensions, *J. Math. Phys.* **5**, 1117–1127.

Temperley, H.N.V.

[1979a] Graph theory and continuum statistical mechanics, in: *Applications of Graph Theory*, eds. R.J. Wilson and L.W. Beineke (Academic Press, London) pp. 121–148.

[1979b] Lattice models in discrete statistical mechanics, in: *Applications of Graph Theory*, eds. R.J. Wilson and L.W. Beineke (Academic Press, London) pp. 149–175.

[1981]   *Graph Theory and Applications* (Ellis Horwood, Chichester).

Thompson, C.J.

[1972]   *Mathematical Statistical Mechanics* (MacMillan, New York).

Toth, B.

[1985]   A lower bound on the critical probability of the square lattice site percolation, *Z. Wahrscheinlichkeitstheorie u. Verw. Gebiete* **69**, 19–22.

Toulouse, G.

[1977]   Theory of the frustration effect in spin glasses: I, *Comm. Phys.* **2**, 115–119.

van Hemmen, J.L., and I. Morgenstern

[1987]   *Heidelberg Colloquium on Spin Glasses* (Springer, Berlin).

Welsh, D.J.A.

[1990]   The computational complexity of problems from statistical physics, in: *Disorder in Physical Systems*, eds. G.R. Grimmett and D.J.A. Welsh (Oxford University Press, Oxford) pp. 305–321.

[1993]   *Complexity: Knots, Colourings and Counting, London Mathematical Society Lecture Note Series*, Vol. 186 (Cambridge University Press, Cambridge).

Whittington, S.G., and C.E. Soteros

[1990]   Lattice animals: rigorous results and wild guesses, in: *Disorder in Physical Systems*, eds. G.R. Grimmett and D.J.A. Welsh (Oxford University Press, Oxford) pp. 321–334.

Wierman, J.C.
  [1981]   Bond percolation on honeycomb and triangular lattices, *Adv. in Appl. Probab.* **13**, 293–313.
Young, A.P.
  [1984]   Spin glasses, *J. Statist. Phys.* **34**, 871–881.
Zuev, A.S.
  [1987]   Estimates for the percolation threshold for a square lattice (in Russian), *Theor. Probab. Appl.* **32**, 551–552.