Enumeration of self-avoiding walks on mixed binary lattices

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We use a new algorithm for calculating the exact number of self-avoiding walks on random binary lattices made of open and closed sites. We provide a simple method for estimating the average value of this number for Monte Carlo–generated lattices. We also present their statistical distribution, and explain the observed trends in this distribution. Finally, we mention several potential applications of these calculations and comment on the relation to the localization-function theory which is to appear in a future paper.

I. INTRODUCTION

There has been a considerable interest in the properties of self-avoiding walks on lattices both recently[1–9] and over the past 25 years[10–15] with many potential applications. A self-avoiding walk (SAW) is a type of random walk with the restriction that each lattice site is visited only once. Properties that have interest include the enumeration of such general walks, the enumeration of walks that end in a closed loop, the calculation of the average end-to-end distance (mean-square radius), the mean-square deviation from the center of gravity (radius of gyration), etc. Most work up to now[8–15] has been limited to perfect lattices (no disorder) where all sites are accessible (open) to a random walker. Several of the properties mentioned above have been studied on such lattices with the use of different methods to investigate problems such as the excluded-volume problem and the Ising model of ferromagnetism,[11] the configuration and dimension[12,13] of polymer molecules, etc.

Considerable interest was shown recently[1–7] for mixed or diluted lattices where some of the sites are declared as inaccessible (closed) to the random walker. This has an immediate consequence of reducing the number of SAW's on the lattices, according to the ratio of open to closed sites. The situation is analogous to a stochastic random walk where the number of sites visited at least once during a random walk is reduced as the concentration of open sites is reduced.[16,17] The interest on this new problem stems from applications in disordered lattices, such as in the estimation of critical exponents,[18–20] where it was recently observed that dilution of the lattice affects the critical behavior of SAW's. This was done[2] with use of the Harris criterion, and instigated the development of other approaches such as renormalization group methods,[2,5] Monte Carlo simulations,[1] and methods of random transfer matrices.[3] However, these approaches do not all agree, and the question is still open. Other applications include the motion of polymers in disordered media[9] and the calculation of the extent of localization[21,22] in the tight-binding model, where the number of SAW's is needed in calculating $L(E)$, the localization function.

We present here a simple method of estimating $\langle C_N(P)\rangle$, the average value of the number of SAW's of length N on a lattice with any concentration P of open sites, if the quantity $C_N(P=1)$ is known. We also give the statistical distribution of $\langle C_N(P)\rangle$ for Monte Carlo–generated lattices.

Depending on the properties examined in this type of calculation, several different methods have been used. It is possible to consider only a statistical random sample out of the total number of walks, and thus be able to extend to high-N values.[1] This method is appropriate for estimating end-to-end distances, radii of gyration, etc., but obviously not for enumerating the total number of walks. In another approach[6] a maximum value of N (of the order of 20) is initially chosen, and starting from a fixed point of origin alternate lattice configurations of the same concentration are considered until this maximum N is realized. At this point all walks are enumerated, thus ensuring that at concentrations P close to P_c the walker is not trapped in a small cluster of open sites, thus severely limiting N. Finally, the average connective constant μ is calculated by extrapolating to $N \rightarrow \infty$; and to achieve such a good extrapolation small-N values were purposely avoided in this approach.

In the present work we perform an enumeration of all SAW's of length N on a given lattice, starting from a random origin. All walks of length $\leq N$ are accounted for, and all possible random dilutions are considered. For concentrations P close to 1.00 our method resembles the previous one.[6] But for P close to P_c we account for *all* walks, rather than only for those which can achieve a maximum N. We do this by developing a very efficient algorithm (described in Sec. II), which permits us, in this concentration region, to average over a large number of runs, typically 1000 or 2000, at a very low computer cost. In these calculations the maximum value of N varied from 9 to 25, depending on the coordination number. Since we are interested in investigating how extended or localized the lattice states become as a function of small and large disorder (see Sec. III) we must include all walks and average over all possible random situations. This was the rationale of our approach.

II. METHOD OF CALCULATION

A lattice of the appropriate topology is generated and kept in the computer memory by establishing at random the character of each site as accessible or inaccessible (open or closed) according to a prescribed concentration, and utilizing a standard IBM subroutine (URAND) for the random number generation. Thus each lattice when generated has an exact concentration P of allowed sites and $1-P$ of unallowed sites. The random walk starts at a randomly chosen position on the lattice. We enumerate the number of walks of length N that are self-avoiding, i.e., they do not cross themselves. If a closed site is encountered no walk can go over it. The simple "brute force" method of doing this calculation is to account for all possible ways of arranging a random walk, checking at each point whether the site has been visited before (in which case it is discarded because it

is not a SAW) or whether the site is a closed one (in which case the walk is not permitted). However, this is an expensive process because it involves a tremendous number of combinations even for moderate N. What is done instead is to enumerate all walks that are self-crossing and all walks that contain at least one closed site. Then this number is subtracted from $C_N(P=1)$, the number of SAW's on a perfect lattice, and we thus arrive at the wanted quantity. This is done by constructing an appropriate matrix whose elements are the identities of all lattice sites, so that all closed sites are easily identified. Then from the value of the coordinates of each closed site in the matrix and by using combinatorial arguments we calculate the number of walks to be eliminated without actually performing them. When a maximum N is specified all walks are computed for all N smaller than or equal to this maximum value. The savings is greater for concentrations that are close to the critical percolation concentration, P_c because if a closed site or loop is encountered early in the walk (which happens with a high probability) then the number of combinations to be eliminated is very large and is calculated at a small fraction of what it would cost to perform the actual walk. A typical run for a three-dimensional simple-cubic lattice (where $P_c=0.31$, for site percolation) for a calculation with $N=9$ and $P=0.35$ takes only a CPU (central processing unit) time of 0.013 sec, while for $P=0.90$ it takes 76 sec, a factor of about 6000, on the IBM 360/67 system.

III. RESULTS AND DISCUSSION

The primary purpose of this work is to derive a method by which one could predict the number of SAW's on a given binary randomly mixed lattice. We first derive a simple formula that gives the average value of this quantity in terms of the number of SAW's on a perfect lattice.

Consider a lattice with a concentration (mole fraction) of open sites equal to P, where $0 < P \leq 1$. A SAW of $N=1$ is a walk one site away from the point of origin. For this case the probability of finding an open site, and therefore having a permissible walk, is equal to P. Then the total number of SAW's of length $N=1$ is

$$\langle C_1(P)\rangle = PC_1(P=1) \ . \tag{1}$$

For a square lattice $\langle C_1(P)\rangle = 4P$, for a simple cubic $\langle C_1(P)\rangle = 6P$, etc. For any length N this quantity becomes

$$\langle C_N(P)\rangle = P^N C_N(P=1) \ . \tag{2}$$

Thus knowing the quantity $C_N(P=1)$ we can easily predict $\langle C_N(P)\rangle$ for any concentration P.

We use three lattices: (1) the directed square, which is a regular square planar lattice, but x and y can only increase for purposes of random walks, (2) a regular square planar lattice, and (3) a three-dimensional simple-cubic lattice. It is rather obvious that for the first case of the directed square lattice,

$$C_N(P=1) = 2^N \ . \tag{3}$$

For the other two lattices Table I contains the values of $C_N(P=1)$, as has been previously reported,[11] and was also found to be the same with the use of our method.

We now perform the calculations for binary lattices using the algorithm described in Sec. II. The average value of several individual runs (i.e., runs on different random lattices with the same concentration P) agrees within about 1% with Eq. (2) for all concentrations and lattice types. This is also a test that the computer programming is indeed correct. But what has also an interest is the statistical distribution of the data as a function of the concentration P of open sites, and also of the length of the walk N. In all cases, for a constant N, we observe that the statistical spread is large close to the critical percolation concentration P_c, and decreases as the concentration of open sites in-

TABLE I. Number of SAW's for a perfect lattice.

N	Square lattice	Simple-cubic lattice
1	4	6
2	12	30
3	36	150
4	100	726
5	284	3534
6	780	16926
7	2172	81390
8	5916	387966
9	16268	1853886
10	44100	
11	120292	
12	324932	
13	881500	
14	2374444	
15	6416596	
16	17245322	

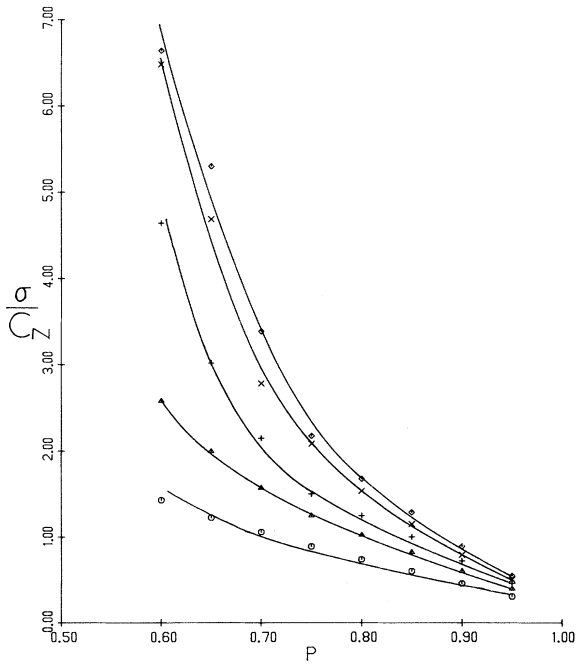

FIG. 1. Ratio of the standard deviation σ over the number of SAW's (C_N) is plotted vs P for $N=5$, 10, 15, 20, and 25, lower to higher curves. The lattice here is the directed square (two dimensional). The number of runs was 2000 for each concentration P. The solid lines are drawn by hand and they are only visual aids.

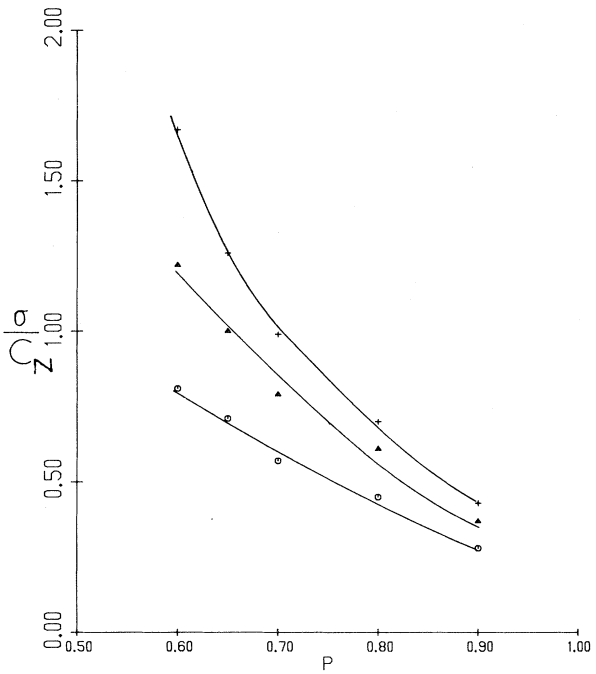

FIG. 2. Ratio σ/C_N is plotted vs P for $N=4$, 8, and 12, lower to higher curves. The lattice here is regular square planar (two-dimensional). The number of runs varied from 1000 (for $P=0.60$) to 100 (for $P=0.90$), due to the increasing cost as explained in the text. The solid lines are drawn by hand and they are only visual aids.

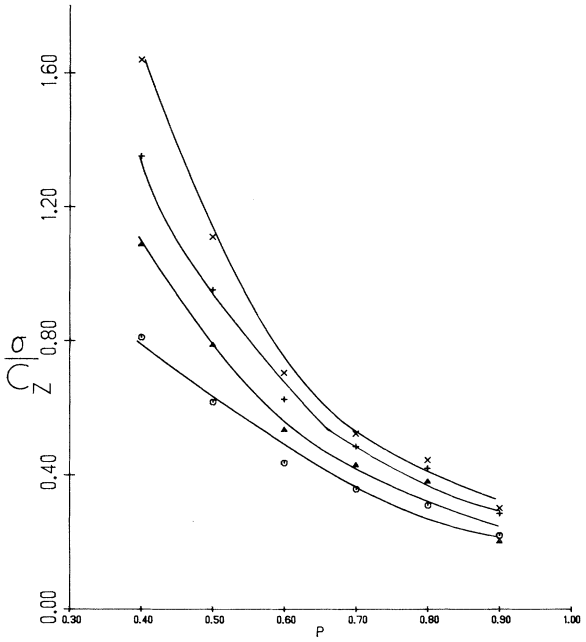

FIG. 3. Ratio σ/C_N is plotted vs P for $N=3$, 5, 7, and 9, lower to higher curves. The lattice here is a three-dimensional simple cubic. The number of runs varied smoothly from 2000 (for $P=0.40$) to 100 (for $P=0.90$), due to the increasing cost as explained in the text. The solid lines are drawn by hand and they are only visual aids.

creases and approaches $P=1$. Also, for a given concentration P, the spread increases as the value of the length of the walk N increases. These trends are all shown in Figs. 1–3. Apparently what happens is that for concentrations close to P_c, where there is an abundance of closed sites, the positioning of each individual closed site relative to the rest plays a very important role, so that small variations in this positioning may result in significantly different C_N values, thus increasing σ (the standard deviation). This is not so in high concentrations, where we have only a few isolated closed sites and their relative positioning does not affect C_N to a large extent, and therefore here σ drops drastically. The same reasoning applies in explaining the variation of σ as a function of N. For a constant concentration P, as N gets longer it spans a greater lattice area which includes a greater number of closed sites, where again their relative positioning plays an important role in determining C_N. These trends are rather smooth in all lattices examined, as it is intuitively expected if we use the above qualitative argument. In general, our numerical results are in good quantitative agreement with the results of Ref. 6 for the high-P range where, as previously discussed, the two approaches are similar. Exact comparisons cannot be made because the reported results[6] are for the $N\rightarrow\infty$ limit, after extrapolation.

In conclusion, we have presented a method for estimating the average number of SAW's on random binary lattices. We reported their statistical distribution on Monte Carlo–generated lattices and qualitatively explained the observed trends. In a previous work[21,22] it has been shown that the localization function $L(E)$ (which is based on Anderson's pioneer work[23]) is equal to one for the square lattice,[21] and larger than one for the three-dimensional simple-cubic lattice[22] when the lattice is in the limit of infinitesimal disorder (all open sites). It is also interesting to investigate now the existence of localized states in the region $P<1$, and it is in this definition of $L(E)$ where the number of SAW's and its statistics are needed. We plan to report these results elsewhere.

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[1]K. Kremer, Z. Phys. B 45, 149 (1981).
[2]B. K. Chakrabarti and J. Kertesz, Z. Phys. B 44, 221 (1981).
[3]B. Derida, J. Phys. A 15, L119 (1982).
[4]G. C. Martinez-Mekler and M. A. Moore, J. Phys. (Paris) Lett. 42, L413 (1981).
[5]A. K. Roy and B. K. Chakrabarti, Phys. Lett. 91A, 393 (1982).
[6]B. K. Chakrabarti, K. Bhadra, A. K. Roy, and S. N. Karmakar, Phys. Lett. 93A, 434 (1983).

[7]A. B. Harris, Z. Phys. B 49, 347 (1983).
[8]K. Kremer, A. Baumgartner, and K. Binder, Z. Phys. B 40, 331 (1981).
[9]K. Kremer, A. Baumgartner, and K. Binder, J. Phys. A 15, 2879 (1981).
[10]H. N. V. Temperly, Phys. Rev. 103, 1 (1956).
[11]M. E. Fisher and M. F. Sykes, Phys. Rev. 114, 45 (1959).
[12]F. T. Wall and J. J. Erpenbeck, J. Chem. Phys. 30, 634 (1959).
[13]F. T. Wall, S. Windwer, and P. J. Gans, J. Chem. Phys. 37, 1461 (1962).
[14]J. L. Martin, Proc. Cambridge Philos. Soc. 58, 92 (1962).
[15]P. J. Gans, J. Chem. Phys. 42, 4159 (1965).
[16]P. Argyrakis and R. Kopelman, Phys. Rev. B 22, 1830 (1980).
[17]P. Argyrakis, Phys. Rev. B 27, 1355 (1983).
[18]R. G. Bowers and A. McKerrell, J. Phys. C 6, 2721 (1973).
[19]B. Shapiro, J. Phys. C 11, 2829 (1978).
[20]M. Napiorkowski, E. H. Hauge, and P. C. Hemmer, Phys. Lett. 72A, 193 (1975).
[21]C. M. Soukoulis and E. N. Economou, Phys. Rev. Lett. 45, 1590 (1980).
[22]C. M. Soukoulis and E. N. Economou, J. Phys. C 14, L221 (1981).
[23]P. W. Anderson, Phys. Rev. 109, 1492 (1958).