Exact computer enumeration of the number of Hamiltonian paths in small plane square lattices

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An algorithm has been developed to permit exact computer enumeration of the number of Hamiltonian paths in plane square lattices. The computational time required prevented us from going beyond the 7×7 plane square lattice. The computer program distinguishes between open and closed Hamiltonian paths (cycles) and also counts the number of configurations with axial or rotational symmetry. The number of independent configurations or "orbits" is thus determined. The number of terms available did not permit us to confirm or disprove the asymptotic relationship proposed by Orland, Itzykson, and de Dominicis for large N, $Z_N=(z/e)^N$, where N is the number of steps in the path, z the coordination number of the lattice, and e the basis of Napierian logarithms. However, for small plane square lattices, the exact enumeration and application of the preceding relationship yields results that differ significantly.

I. INTRODUCTION

A Hamiltonian path (HP) is a path that visits each point of a given lattice once. A HP may be open (noncyclical) or closed (cyclical). Examples of open and closed HP are given in Figs. 1 and 2 for plane square lattices (PSL) with which we shall be exclusively concerned in this article. Cyclical configurations, in the strict sense, are only possible for even PSL denoted by C_{2k}, where $2k$ is the number of points along one side of the PSL. This is so because, as may be shown, the starting and ending points of the HP's in odd PSL, denoted C_{2k+1}, necessarily lie on odd diagonals (Fig. 3). However, in odd PSL, one may define as "pseudocycles" those configurations whose end points are adjacent on the same diagonal.

Exact enumeration of the number of HP's in a arbitrary lattice in two or more dimensions is an unsolved problem of combinatorial analysis. Such exact enumeration is of interest, for its own sake, and because the number of HP's is related to several problems in polymer physical chemistry, such as the entropy of disorientation of crystalline polymers to the amorphous state or the configurational (combinatorial) entropy of a globule made up of one or more giant macromolecules. Flory[1] was the

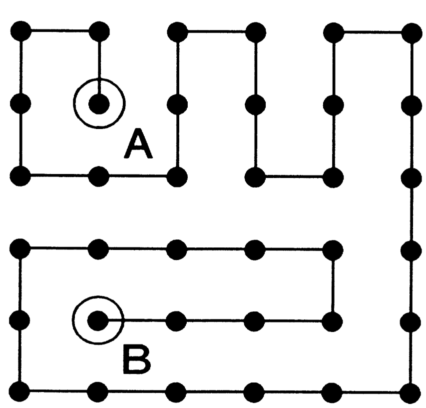


FIG. 1. Open Hamiltonian path.

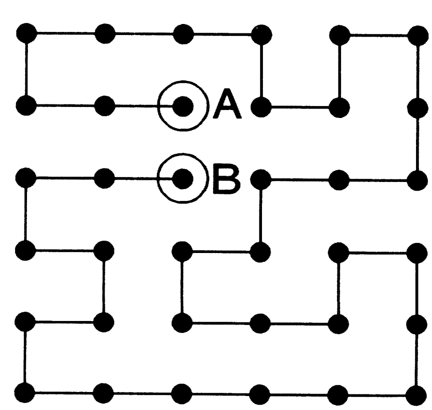


FIG. 2. Closed Hamiltonian path (cycle).

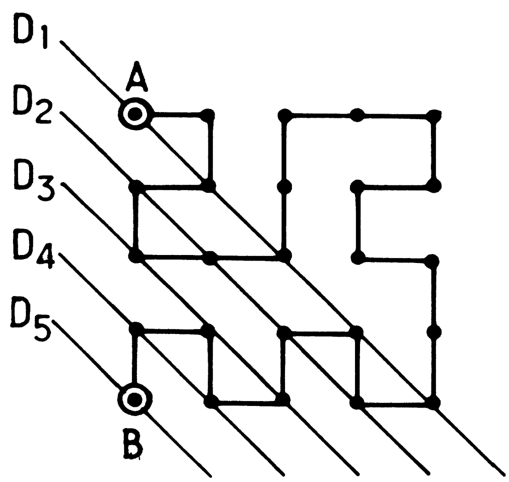


FIG. 3. Hamiltonian paths are impossible in odd plane square lattice as end points necessarily lie on odd diagonals.

first to give an estimate of the number of HP's in relation to his determination of the combinatorial entropy of mixing solvent with polymer molecules. Flory's result is

$$Z_F=[(z-1)/e]^N \, . \tag{1}$$

Here z is the coordination number in the lattice (= number of nearest neighbors, equal to 4 for the PSL), N is the total number of steps in the path, equal to n^2 minus one, where n is the number of points at each side, and e is the base of Nepierian logarithms. As shown by Gujrati and Goldstein,[2] Eq. (1) underestimates the number of HP's. In the particular case of the PSL these authors show that the number of HP's lies between that of the Manhattan walks[3] (traffic regulations in Manhattan) and the number of configurations of two-dimensional ice.[4] The number of HP's varying as a^N, this fixes the following bounds for a:

$$1.338 < a < 1.539 \, . \tag{2}$$

More recently, Orland, Itzykson, and de Dominicis[5] obtained the following asymptotic value for the number of closed HP's or cycles:

$$Z_{\text{or}}=(z/e)^N \, . \tag{3}$$

This equation closely resembles that of Flory, $z-1$, being replaced by z, but direct comparison is not significant since, as stated by the authors, it applies only to cycles

TABLE I. The number of Hamiltonian paths as a function of the number of steps by Flory's equation [Eq. (1)], the number of cycles by Eq. (2) of Orland *et al.*, and exact enumeration.

n	2	3	4
Z_F	1.34	2.20	4.39
Z_{Or}	3.2	23.0	328
Exact enumeration			
Total	4	16	276
Cycles	4	0	12

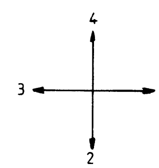
[see Eqs. (4) and (6) of Ref. 5]. We shall come back to this point in the discussion. Equation (3) overestimates for small PSL the number of HC's as shown in Table I. It may be of interest to have a computer exact enumeration of the number HP's in small PSL in order to extend the above table and make the comparison more significant, as Eq. (3) is an asymptotic one. To this end a special algorithm has been developed which will now be described in detail.

II. THE ALGORITHM

A. Description of the algorithm

1. *Initialization stage*

Let us first denote by the four integers 1, 2, 3, and 4 the four possible directions in a PSL and by x and y the coordinates of any lattice site:



Starting from an arbitrary point $A_0=(x_0,y_0)$, let $X=(x,y)$ be the running point on the lattice. At each position of the running point all possible directions are stored up in the computer memory. Now the running point X is made to progress in one of the available directions to an adjacent point, always preferring the available direction which corresponds to the smaller integer between 1 and 4. Two possibilities may now occur: eigther the process may continue to its end, i.e., all lattice points have been visited once. In this case a HP is recorded and the initialization stage is over; or, the progression has to be stopped before all lattice sites have been visited. Let us assume that the latter alternative has occurred. The computer is then ordered to go backwards along the path followed to the first point P were there are one or more directions which have not been tried. At this point, a new direction is followed, trying first that which corresponds to the smaller available integer. If all directions starting from P have been tried and yet no HP has been found, the computer is order backwards along the path to the second point, let it be P', where there are available directions which have not been tried. This forward and backward motion is repeated until a first HP is found. When this happens a first HP is recorded and the initialization stage is over.

2. *Computation stage*

Starting now from the end point of the first found HP, the computer is ordered to move backwards along its path until a point Q is found where available directions which have not been followed have been memorized. A new direction is now taken, in the strict order corresponding to the smaller available integer. When all possible directions at Q have been tried, the computer is ordered back to the second point Q', where available directions have been memorized and a new direction tried.

This process of forward and backward motion is repeated until the initial point A_0 is reached. At point A_0 a new direction, if available, is tried, otherwise a new starting point is chosen.

This process of alternate forward and backward motion, recording a HP in case of success and nothing in case of failure, clearly constitutes an ordered and exhaustive counting of all possible HP's starting from point A_0. The computer is made to distinguish between open and closed HP's, and records them us such. In principle, all lattice points should be taken as starting points to have an exhaustive count of HP on the lattice. However, as shown in Sec. II C, symmetry considerations permit us to reduce the number of starting points.

B. Compatibility tests

In order to increase the performance of the algorithm, the two following tests of compatibility of the path followed have been introduced.

1. Compatibility test of connectivity

Consider the path indicated in Fig. 4; it is clear that no HP may be obtained if the path goes to point C, because then the square is divided in two domains α and β which are not connected. The test of connectivity ensures that at each point during a progression phase, the free points (points not yet visited) form a connected domain. To this end, at each step an arbitrary free point is "colored" and the color diffused form neighbor point to neighbor point. The bounded (= already visited) points do not afford coloration. When the coloration process is over, the sum is made of colored and bound points. If the domain of free points is connected, this sum equals the total number of lattice sites; otherwise, this sum is less than the total number of lattice sites because the color cannot cross the boundary of bound points. This coloration procedure somewhat increases the time required to progress by one step, but finally saves considerable time, allowing the computer to avoid trying impossible directions.

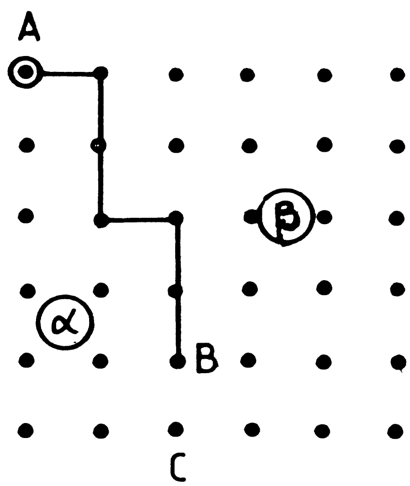


FIG. 4. Going from B to C is forbidden; all free (not yet visited) points should form a connex domain.

2. Compatibility test of available directions at free points

Consider now the path followed in Fig. 5. A little thought shows that point $E=(1,2)$ and $G(3,1)$ can only be reached from points $D=(1,3)$ and $F(4,1)$. Thus, E and G are necessarily end points of the path. As a path cannot have two end points, step BC has to be discarded as a permitted direction. Further, point E is necessarily the end point of the path, so that from B the only possible direction is upwards to G. To take advantage of these remarks, one has to define the "degrees of liberty" of free points. By definition, the degree of liberty of a free point equals the number of neighboring free points. This definition is illustrated in Fig.5. At each step of the progression phase, the table of degrees of liberty of the free points is adjusted. If two free points having one as degree of liberty appear which are not first neighbors, a situation of compulsory next direction to follow generally arises, unless the last step has to be discarded as leading to an impossibility. The computer is ordered to proceed accordingly. This second test is also time saving.

C. Symmetry considerations and starting points on the lattice

As pointed out in Sec. II A, the number of starting points may be reduced using symmetry considerations. Let us first consider oriented paths, that is, a given path starting from point A to end at point B is distinguished from the same path starting at B to end at A. In Fig. 6 an even PSL is represented together with three symmetry axes Δ_1, Δ_2, and Δ_3. We first consider all paths starting from the points lying between axes Δ_2 and Δ_3 and on Δ_3 as indicated. By appropriate symmetries though the symmetry axes, all oriented paths starting at any point on the lattice are obtained. Thus, it suffices to enumerate the HP obtained taking as starting points the surrounded points. To obtain the total number of oriented HP's, the number of HP's obtained from each surrounded point has

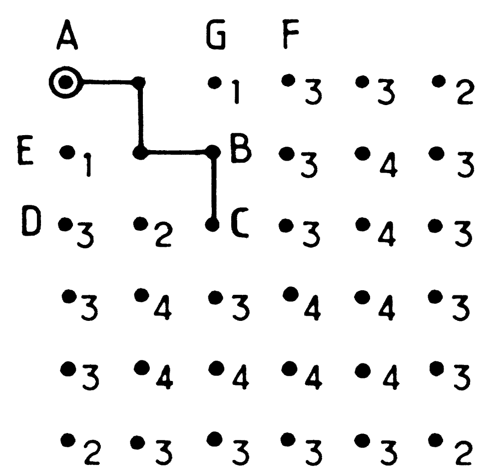


FIG. 5. No progression path is allowed when there is a simultaneous appearance of two or more lattice points having one as degree of liberty, unless these points are connected by a continuous line of points also having one as degree of liberty.

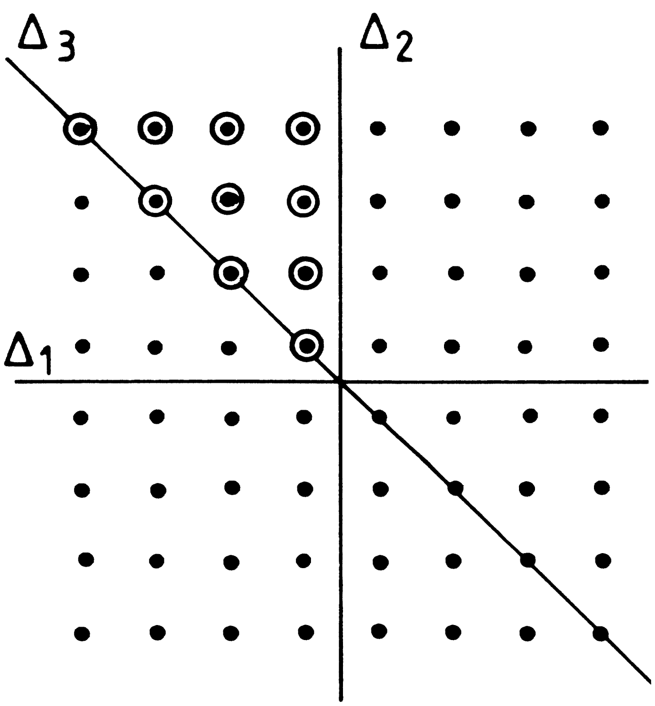


FIG. 6. Starting points which have to be considered in an even plan square lattice.

to be multiplied by an appropriate factor, which is either 4 or 8. The total number of "nonoriented" HP's is that number divided by two.

The same considerations as above apply to odd PSL, with two differences: (a) starting points on even diagonals do not have to be considered, as these cannot lead to HP's, and (b) there is a central point (CP) with a weight of 1, instead of 4 or 8 for the other starting points.

D. Symmetrical HP's and orbits

So far we have considered oriented or nonoriented HP's, irrespective to whether some of them may be obtained from others through simple symmetries. It may be of some interest to know the number of HP's which may not be obtained from others through simple symmetries. Two kinds of symmetrical configurations have, in fact, to be considered: (a) configurations invariant through a rotation of angle π, which will be defined as type-1 symmetries, and (b) configurations invariant through an axial symmetry, which will be defined as type-2 symmetries.

These two kinds of symmetries are found by the computer through the following procedure: let us denote 1 (left), s (straight), and r (right), the relative directions formed by two consecutive steps along the HP (Fig. 7). If there is a type-1 symmetry, in symmetrical positions about the central directions (which one may replace by a point if the total number of directions is even), letter 1 is replaced by letter r and vice versa, while to each s should correspond an s. On the other hand, for type-2 symmetries, the same letter should always be found at equal distances from the central direction. The latter case is illustrated in Fig. 7. When a HP is found, all successive relative directions are memorized and the computer

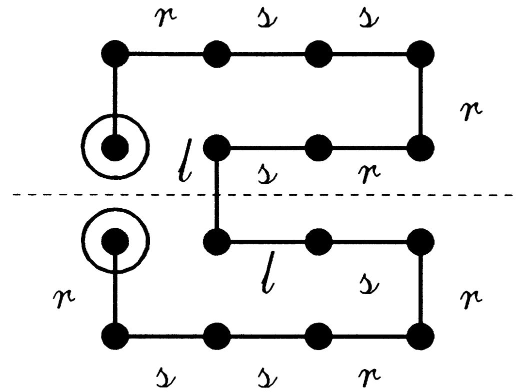


FIG. 7. The figure shows the relative directions followed by two consecutive steps in the path, to detect the presence or absence of symmetries. The path on the figure has a type-2 symmetry (see text).

searches for symmetries using the above scheme. Thus, all HP's are classified as sym0, sym1, and sym2 configurations. These symmetry classifications permit us to define the "orbits" of the PSL. These, in short, are all configurations constituting HP's which cannot be obtained from one another through some symmetry. If a HP displays no symmetry, it is part of a subset (or orbit) of eight configurations, each of which may be obtained from an arbitrary one by rotation or axial symmetry. On the other hand, if the HP displays a type-1 or type-2 symmetry, it is part of a subset of four elements. The sum of all orbits is the number of "independent" HP on the lattice.

III. RESULTS AND DISCUSSION

The algorithm described in Sec. II permitted enumeration of HP's up to the 7×7 PSL, for which the computation time on an IBM 3090 computer was about 3 h; the time required to determine the HP of the 8×8 PSL is prohibitive, as it increases more rapidly than exponentially when going from C_n to C_{n+1}. The results are summarized in Table II, together with the values obtained from the asymptotic relationship, Eq. (3). The table shows that depending on parity, the HP's display type-1 or type-2 symmetry, but never both.

Let us now define

$$u_n=[\ln(Z_{n+1}/Z_n)]/(2n+1)\ . \tag{4}$$

Following Eq. (3), the suite u_n should tend to the constant value 0.3862. . . as n becomes large. From Table II one finds

u_2	u_3	u_4	u_5	u_6
0.3218	0.3749	0.3057	0.3610	0.3136

Unfortunately, the number of terms is too limited to reach any conclusion regarding the convergence of the terms to the above-indicated theoretical value. A last point which will be discussed is the following: Orland *et al.*[5] state that the base $a=z/e$ in Eq. (3) applies only to

TABLE II. Exact computer enumeration of the number of Hamiltonian paths and of cyclical Hamiltonian paths (cycles) as a functions of their symmetry (see text) and of the number of points in the square side. Z_{Or} is the number of cycles determined by Eq. (3). The number of orbits is also given.

n	2	3	4	5	6	7
			Noncyclical			
sym0	0	16	168	4256	190 456	13 531 224
sym1	0	4	0	68	0	4056
sym2	0	0	12	0	300	0
			Cyclical			
sym0	0	0	80	0	38 416	0
sym1	0	0	0	0	0	0
sym2	4	0	16	0	176	0
Total	4	20	276	4324	229 348	13 535 280
Orbits	1	3	38	549	28 728	1 692 417
Z_{Or}	3.2	23.0	328	10 623	744 062	112 847 720

cyclical HP's. Noncyclical HP's would have, following the authors, a base equal to twice the above value, i.e., in the case of the PSL, the value 2.9430.... This value, however, is beyond the bounds set by inequalities (2). One may further observe that, as shown by Hammersley and Fisher and his co-workers,[6-8] the numbers of self-avoiding walks (SAW) U_N and self-avoiding cycles (SAC) W_N of N steps are, respectively, given by

$$U_N = u_0 N^{\gamma-1}\mu^N , \tag{5a}$$

$$W_N = w_0 N^{\alpha-2}\mu^N . \tag{5b}$$

Here u_0 and w_0 are constants, γ is the critical exponent of the magnetic susceptibility, α is the critical exponent of the specific heat, and μ is the "effective" coordination number[7] related to, but inferior to, the lattice coordination number z. In the PSL, $\mu=2.6389$. From 5(a) and 5(b) one concludes that the ratio W_N/U_N varies as a power of N, not exponentially with N. Now the HP's are a special case of self-avoiding walks (close-packed SAW) so that one may suppose that asympotically both the number of HP's and HC's should display the same base, possibly z/e as indicated by Eq. (3). If this is correct, the base $2z/e$ for the number of open paths is not relevant.

As already indicated, our algorithm did not permit us to go beyond the 7×7 PSL. No definite conclusion may therefore be reached regarding the relevance of Eq. (3), which was a primary aim of the investigation when initiated, as Eq. (3) is attractive for its simplicity and may be very useful, since, to the authors' knowledge, no other approximate asymptotic relationship has been proposed. More powerful algorithms, if such may be deviced, may permit us to gain a few more squares, perhaps up to the 10×10 PSL. Exact enumeration on truly large (say 100×100) PSL seems, however, presently beyond the reach of informatic means and procedures, unless truly new analytical and computational methods could be developed.

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