Physical Sciences Section

Pakistan J. Sci. Ind. Res., Vol. 21, Nos. 3-4, June - August 1978

EXACT ENUMERATIONS AND MONTE CARLO SAMPLING OF SELF-AVOIDING RANDOM WALKS

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(Received January 5, 1978)

Abstract. Two methods for the computer based enumerations of self-avoiding random walks according to their order are described. One is an exact enumeration method and the other is a Monte Carlo method based on the 'slithering snake' technique of Wall and Mandel. It is suggested that such a classification of random walks according to their order helps in the study of polymers in different solvents.

INTRODUCTION

A self-avoiding random walk (SARW) is a random walk with the restriction that no point in space may be visited more than once [1]. This means that in a SARW neither step reversal nor the formation of any closed loops is allowed. Such a restriction makes a SARW non-Markovian in the sense that the probability at nth step (for any n, no matter how large)depends on the probabilities for all the previous $n-1$ steps, because while taking the nth step all of the previous $n-1$ steps must be remembered in order not to intersect them. It is due to this non-Markovian nature that SARW has so far defied exact mathematical analysis. In the absence of such an analysis exact and numerical techniques have been used for studying SARW. An example of the approximate method is the transition matrix approach in which a SARW is approximated by a restricted walk with limited number of restrictions [2]. Such a walk is Markovian and can be described by a transition matrix which relates the n-step walks to the $(n-1)$-step walks. For a small number of restrictions the transition matrix can be diagonalized and its eigen values calculated. The order of the transition matrix, however, increases very rapidly as the number of restrictions are increased which makes it very difficult to study random walks with more than a very small number of restrictions with this method. The numerical techniques for studying random walks fall into two categories: One is the exact enumeration method in which all of the walks of a relatively small number of steps (about 16–20) are enumerated and the results so obtained are extrapolated to walks corresponding to larger number of steps [3]. The other method makes use of Monte Carlo sampling technique which can be used to study walks of much larger number of steps [4].

In the present work the concept of order of a walk is introduced. It is defined to be the number of steps with at least one identical nearest neighbour. According to this definition n-step walk with maximum number of kinks is of order zero and the one without any kinks – the straight chain – is assigned the order $n-1$. Exact and Monte Carlo enumeration methods of self-avoiding random walks classified according to their order are described and some results obtained with these methods are presented in the last section. It is also shown that such a classification of random walks enables one to get results for SARW with biased probability in the forward direction from the results for walks with equally likely probability of step in all directions.

II. PROCEDURE

A. *Exact Enumeration.* In the enumeration of random walks on the computer there are two hurdles: one related to the computer storage and the other related to the computer time, both of which are necessarily finite. The number of n-step self-avoiding walks on a lattice of coordination number z, for example, is of the order of $(z-1)^n$. Also an n-step walk may wander around anywhere in a region of size $(2n)^d$, d being the dimensionability of the lattice. Thus the total space requirement for storing all of these walks comes out to be of the order of

$$(2n)^d (z-1)^n$$

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For a 10-step walk on a square lattice this number is about ten million and for a 10-step walk on a simple cubic lattic this number is about twice as big. One must, therefore, devise means to reduce these numbers to managable size.

The first obvious step is to make use of the symmetry of the lattice. For example only one direction, say the $+x$-direction, may be chosen for the first step out of *the* z equally likely possible directions. Similarly, out of $(z-2)$ possible directions for the 2nd step which are at an angle to the first step one needs only choose those in the first quadrant. This reduces the storage (and time) requirements by a factor of about $1/z\,(z-2)$; i.e. by a factor of 8 for a square lattice and a factor of 12 for a simple cubic lattice. Another major reduction in the storage requirement can be achieved by representing a step along a given bond by an integer associated with that bond. If the bonds meeting at a point are numbered $(b_1, b_2, \ldots b_z)$ then a given n-step walk may be written as a string of numbers:

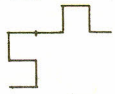
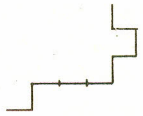
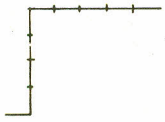
$$b_{\alpha 1}\, b_{\alpha 2} \cdots b_{\alpha n}$$

which are chosen from amongst the set of numbers $(b_1 b_2 \ldots b_z)$ subject to the restriction that the walk be a self-avoiding walk. For a square lattice one may use the set of numbers $(1, 2, -1, -2)$ to represent the walks along the four possible directions and for a simple cubic lattice a possible set of integers is $(1, 2, 3, -1, -2, -3)$. Some examples of such strings along with their corresponding graphical presentation are given in Table 1.

Further reduction in the computer storage requirements can be achieved by packing several steps into a single computer word. For the square and simple cubic lattices, for which the integers representing the steps are between -2 and $+2$ and between -3 and $+3$ respectively, one needs only three bits to write these numbers. Consequently, one may pack upto 20 steps into a single CDC word which is made up of 60 bits. This means that each walk of upto 20 steps may be represented by single word in a CDC machine. After implementing all these measures the storage requirements are reduced from about $(2n)^d(z-1)^n$ words to about $[1/z(z-2)]\,(z-1)^n$ words.

In view of the symmetry considerations mentioned above, for enumerating random walks on a square lattice the first step is always taken in the $+x$- direction and the 2nd step is taken either in the $+x$-direction or the $+y$-direction. These initial constraints and the classification of walks according to their order leads to the following

Table 1. Some examples of a 10-step self-avoiding random walks corresponding to different orders.

Order	Numerical Representation	Graphical Representation
0	12-12-1212-12	
1	12-121121-21	
2	12111212-12	
3	1121-211221	
4	12122-1-1-1-2-2	
5	122211-2-2-2-1	
6	111222-1-1-2-2	
7	1222211111	
8	1111112222	
9	1111111111	

systematics;

i) All walks having odd order end with $\pm x$-step as the last step.

ii) All walks having even order end with $\pm y$-step as the last step.

Therefore adding a step to an n-step walk identical to its last step we get an $(n+1)$-step walk of the same order as the one before adding the step, and adding a step to an n-step walk different from the last step we get an $(n+1)$-step walk with its order reduced by unity.

The self-avoiding nature of the walk is realized in the following way: Firstly reversals are not permitted; i.e. +1(+2) and -1 (-2) do not follow one another. Secondly the formation of closed loops is not permitted: Now on a square lattice a closed loop may be formed in an even number of steps greater than or equal to 4. Moreover the components of the cumulative distance covered during these steps along the: x- and the y-directions must both vanish for a closed loop. Thus all walks for which these components both vanish for the last even number ($\geqslant 4$) of steps of the walk are discarded as unsuccessful walks.

B. *Monte Carlo Method.* For the Monte Carlo sampling of self-avoiding random walks classified according to order we have adopted the 'slithering snake technique' of Wall and Mandel [4]. It may be recalled that in this method the head of a chain of fixed contour length is moved one space in a lattice with all the other elements of the chain moving forward along the old contour. Possible moves of the head are selected at random and for moves precluded by double occupancy the old configuration is retained, with heads and tails interchanged, and then counted as if a move were made.

Since the procedure outlined above involves adding a step at the head of the walk and chopping off the step at its tail-end, the following four possibilities are of interest for determing the order of the new configuration.

i) The step added at the head of the walk is identical to the step preceding it.
ii) The step added at the head of the walk is different from the step preceding it.
iii) The step chopped off at the tail-end of the walk is identical to the step succeeding it.
iv) The step chopped off at the tail-end of the walk is different from the step succeeding it.

The order of the walk remains unchanged in situations where either (i) and (iii), or (ii) and (iv) are true, it is enhanced by unity in cases when (i) and (iv) are true and it is reduced by unity when (ii) and (iii) are true.

III. RESULTS AND DISCUSSION

In this section we present some of the results obtained with the above methods for an 'unbiased' self-avoiding random walk, i.e. a random walk in which steps in all allowed directions are equally likely. A detailed discussion of these results is deffered to a subsequent paper. In this section we also briefly describe a method for using these results for extending SARW as a model for the study of polymers in different solvents.

In Fig. 1 we present the quantities $C_n(r)$ and $\frac{1}{n} \langle R_n^2(r) \rangle$ as functions of the walk order r for a 10-step walk on a square lattice. One set of curves corresponds to the exact results and the other to the Monte Carlo results. Following the standard notation in the literature we have defined $C_n(r)$ to denote the number of 'successful' walks of order r and $\langle R_n^2(r) \rangle$ denotes the mean square end-to-end distance for n-step walks of order r. It may be noted that our results for (R_n^2), defined as the mean square end-to-end distance for an n-step walk averaged over all orders.

$$\langle (R_n^2) \rangle = \frac{1}{C_n} \sum_{r=0}^{n-1} C_n(r) \langle R_n^2(r) \rangle$$

with

$$C_n = \sum_{r=0}^{n-1} C_n(r),$$

for both the exact and the Monte Carlo enumerations are the same as the corresponding earlier results [5] (see also Table 2). Our results for C_n, defined above, also agree with those of Fisher and Sykes[3] after we carry out the following simple transformation which is necessitated by

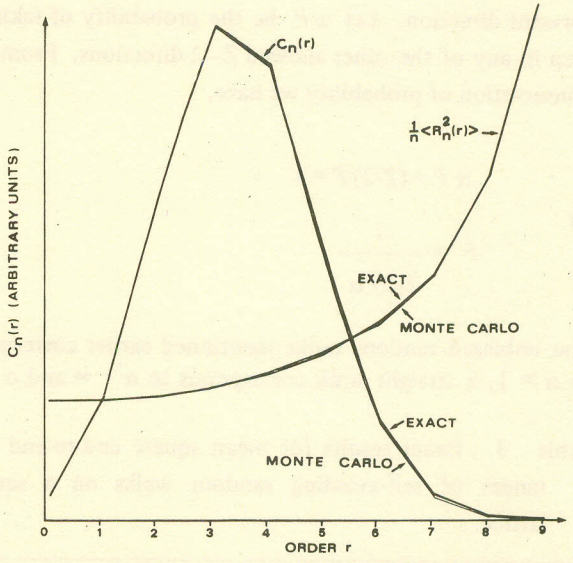


Fig.1. Exact and Monte Carlo results for a 10-step self-avoiding walk on square lattice corresponding to $\alpha = 1$

$$C_n = \sum_{r=0}^{n-1} C_n(r) = 5513$$

$$\frac{1}{n} \langle R_n^2 \rangle = \frac{1}{nC_n} \sum C_n(r) \langle R_n^2(r) \rangle = 2.625$$

Total attempted walks for the Monte Carlo results = 180000.

Table 2. Mean square end-to-end distance for self-avoiding random walks on a square lattice: exact and Monte Carlo results.

n	R_n^2	C_n
8	19.0446	740
9	22.3769	2034
10	26.2492*	5534
11	30.02068	15037
12	34.1908	40617
20	71.9±0.1†	
40	201.2 ± 1.0†	

*Exact as well as Monte Carlo results.

†Monte Carlo results.

the symmetry considerations mentioned earlier;

$$C_n = \frac{1}{2}\left(\frac{1}{4} C_n^F + 1\right),$$

where C_n^F refers to the corresponding quantity used by Fisher and Sykes. Table 2 also gives some of our exact results for C_n for the walks we have so far enumerated.

We now briefly discuss the extension of the above results to a self-avoiding random walk with a bias in the forward direction. Let αP be the probability of taking a step in any of the other allowed Z−2 directions. From the conservation of probability we have,

$$\alpha P + (Z\text{-}2) P = 1$$

or

$$P = \frac{1}{Z\text{-}2+\alpha}$$

The unbiased random walks mentioned earlier correspond to $\alpha = 1$, a straight walk corresponds to $\alpha = \infty$ and $\alpha = 0$ gives random walks with bond angles 90°. Physically speaking small values of α would correspond to polymers in 'poor' solvents where they would tend to contract and large values of α correspond to polymers in 'good' solvents where they would tend to elongate. It may, however, be noted that α does not necessarily vanish for extremely poor solvents as, for $\alpha = 1$, $< R_n^2(r) >$ has a minimum value for values of r greater than zero (see table 3 and the following discussion).

Table 3. Exact results for mean square end-to-end distances of self-avoiding random walks on a square lattice.

r	$\frac{1}{9}<R_9^2(r)>$	$\frac{1}{10}<R_{10}^2(r)>$	$\frac{1}{11}<R_{11}^2(r)>$	$\frac{1}{12}<R_{12}^2(r)>$
0	2.072	2.178	2.27	2.407
1	2.037	2.164	2.25	2.361
2	2.156	2.257	2.33	2.427
3	2.40	2.414	2.37	2.539

According to the above definition of a biased random walk the probability is αP for each pair of identical consecutive steps and it is P otherwise. Thus the total probability to get an n-step random walk with r identical consecutive steps is $\alpha^r p^n$. As it is obvious r is nothing but the order of the walk. The α -dependance of the mean square end-to-end distance of a 'biased' self-avoiding random walk may, therefore, be calculated from order-dependent mean square end-to-end distance of the corresponding 'unbiased' walk as follows,

$$< R_n^2(\alpha) > = \frac{1}{C_n(\alpha)} \sum_{r=o}^{n-1} \alpha^r \; < R_n^2(r) >$$

where

$$C_n(\alpha) = \sum_{r=o}^{n-1} \alpha^r \; C_n(r).$$

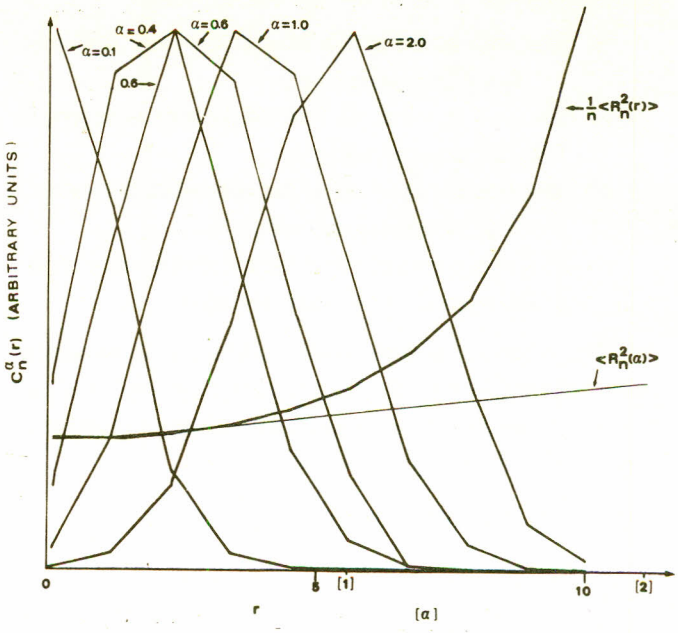


Fig. 2. Exact results for 10-step self-avoiding random walk. $C_n^2(r)$ vs walk order 'r' for different values of α and

$$< R_n^2(\alpha) > = \frac{1}{nC_n(\alpha)} \sum_r \alpha^r C_n(r) \; < R_n^2(r) > \text{ vs } \alpha$$

In so far as α is related to the polymer-solvent interaction, the above-described procedure, therefore, enables one to study single polymers in solutions with the help of 'unbiased self-avoiding random walks. In Fig.2, we present some exact results for a 10-step self-avoiding random walk obtained with this procedure.

Acknowledgements. The author expresses his deep gratitude to the Director and the staff of the International Centre for Theoretical Physics, Trieste, for the kind hospitality extended to him during his stay at Trieste. He also thanks the members of the Physics Faculty of the University of Trieste, particularly, Dr Danial Triliani, for their help in connection with computer work. The present work could not have been done without the help of the staff of the Computer Centre of the University of Trieste, and the author expresses his thanks to the Director and the staff of Centro de Calcolo of the University of Trieste, particularly Signora Adda Lagonegra,who helped write the subroutines for packing several numbers into a single CDC word. Helpful discussions with Professor R.A.Tahir Kheli and with colleagues at the Pakistan Institute of Nuclear Science and Technology are also acknowledged.

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