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Correlated random-walk simulations in simple and binary lattices

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Random-walk simulations were performed on one-, two-, and three-dimensional, simple and binary lattices with several coordination numbers containing about one million sites. The random walk included a correlation parameter l (Gaussian distribution with given standard deviation) representing a partial directional memory. The walks on the random binary lattices were constrained to sites of one component only (concentration C) with the sites of the second component acting as reflecting microboundaries. All simulations were restricted to the percolating cluster. The simple lattice simulations are compared with the well-known asymptotic analytical expressions for simple random walk ($l = 1$) and with an expression for correlated walks ($l \gg 1$). The visitation efficiency increases, as expected, with C. It also increases with l for simple and high-C lattices. However, for lower-C lattices the visitation efficiency *decreases* with l, thus giving rise to "crossover concentrations." Our results are given in a series of figures of the efficiency or the number of sites visited versus the number of steps, showing the effects of concentration (C), and correlation (l). Applications to exciton percolation and coherence are mentioned.

I. INTRODUCTION

Random walks on lattices of various topologies have been studied extensively in the past owing to the large number of applications that they encompass. For simple, one-component lattices the problem has been solved analytically for several system characteristics, such as the number of distinct sites visited at least once after a certain number of steps, the first passage times, etc.[1-5] These solutions seem to hold for several dimensionalities, but are limited to simple random walk; i.e., the walker is allowed jumps only to adjacent sites with a total loss of memory after each jump. More complicated situations cannot be handled using these formalisms, as would be desirable, but certain phenomena of interest contain these complexities. For example, the connection between excitonic energy transfer in molecular solids and the random-walk mathematical models has been recently demonstrated.[6] The formalism of the hopping model assumes that a resonance type of interaction between neighboring molecular sites causes a transfer of energy between these sites. It is assumed that this transfer follows a random pattern on the average and, therefore, a method based on random-number theory would be applicable to studying this case. This type of energy transfer has been suggested for the exciton percolation behavior in binary crystals (such as for benzene,[7] naphthalene,[8,9] and the photosynthetic units of green plants[6,10-12]). The impurities, dislocations, phonons, etc., that one deals with in molecular crystals necessitate a more complex formalism than usually employed for a pure, rigid, and perfect lattice. In addition, some "coherence of motion" at low temperatures has been suggested for these systems.[13] This leads us to believe that a correlated random-walk model might be appropriate.[8,9] When all these factors are considered, one quickly realizes that the problem is formidable if an exact closed-form solution is sought. We thus resorted to a numerical method, using simulation processes on random lattices that incorporate the complete details of the motion. All calculations are performed on a high-speed computer. We indicate how our results can be applied to the problem of energy transport in molecular solids.

II. RANDOM-WALK METHOD AND COMPUTATIONS

A random binary square lattice made of A and B sites is simulated and kept in the computer memory for the two-dimensional topologies investigated. Several such layers are used for the three-dimensional ones. A linear chain, of course, forms the simple one-dimensional case. The standard IBM subroutine RANDU is used (in its more efficient variant, URAND of the Michigan Terminal System) to decide whether the site in question is A or B according to the given concentration of A, C_A, where C_A ranges from 0 to 1.0. Therefore the lattice is built in a completely random fashion. We have checked the random-number generation routine URAND against a Tausworthe random-number generator[14-16] and found, within our precision, complete consistency. We also compared our routine computer program with several different versions and found complete consistency. The size of the lattice N (number of sites) is an important parameter. One asks the question: How big a lattice is necessary so that the results will be representative and can be easily extrapolated to the case of an infinite lattice? One

would like (because of economics) to work with the smallest such lattice. The answer to this is not unique, but depends on the type of random walk performed. In some instances we used lattices containing a quarter- or a half-million sites, but in other cases we had to increase the size to over one million. It is intuitive that one-dimensional runs need a smaller number of sites than the two-dimensional ones, which in turn need a smaller number than the three-dimensional ones.

Coupled with the size of the lattice is the question of the boundary conditions. In order to avoid interruptions in the random-walk process at the ends of the finite lattice, cyclic boundary conditions are employed (so that the lattice repeats itself indefinitely). However, for most computations we employ a large enough lattice so that the walker rarely hits the boundary. In this way one is assured of not having artificial revisitations induced by the small size of the lattice.

The origin of the motion is randomly chosen and located on a specific lattice site. Then the random walker starts moving to adjacent sites. The direction is again chosen at random, say, from the four available choices of the nearest neighbors (when a square-lattice symmetry with nearest-neighbor jumps is considered). The programing allows motion *only* on the terrain of A-type sites but no access is allowed onto B-type sites. This means that the species concentration (or A/B ratio) determines what portion (and patterns) of the lattice area are allowed to the random walker.

What we compute is the number $n(t)$ of distinct sites visited at least once during a random walk after a specific number of steps s, these sites being all A sites, since all B sites are inaccessible. It may be surprising to notice that these statistical situations do not exhibit a large variance, because owing to the large number of operations occurring in each run there is an internal averaging taking place each time so that one does not have to average over a large number of runs before a particular behavior can be discerned. As an example we show in Fig. 1 the distribution of results for 100 runs of $s = 200\,000$ steps, each on a two-dimensional lattice with four equal interactions, where we plot $n(t)$ versus the frequency of the result. The average result of these 100 runs is 44 800 sites visited, the median is 45 200 sites, and the standard deviation is 4000 sites.

Also of interest is the quantity $n(t)$ divided by the total number of steps, which is the number of sites visited per step [in a way a normalized $n(t)$ quantity]. We call this quantity, $\epsilon = n(t)/s$, the *efficiency* of the visitation process, because it simply shows for each particular run the ability to visit a certain number of sites (or, in other words,

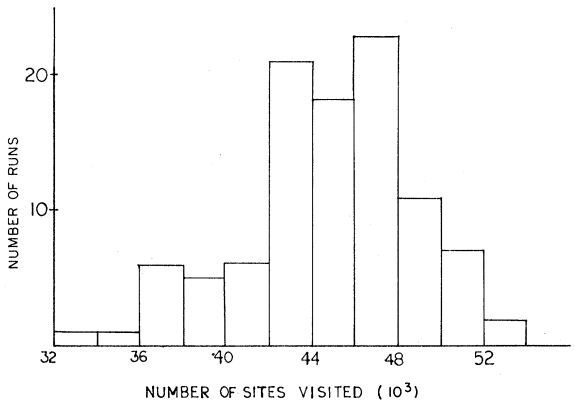

FIG. 1. The distribution of results for the number of sites visited for 100 runs on a two-dimensional one-component lattice of size 1022×1022. The number of sites visited after 200 000 steps is plotted versus the frequency of each result. See text for more statistical details.

how efficient the process is). Obviously $\epsilon \leq 1.0$, where the equality holds only in the limit when each site is visited only once. On the other hand, when only a small number of sites are visited with a high revisitation frequency, then $\epsilon \to 0$ in the limit of a very large s. The novelty of our calculations lies in estimating the efficiency values under different sets of conditions in a rather generalized model (system independent). The utility of these quantities will easily be seen later through some sample calculations.

After each hop there is an option in which all memory is lost, in which case the process will repeat itself anew for a total number of steps s, or alternatively, the memory is retained and the same direction of motion is then followed. The number of steps for which memory is retained can be treated as a variable. The latter is one of the main points of interest in this study

We can extend the random-walk process to include direct hops to next nearest neighbors, next-next-nearest neighbors, etc. The program gives the option of assigning different hopping probabilities to different kinds of jumps. This probability will depend on the specific application at hand.

The total number of sites in the lattice is N. Thus, N_A is the upper limit for the number of sites $n(t)$ that can be visited. As mentioned above, this case of $n(t) = N$ is possible only for high C_A (i.e., when $C_A \to 1.0$) where all A sites in the lattice are connected. However, as C_A decreases, the number of available A sites decreases even faster because finite clusters of A become more abundant. A cluster of A sites is a set of connected A sites completely surrounded by B sites. Since all B sites are inaccessible, *all A clusters but one are also inaccessible to a given*

walker. Again, the smaller C_A, the smaller is the available number of A sites. We focus on the largest cluster available in the crystal, the so-called maxicluster. Its size is strongly concentration dependent.[17] All random-walk motion is then restricted to this maxicluster.

Percolation theory which has been developed recently for the treatment of random binary systems in terms of cluster distributions[18] has shown[17-19] that the size of the maxicluster increases dramatically at the critical site-percolation concentration C_c, while it rapidly drops to small values below it. At this particular critical concentration, the infinite, extended cluster appears for the first time. Well below C_c it is obvious that,[6] for a large number of steps, $n(t)$ will usually be about equal to m, a number we can predict from percolation theory (m is the size of a finite cluster). Therefore, we focus on the region $C \geq C_c$.

The simplest case occurs when all memory is lost after $l=1$ jumps. We call l the correlation or coherency parameter or just coherency. A more complex case occurs when we allow the random walker to make l jumps in a row in the same direction, which is similar but not equal to making a jump of length $l=k$, where k is an integer. We then say that memory is retained through all l jumps and the same direction of motion is followed until the end of the vector l or until an inaccessible site is encountered. Of even greater interest is the more general case where l is the average or most probable value of a distribution rather than a constant. This idea has been utilized earlier[4] and solved analytically, but only for a one-dimensional, pure (one-component) lattice, using exponentially distributed jumps. In our case the coherency of the given jump is characterized by a Gaussian distribution where we define the mean and the standard deviation of the line shape. As in the case of $l=1$, at the end of these l hops all memory is lost, while within them it is perfectly retained, i.e., all successive l jumps are completely correlated, directionally. We note, however, that in our model this correlation is completely broken as soon as the hopping path is blocked by a B site. In this case the walker is started anew at the last A site.

III. RESULTS

In Table I we show the number of distinct sites visited at least once during a random walk of 200 000 steps for the several different conditions discussed above, i.e., as a function of dimensionality, number of interactions, binary system concentration, and coherency. Notice that the values of the number of sites visited for $C_A=1.0$ and high l compare within a few percent with a heuristically derived limiting formula[9] giving (except for one dimension)

$$n(t)=s(b-2)/(b-1) \quad (N \gg s \gg 1 \gg d \gg 1), \quad (1)$$

where b is the number of bonds (directions) per site. This formula gives $n=133\,000$, 160 000, and 171 000 for $b=4$, 6, and 8, i.e., square, simple-cubic, and "square-1, 2" lattices, respectively.

The Table I cumulative results ($s=200\,000$ steps) were chosen for the naphthalene system, where s corresponds to the average lifetime of a singlet excited state. In Figs. 2–6 we show a more complete picture in terms of the efficiency as a function of the number of steps (or time). Below we treat each dimensionality case separately.

A. One-dimensional case

This is the most tractable case, as one would intuitively think. The standard procedure[1-5] is to set up the generating function

$$G(z,l)=\sum_0^\infty z^n P_s(l)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{e^{-il\phi}}{1-z\lambda(\phi)}\,d\phi\,, \quad (2)$$

where l is the site variable, $P_s(l)$ is the probability that a walker starting from the origin arrives at l for the first time after s steps, $\lambda(\phi)=\frac{1}{2}(e^{i\phi}+e^{-i\phi})=\cos\phi$ (if the probability is 0.5 for going to the right or the left). The properties of interest such

TABLE I. The numbers of sites visited (in thousands) during a random walk after 200 000 steps for several conditions.

	One-dimensional linear		Two-dimensional square			Two-dimensional 8 interactions			Three-dimensional simple cubic	
C_A	$l=1$	$l=10$ $d=3$	$l=1$	$l=10$ $d=3$	$l=100$ $d=30$	$l=1$	$l=10$ $d=3$	$l=100$ $d=30$	$l=1$	$l=10$ $d=3$
1.00	0.69	2.12	44.6	125.2	140.2	63.6	149.4	161.2	125.2	155.3
0.85			34.8	66.1	58.3					
0.75						41.6	97.0	103.9	100.4	125.8
0.70			17.4	7.8	0.82					
0.50						17.0	22.7	19.5	17.5	42.5

as mean first-passage time to trapping, mean recurrence times, mean excursion from the origin, etc., are related to a number of moment properties and can readily be calculated. It is shown[4] that for an N ring (one-dimensional model with cyclic boundary conditions made of N lattice sites) containing one trap site, the number of steps for trapping is given by

$$\langle s\rangle = \tfrac{1}{6}N(N+1), \tag{3}$$

while the number of distinct sites n visited at least once after s steps is given by

$$\langle n\rangle = (8/\pi)^{1/2}s\,. \tag{4}$$

If one is to include coherence, the generating function is much more complex[4] now because one needs to evaluate the quantity

$$\lambda(\phi) = \sum_{k=-\infty}^{\infty} P(k)e^{ik\phi}, \tag{5}$$

where k is the distance in lattice spacings between the initial and final sites of transfer. When this complete form is used it is found that[4] the equivalent to Eq. (3) but including coherence is

$$\langle s\rangle = \frac{(1-e^{-a})^2N^2}{(1+e^{-a})6}, \tag{6}$$

where the parameter a determines the relative probabilities that a walker takes steps of different lengths in one direction. No solution exists to give the equivalent to Eq. (4) for coherence values $l \neq 1$.

We compare our simulation results, where possible, with the above formalisms. For a one-dimensional lattice it is obvious that one cannot perform a meaningful simulation on a binary (guest-host) system because one or two single host (inaccessible) sites would severely limit the range of motion by blocking the transfer completely. Figure 2 shows our efficiency calculations for a one-component lattice. It is seen in this figure that the case of $l = 10$ shows a considerably greater efficiency, indicating that the long "stretches" in one dimension are more efficient than the "back-and-forth" oscillatory motion of short steps. The exact analytical result for $l = 1$ is also plotted in the same figure and it is seen that it is in good agreement with our simulation result for the totally stochastic case ($l = 1$). There is no solution, however, for which to compare our $l = 10$ simulation result.

B. Two-dimensional case

For the simple case of the coherence parameter $l = 1$ for a one-component lattice, one proceeds in a similar fashion as in Sec. III A and the equivalent equations are for a square and triangular lattice, respectively,

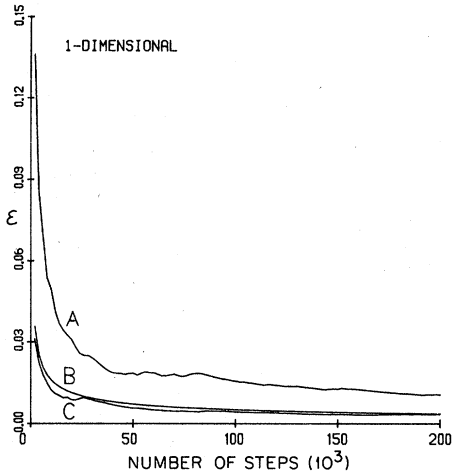

FIG. 2. Efficiency calculations for a one-dimensional one-component chain (average of five runs each). Two cases are shown, one for $l = 1$ (curve C) and one for $l = 10$ (with standard deviation = 3.0), curve A. The "exact" analytical limit (for $l = 1$) as given by Eq. (4) is also plotted on the same graph, curve B.

$$\langle s\rangle = (1/\pi)N\ln N + 0.19506N, \tag{7a}$$

$$\langle s\rangle = (\sqrt{3}/2\pi)N\ln N + 0.235214N, \tag{7b}$$

for large N. The equivalent to formula (4) for the two-dimensional case is

$$\langle n\rangle = \pi s/\ln s \tag{8}$$

for s very large. For square lattices where the connectivity between adjacent sites is not always unity the formula equivalent to (8) is[20]:

$$\langle n\rangle = \frac{2\pi\sqrt{k}}{k+1}\,\frac{s}{\ln s}, \tag{9}$$

where k here is a measure of the periodicity of the connections. There is no formalism to cover either the more complex binary lattices or values of $l \neq 1$. Our simulations, therefore, provide new insight into these properties.

Figure 3 shows the efficiency results for a two-dimensional lattice with four interactions in each site. The cases of $l = 1$, 10, and 100 are plotted (with standard deviation equal to 0, 3.0, and 30.0, respectively) for three guest concentrations, $C(\text{guest}) = 1.0$, 0.85, and 0.70. The lattice employed was 1022×1022 sites in size in each case. Comparison with the "exact formalism" poses some difficulties even for the $C_A = 1.0$ case. According to Eq. (8) the number of sites visited after s steps is equal to $n(t) = \pi s/\ln s$, but this appears to be valid only for very large values of s, of considerably higher magnitude than the values we employ in this study.[9] Therefore, no meaningful

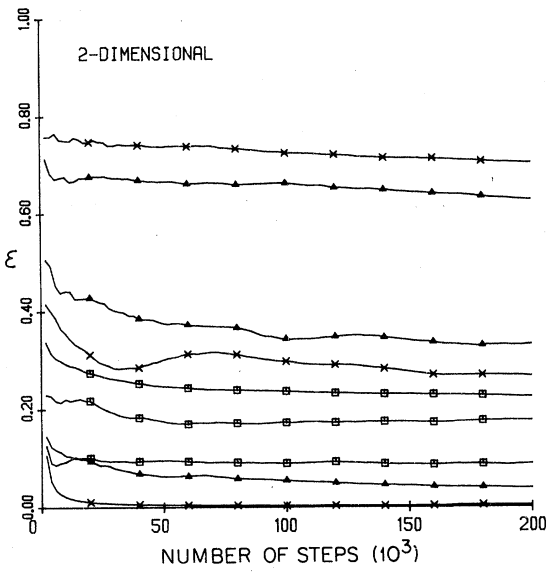

FIG. 3. Visitation efficiency versus the number of steps as a function of the coherency l and the guest concentration. We report here the cases of $l=1$ (square), $l=10$ (triangle), and $l=100$ (×) (averages of Gaussian distributions with a standard deviation of $d=0$, 3.0, 30.0, respectively). The several curves in each case correspond to different guest concentrations as follows: 1.0 (pure crystal), 0.85, and 0.70, respectively, from top to bottom. The lattice size is a square of 1022×1022, and only the four nearest-neighbor interactions are considered here. All four carry equal probability. The crossover concentration can easily be detected in each case (see text). The results are averages of several runs, typically 5–30 runs (depending on the fluctuations that each case had).

comparison can be made here [this analytical formula gives $n(t)=51\,476$ sites visited, compared with our simulated value of 44 800]. Obviously our scheme also gives values of $n(t)$ for small values of s, in contrast to the limiting analytical form. Moreover, our emphasis in this study is on concentrated binary lattices ($C_A=0.85$, 0.70) where no analytical formula is available.

As expected, ϵ decreases with time (i.e., with the number of steps) in all cases, but after a certain point it remains roughly constant. This apparent limiting value is the most important numerical information in these plots because it largely determines the efficiency of the corresponding transport mechanism over long times. Table II summarizes all these limiting values for all three cases for the four-nearest-neighbors topology (d is standard deviation).

TABLE II. Limiting ϵ as a function of guest concentration (square lattice topology).

C_A	$l=1$	$l=10$ $d=3$	$l=100$ $d=30$
1.00	0.22	0.67	0.70
0.85	0.18	0.33	0.27
0.70	0.07	0.04	0.01

We note the following: The case of $l=10$ is more efficient than $l=1$ for $C_A=0.85$, while $l=1$ is more efficient than $l=10$ at $C_A=0.70$. We call the intermediate range the crossover concentration (C_x) for the two cases compared. This is typical of a certain trend. If one plots ϵ (limiting) vs C, Fig. 4 results. First, one should observe that there is a quasilinear relationship exhibited by all cases. Second, C_x can be easily deduced at the point where the lines cross. Therefore

$$C_x \simeq \begin{cases} 0.74 \text{ for } l=1,\ 10 \\ 0.79 \text{ for } l=1,\ 100 \\ 0.95 \text{ for } l=10,\ 100. \end{cases}$$

We also observe that the greater the l value, the steeper is the curve of the corresponding line.

The reason for the above behavior of ϵ with concentration becomes intuitive only after some reflection. At the high guest concentration the random walker encounters few obstacles, so a long coherence length enhances the chances of visiting new sites and therefore enhances ϵ. However, at low concentrations the opposite occurs because of the labyrinths that are now present due to the cluster formations and the many "host" boundaries which constantly interrupt the long jumps, forcing an abundance of revisitations. When investigating a particular phenomenon re-

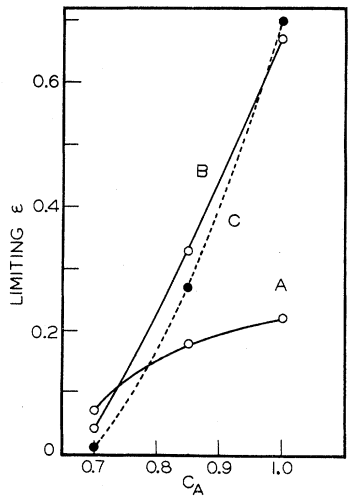

FIG. 4. The limiting visitation efficiency (from the calculations of the previous figure) versus guest concentration as a function of the coherence parameter l. The cases of $l=1$ (curve A), 10 (curve B), and 100 (curve C) are reported here (with a Gaussian distribution having standard deviations of $d=0$, 3.0, 30.0, respectively). Only the four nearest neighbors are considered here. See text for details.

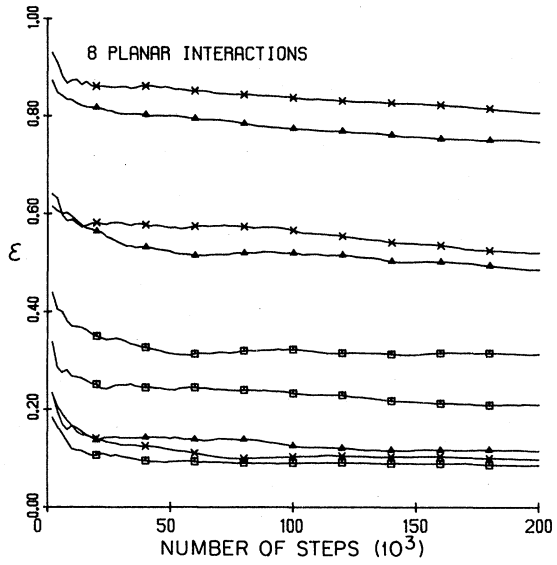

FIG. 5. Visitation efficiency versus the number of steps with the coherency l and the guest concentration as parameters for the square-1, 2 lattice. The guest concentrations reported here are 1.0, 0.75, and 0.50, from top to bottom. In these simulations, besides the four nearest neighbors, we have added four next-nearest ones (eight in all). All eight interactions carry equal probability; the lattice used and the symbols are as in Fig. 3. The results are averages of several runs, typically 3–10 runs (depending on the fluctuations that each case had).

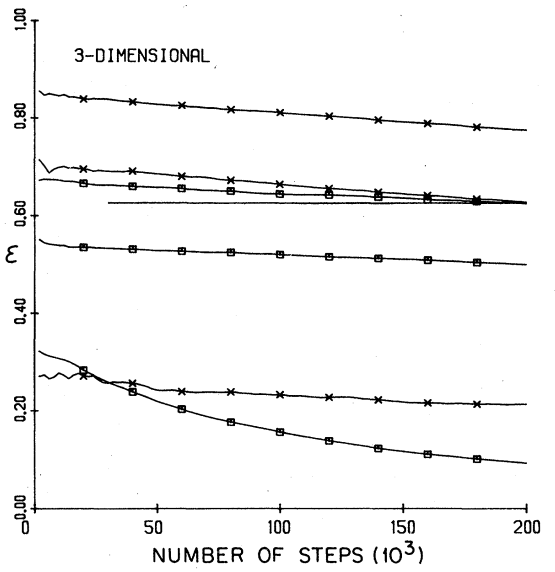

FIG. 6. Visitation efficiency versus the number of steps with the coherency l and the guest concentration as parameters. These simulations are for the three dimensional case ($101\times101\times101$) with a total of six interactions, four in-plane and two out-of-plane. The coherency values shown are for $l=1$ (square) and $l=10$ ($\times$) with standard deviation equal to 3.0. The guest concentrations reported here are 1.0, 0.75, and 0.50, from top to bottom. The results are averages of several runs, typically 3–30 runs (depending on the fluctuations that each case had). The solid line represents the prediction of the exact formalism [Eq. (1)]. Note also that Eq. (1) gives $\epsilon = 0.8$ for large S.

garding its coherence values, a set of binary systems can be utilized for establishing its characteristics, because the dependence of ϵ on C can indicate, at least qualitatively, the magnitude of the coherency. Figure 5 shows the efficiency calculations for two-dimensional lattices with eight interactions. We know of no analytical formula with which to compare these calculations or which predicts the crossover phenomenon described above.

C. Three-dimensional case

Here, again owing to the increased complexity of the problem, only the simplest cases have been treated analytically. It was found[1-3] that for simple cubic, one-component lattices with $l=1$,

$$\langle s\rangle = 1.5164N, \tag{10}$$

$$\langle n\rangle = 0.629\,462\ s. \tag{11}$$

Our calculations, emphasizing the more complex systems, are shown in Fig. 6 for a three-dimensional simple cubic lattice with six interactions. The analytical form [Eq. (11)] predicts a constant limiting value of 0.629 462 for the efficiency (this is also plotted in Fig. 6) throughout a wide s range. For an s value of 200 000 this gives an $n(t)$ value of 125 890 sites visited, compared with the 125 200 sites in our simulated value, i.e., in excellent agreement. Summarizing the comparison of the $l=1$ simulations with the limiting analytical forms we conclude that we have very good agreement for the cases of the one-dimensional and three-dimensional lattices, but we seem to be outside the range of validity for the two-dimensional limiting analytical formula.

IV. DISCUSSION

We developed a Monte-Carlo-simulation method to derive random-walk efficiencies for binary lattices for a range of topologies, concentrations, and coherence (correlation) parameters. This technique is based on computer programs we developed in this laboratory, treating all the problem characteristics as adjustable parameters, and thus it is quite general. We have utilized[8,9] this approach for the exciton migration in a naphthalene system ($C_{10}H_8/C_{10}D_8$) to calculate efficiencies for totally random walks ($l=1$) and partially coherent walks ($l>1$). As we have reported earlier,[9] in this system our calculations showed that the large coherence values favor the migration at high guest concentrations, but hinder it at low concen-

trations (which are still above the critical percolation concentration). The reason for this turning point has been discussed above. This effect may be rather important for the study of coherence parameters.[8,9] It obviously has a relationship with the cluster distributions.[17,18] This was also our main motivation for performing random- and correlated-walk simulations on binary lattices.

Fluorescence spectra of mixed crystals provide a very good measure of the transport efficiency since one can monitor the excitation quantitatively by looking at emission from the various species present. One can vary the guest-to-host ratio by growing a series of crystals over the total binary concentration range. Then, the visitation efficiency for each crystal can be measured, and using l as an adjustable parameter one can find the best fit for the experimental behavior in terms of a value of the coherence length. Such a detailed study[21] will be reported elsewhere (for a preliminary report see Ref. 8).

We note that all our simulations were performed above the critical percolation concentration and did not include walks on miniclusters.[6] We also emphasize that each of the l sites in the l-correlated walks is nominally "visited." A summary of work on long-range hops, related to long-range clusters,[22] is in preparation.

ACKNOWLEDGMENT

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