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The number of selfavoiding rings on a lattice

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Abstract. The numbers of n step selfavoiding returns to the origin are given up to $n = 14$ for the face-centred cubic lattice, $n = 16$ for the body-centred cubic lattice, $n = 18$ for the triangular lattice, $n = 20$ for the simple cubic lattice and $n = 26$ for the square lattice, inclusive. The technique used to obtain the data is described in outline.

1. Introduction

It is the primary purpose of this paper to report some numerical results for the number of selfavoiding rings on a crystal lattice (table 3). These numbers have direct application to the lattice model of a polymer (Hiley and Sykes 1961, Martin *et al* 1967), to the specific heat of the Ising model (Rushbrooke and Eve 1962, Sykes *et al* 1967, 1972c) and are also required in the derivation of susceptibility expansions for the Ising model (Sykes 1961, Sykes *et al* 1972a, 1972b). Following the literature we denote the number of n step self-avoiding returns to the origin by u_n; for a regular lattice $u_n = 2np_n$, where p_n is the number of embeddings per site of a selfavoiding ring (or polygon). The determination of successive u_n is a problem of classic difficulty (Wakefield 1951, Domb 1960). We do not give a detailed account of our calculations; rather we wish to communicate the broad outlines of the technique. The technique is of interest in itself and can be applied to other lattices and to other enumerative problems.

2. Direct method

The direct method of obtaining the number of rings on a lattice consists in counting all the possibilities; computer enumeration seems the only practical method for large rings. Since the first application of computers by Rushbrooke and Eve (1959) very little progress has been made in overcoming the serious obstacle presented by the rapid increase in the number of rings with the number of steps.

To take a specific example, the direct enumeration of the number of 11-step returns on the face-centred cubic lattice using the fastest available computer is estimated to take

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several hours and the time increases by a factor of about nine at each additional step. By fully exploiting the symmetry of the lattice it is possible to reduce the computer time needed by a factor which for the face-centred cubic lattice cannot exceed 96. The symmetry of the initial step is twelvefold and this economy can be improved upon by taking account of any symmetry in subsequent steps. For example, the 1404 possible choices of the first three steps fall into 21 sets, and only one representative of each set need be counted; in this way computer time is reduced by a factor of about $1404/21 \simeq 67$. This is already a substantial saving, and classification of further steps becomes rapidly less worthwhile.

Using the three-step classification the value $u_{12} = 3\,235\,366\,752$ was obtained as a result of an enumeration of 47 392 668 embeddings on a KDF9 computer at the National Physical Laboratory at Teddington in 1967 using a program developed by one of us (JLM). The total time was 3 h 13 min, implying a counting rate of just under a quarter of a million successes per minute. Using the same procedure, u_{13} would require some 28 h and u_{14} some 243 h. Only the use of a faster computer would result in further time economies but since the number of rings to be enumerated is increasing by a factor of nearly nine at each new step there are obvious limitations to the method. It is desirable to make the most efficient use of the available computer time; to do this we have proceeded indirectly, as described in the next section.

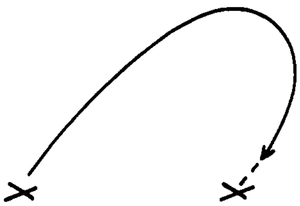
3. Indirect method

The indirect method we have used is based on a study of the distribution of selfavoiding walks which end at points close to the origin. We take the face-centred cubic lattice as an example. If we denote the lattice sites by cartesian coordinates the lattice consists of all points (x, y, z) for which x, y and z are integers and $x+y+z$ is even. The technique is to determine the number of selfavoiding walks of n steps, denoted by $b_n(x, y, z)$, to each point for two values of n, say r and s, and to form the sum

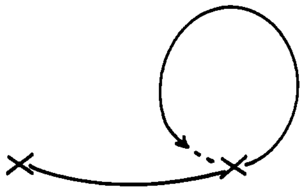
$$B(r, s) = \sum_{x,y,z} b_r(x, y, z) b_s(x, y, z). \tag{3.1}$$

If r is small the distribution need only be determined for points close to the origin. The sum $B(r, s)$ includes all the rings corresponding to u_{r+s} together with certain overlaps; the counting of these overlap configurations requires less computer time and the rings can be calculated by subtracting the failures in (3.1). We illustrate the method by giving some details of the calculation of u_{13} and u_{14} for the face-centred cubic lattice.

We first construct table 1, which gives the number of ten-step selfavoiding walks to each of the 15 distinct classes of point also accessible in 4 steps. The computer program earlier used to count rings, derived these data in $8\frac{1}{2}$ h; the twelve-fold starting symmetry is lost if the end point of a walk is specified but the number of initial vectors can usually be reduced by some symmetries. Details of the initial and final vectors were recorded. We next constructed table 2, which gives the number of eleven-step selfavoiding walks to the 8 distinct classes of point accessible in 3 steps. By direct enumeration this would take about 40 h; however if each walk of table 1 is extended by one further step, which is not an immediate reversal, the resulting distribution will correspond to only two types of walk:



α: selfavoiding walk



β: tadpole-type walk

Table 1.

Typical point	Symmetry	b_{10}
0, 1, 1	12	31484244
0, 0, 2	6	36360872
1, 1, 2	24	37179840
0, 2, 2	12	37164700
0, 1, 3	24	36765592
2, 2, 2	8	35450940
1, 2, 3	48	34063492
0, 3, 3	12	30630980
0, 0, 4	6	32637592
1, 1, 4	24	30772624
0, 2, 4	24	28859590
2, 3, 3	24	26852148
2, 2, 4	24	24999738
1, 3, 4	48	23121298
0, 4, 4	12	17843074

Walks of type β are less numerous than those of type α and by counting type β directly, and subtracting off, we obtain the data in table 2. The entry for the point (0, 1, 1) is of course directly related to u_{12}.

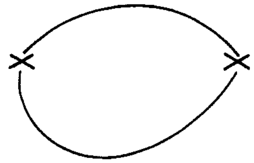
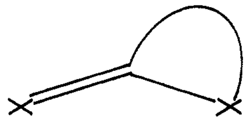
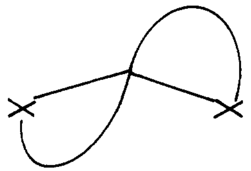
Table 2.

Typical point	Symmetry	b_{11}	b_2	b_3
0, 1, 1	12	269613896	4	264
0, 0, 2	6	312284536	4	144
1, 1, 2	24	320861342	2	432
0, 2, 2	12	322624804	1	144
0, 1, 3	24	321262541	—	216
2, 2, 2	8	312411672	—	48
1, 2, 3	48	302790797	—	144
0, 3, 3	12	277824572	—	12

We next form the sum $B(2, 11)$ over all points; only the four classes within two steps of the origin contribute. From table 2

$$B(2, 11) = 39709137936 \tag{3.2}$$

and this total is made up of three possible combinations of the two bridges:

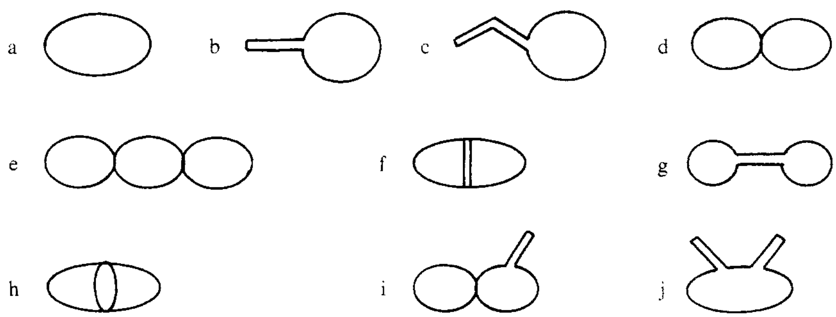
	Type	Total number of cases
A		28074857616
B		1597052112
C		655758984

The total number of cases for A, which is just u_{13}, is obtained by elimination. The number of cases for B can be calculated; the number for C is found by computer.

To calculate u_{14} the sum

$$B(3, 11) = 432541351992 \tag{3.3}$$

is calculated from table 2. From this number must be subtracted all the possible intersecting pairs. There are now ten fundamental combinations represented in outline by:



A certain amount of computer time is needed to derive the extra configurational information; to derive u_{14} for the face-centred cubic lattice we used about 20 h which, although an improvement on the some 243 h estimated for the direct method, still represents a substantial amount. Essentially the economy has been effected by using computer enumeration of failures, which are less numerous, rather than successes. The technique closely parallels the chain counting theorem (Sykes 1961, Martin and Watts 1971) used to estimate the number of selfavoiding walks recursively. Recently a generalization of this recurrence relation has been obtained (JLM) and incorporated in a computer program (MGW): We have used this program, and the technique outlined above, to derive data on other lattices.

4. Summary

We conclude by summarizing in table 3, all the available data for five crystal lattices. So long as such data are obtained by direct enumeration the techniques we have outlined will always effect some economies and enable the available computer time to be used to the best advantage.

Table 3.

	SQ	SC	BCC	T	FCC
u_3	—	—	—	12	48
u_4	8	24	96	24	264
u_5	—	—	—	60	1680
u_6	24	264	1776	180	11640
u_7	—	—	—	588	86352
u_8	112	3312	43776	1968	673104
u_9	—	—	—	6840	5424768
u_{10}	560	48240	1237920	24240	44828400
u_{11}	—	—	—	87252	377810928
u_{12}	2976	762096	37903776	318360	3235366752
u_{13}	—	—	—	1173744	28074857616
u_{14}	16464	12673920	1223681760	4366740	246353214240
u_{15}	—	—	—	16370700	
u_{16}	94016	218904768	41040797376	61780320	
u_{17}	—	—	—	234505140	
u_{18}	549648	3891176352		894692736	
u_{20}	3273040	70742410800			
u_{22}	19781168				
u_{24}	121020960				
u_{26}	748039552				

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