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On listing linear graphs

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Abstract. A method is described for the efficient generation of lists of graphs which can be embedded on very loose-packed lattices.

1. Introduction

This paper is concerned with the problem of listing connected linear graphs which have nonzero lattice constants on very loose-packed lattices. The problem arises from the investigation of many-body systems by the method of exact series expansion. Such methods are well established in the fields of phase transitions and critical phenomena and are reviewed by Domb and Green (1974). Here we are concerned with the details of some of the general techniques used in applying the method, though not with any particular model in mind. This paper follows the study of the Ising ferromagnet above the Curie temperature by Sykes *et al* (1974) which contains a bibliography and some details of the terminology we shall use.

The techniques to be described here are very much concerned with the enumeration and identification of particular subgraphs of a graph. This problem also arises in the calculation of the weight which determines the contribution of a graph to a particular model of a physical system (Sykes and Hunter 1974, Domb 1972a, b). One of us (S McKenzie 1975) has used some of these techniques to extend the high-temperature series expansion of the zero-field susceptibility of the Ising model.

Very loose-packed lattices such as the honeycomb, diamond and hydrogen peroxide lattices have been used in studies of polymers, where the diamond lattice models the tetrahedral carbon–carbon bond angle, and in studies of the Ising model on the honeycomb lattice (Sykes *et al* 1972) and on the hydrogen peroxide lattice (Betts 1970). The interest for the Ising model is that a series of lattices with coordination number 3 of differing dimensionality can be constructed of which the honeycomb and hydrogen peroxide lattices are the first two members of the series. Because of the low coordination number only a very restricted class of graph contributes to the series expansion for any model. Because the series expansions behave in a similar fashion to those of more highly coordinated lattices, attempts to understand the fundamentals of critical phenomena such as those of Domb (1972a, b) can concentrate on this restricted class of graph. Furthermore, not only is the class of graph restricted but the actual number of graphs which need to be taken into account is also a very small subset of all possible graphs of that class. It is the problem of efficiently finding these subsets to which this paper is addressed.

The number of weak embeddings (G, H) of a graph G on a graph H is the number of subgraphs of H which are isomorphic to G (Sykes *et al* 1966). For the purposes of this paper a lattice is defined as a locally finite infinite graph which is regular. The concept of regularity will be defined precisely in a subsequent publication but basically it means that every vertex is equivalent to every other vertex. Examples of lattices can be found in table 1. The lattice constant $p(G, \mathscr{L})$ of a graph G on a lattice $\mathscr{L}$ is the

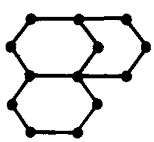
Table 1. Classification of lattices. The polygons which occur on each lattice are listed by the number of edges.

Group	Lattice	Dimension	Coordination number	Polygons
Close-packed	Triangular	2	6	3, 4, 5, 6, ...
	Face-centred cubic	3	12	3, 4, 5, 6, ...
	Hexagonal close-packed	3	12	3, 4, 5, 6, ...
Loose-packed	Simple quadratic	2	4	4, 6, 8, 10, ...
	Body-centred cubic	3	8	4, 6, 8, 10, ...
	Simple cubic	3	6	4, 6, 8, 10, ...
Very loose-packed	Honeycomb	2	3	6, 8, 10, 12, ...
	Diamond	3	4	8, 10, 12, 14, ...
	Hydrogen peroxide	3	3	10, 14, 16, 18, ...

number of weak embeddings of G on $\mathscr{L}$ *per lattice site*. Usually the lattice constant of a graph varies from lattice to lattice. When $p(G, \mathscr{L}) \equiv 0$, we shall say that G does not occur on $\mathscr{L}$. Many problems can be formulated in a series expansion, the coefficients of the terms of which can be represented graphically. The contribution of each graph to the series expansion is a weight factor, dependent on the problem, multiplied by the lattice constant for a particular lattice $\mathscr{L}$. Hence only graphs which occur on $\mathscr{L}$ will contribute to the series expansion for $\mathscr{L}$. It is therefore sensible to list for each lattice only those graphs which occur on the lattice.

Lattices may be divided into three broad groups classified by the smallest polygon which occurs on the lattice. The groups are known as close-packed, loose-packed and very loose-packed, for which the smallest polygons are respectively the triangle, the square and the hexagon or larger (table 1). Furthermore, only polygons with an even number of edges can occur on loose-packed and very loose-packed lattices.

For a graph to occur on a lattice an elementary requirement is that each cycle of the graph must be isomorphic to a polygon which occurs on the lattice. For example, the graph  occurs on the close-packed lattices but not on any loose-packed or very loose-packed lattices since it contains triangles. The second elementary requirement is that no vertex of a graph has a valence greater than the coordination number of the lattice. For example, the graph



does not occur on the honeycomb lattice although each cycle occurs. A procedure for generating a list of graphs for a lattice which takes account of these two elementary requirements is reasonably efficient for the close-packed and loose-packed lattices, where by efficiency we mean the ratio of the number of graphs which occur on the lattice to the total number generated.

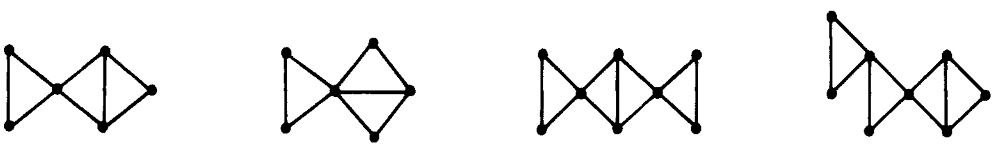
The two elementary requirements do not take into account higher-order restrictions which involve forbidden subgraphs. That is, if a graph G does not occur on a lattice then a graph H, one of whose subgraphs is isomorphic to G, will not occur. For example, the graph  does not occur on the simple cubic lattice although it contains only even cycles, so that the graph  cannot occur on the simple cubic lattice. These higher-order restrictions apply with most force when generating lists for the very loose-packed lattices. The general principle of the method we have adopted is to generate only those graphs all of whose subgraphs are known to occur on the lattice.

2. The method

In this section we shall quote without proof a number of graph theoretical results. Most of the statements are fairly obvious, but we shall give examples where a statement is not immediately apparent.

As mentioned in the introduction the purpose of the procedure we shall describe is to generate a list of graphs all of whose subgraphs occur for a particular lattice. It is necessary in creating and using a list of graphs that each graph be given an unambiguous name. We have used the nomenclature described by McKenzie (1975). This nomenclature relies on the distinction between a topology and a realization of a topology. The method to be described will generate realizations of a topology. Hence the method is based on properties, such as cycle index, which are held both by a topology and all its realizations.

Given a list of graphs which are at least two-point connected (star graphs) and which occur on the lattice, it is easy to construct a list of graphs which are less than two-point connected since such graphs are mixed trees, each block of which is a star graph. For example, knowing that the graphs  and  occur, then the graphs



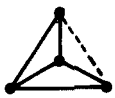
should also occur, assuming that the coordination number of the lattice is greater than 4. Hence the problem is reduced to creating a list of star graphs which are known to occur.

To do this we have used the fact that all realizations of a topology which is at least two-point connected and which contains no loops are also at least two-point connected. If we call such topologies star topologies then star graphs are realizations of star topologies, and conversely the topology of a star graph is a star topology. The problem of enumerating star topologies has been solved by Heap (1966) who gives a list of such topologies up to cycle index 5. Heap has since produced a complete list of cycle index 6 topologies and a partial list of cycle index 7 topologies. The procedure described here is to generate a list of star realizations which are known to occur for each star topology.

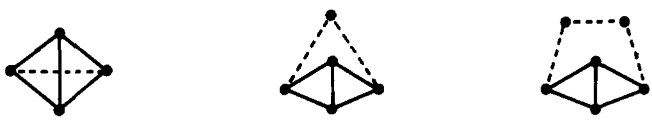
The crux of the method is to form the set of maximal subtopologies of a star topology by removing each bridge of the topology one by one. There are four possible situations from which a bridge may be removed namely: the bridge connects two nodes of valence higher than 3; the bridge connects a node of valence 3 to a node of higher valence; the bridge connects two nodes of valence 3 and the antinodes formed in removal of the bridge lie either on the same bridge or on two different bridges of the subtopology so formed. In each case the cycle index of each maximal subtopology is one less than that of the topology. Only the subset of the set of maximal subtopologies which are star topologies needs to be retained. This subset contains at least one member.

We now suppose that we have lists of realizations of the maximal subtopologies; that these lists are complete up to the desired number of lines; and that the lists contain only graphs which occur on the lattice. We then generate a list of realizations of the topology from the list of realizations of one of the maximal subtopologies by replacing the bridge removed.

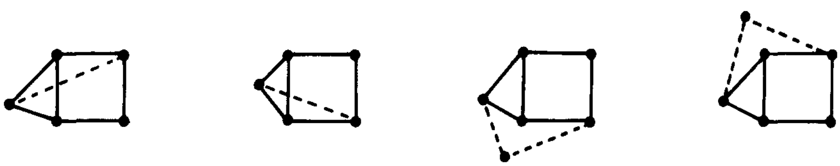
To illustrate the method by an example, suppose that we wish to generate realizations up to eight lines of the topology given that the realizations , and of the topology occur on the lattice. If the bridge removed is as shown below:



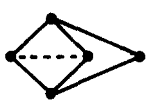
the resulting maximal subtopology is of the given topology namely . From the realization we then generate the realizations



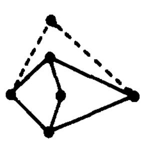
of the topology . From we generate



and from we generate



and



Not all the generated realizations are distinct and duplications must be removed.

Furthermore, this method of generating realizations of the topology from a list of realizations of *one* of the maximal subtopologies may create a realization for which a realization of one of the *other* maximal subtopologies does not occur. The generated list is therefore checked to ensure that, for each member, all subgraphs which are realizations of the other maximal subtopologies are present in the list of realizations of the maximal subtopologies. This amended list contains all realizations of the topology such that for each member of the list, all subgraphs which are realizations of the maximal star subtopologies are known to occur on the lattice.

The amended list is now checked to see if all the generated graphs occur on the lattice. Those which do not occur are removed to produce a final list. By these means we have produced a list of graphs of cycle index c, all of which occur on the lattice, from a list of graphs of cycle index $(c-1)$. The method is therefore iterative, proceeding from low cycle index to high cycle index. Hence we start with a list of polygons which are known to occur and create a list of cycle index 2 graphs which are known to occur. Thus in creating the list of cycle index c graphs from cycle index $(c-1)$ we are sure that all subgraphs of cycle index less than (c) are known to occur.

3. Discussion

To summarize, the method we have described above generates a list of graphs of cycle index c which occur on a given lattice from a known list of graphs of cycle index $(c-1)$. The method builds a list of realizations of a topology from the known list of realizations of one of its maximal subtopologies, checks each new realization for forbidden subgraphs belonging to other maximal subtopologies and finally rejects any new realization which does not occur on the given lattice.

The procedure has been programmed for use on an IBM 360 computer. The major problem in using this method is to reduce to a minimum the number of realizations generated which duplicate realizations which have been generated previously. For example, from  we may generate  (α) while from  we may generate  (β). Removing the distinction between broken and full lines it can be seen that (α) and (β) are isomorphic. The solution of this problem is too technical to go into in much detail but it is obvious that symmetry plays an important role. Both the symmetry of the topology and that of the maximal subtopology are taken into account. For this reason the canonization procedure described by McKenzie (1975) which produces an explicit realization of the bridge group of a topology is particularly convenient. One technique which is particularly economical is to start replacing the bridge removed at the number of lines of any equivalent bridge in the realization of the maximal subtopology. An equivalent bridge to the bridge removed is a bridge of a topology which occupies an equivalent position in the topology under the operation of the bridge group of the topology. The technique depends on ordering the realizations of the maximal subtopologies by the number of lines and on starting to generate graphs from the realizations with the smallest number of lines.

The method has been used to generate lists of graphs which occur on the diamond lattice up to 26 lines and hydrogen peroxide lattice up to 35 lines. The efficiency of the process is normally greater than 80% at any stage. For example, for the diamond lattice 527 realizations at 23 lines of the topology  were generated of which 436 occur. If the lattice were close-packed one would expect 27 456 realizations with this number of lines. Readers interested in problems which involve the kind of graph list described in this paper are invited to contact either of the authors who may well be able to supply relevant information.

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