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Correlated random walk in continuous space

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We present a model for diffusion with correlated motion in continuous space. Correlation is implied as the retention of the directional memory of the moving particle between successive scattering events. We use a model borrowed from the field of polymers, based on a scattering angle θ, which is analogous to the bond angle between two monomers in a chain molecule. We monitor via Monte Carlo computer simulations the usual random walk properties, such as the mean-square displacement, the number of sites visited (where the underlying continuous space is binned in boxes), etc., for two-dimensional spaces, as a function of time, and the correlation parameter. This type of motion belongs asymptotically to the same class as the regular random walk. For short times one observes a crossover that is strongly dependent on the correlation parameter in a scaling form, which is calculated numerically. [S1063-651X(96)00407-2]

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I. INTRODUCTION

Correlation in diffusional motion has been shown in the past [1–3] to be a very important and sometimes a necessary idea for the explanation of several different experimental systems. For example, it has been used to explain hydrogen diffusion in group VB metals at higher temperatures [1], vacancies in solids [2], motion of excitons at low temperatures in mixed naphthalene crystals [3], etc. Correlated walks are a special case of random walks, in which the moving particle has a retention of the directional memory over a certain number of trajectory steps. Thus, the options available to the moving particle at each step, regarding the direction of the next step, depend on its past history, i.e., previous λ steps, where λ signifies the degree of correlation. It is sometimes referred to as persistent motion, or coherent motion, to denote the particular characteristic of the motion that distinguishes it from totally stochastic motion (regular random walk) by preserving the memory of the direction of the previous step(s). Up to now it has been studied on regular [4,5] and fractal [6] discrete lattices. In the present work we extend these lattice models to continuous space. It is generally believed that [4] continuous space and lattice models behave identically, at least as far as simple random walks are concerned. This similarity is also checked here.

Due to the nature of the problem we use a model that is based on the scattering angle θ. The value of this angle quantitatively determines the extent of correlation. This model is equivalent to the ones used in chain molecules (usually hydrocarbons, polymers, etc.), where the particle steps are the connecting bonds between two consecutive atoms, while the angle θ is the bond angle [7]. The root mean-square displacement of random walks is simply the polymer end-to-end distance. However, depending on the problem at hand, one may have to consider a self-avoiding walk in the polymer case, rather than a usual random walk, if the excluded volume principle applies. At any rate, the angle model can not be generally formulated on a lattice, where the bond angles have only a few fixed values (e.g., 90°, 60°, etc.), and thus continuous space comes naturally. Due to the large number of configurations (or step combinations) the problem can only be treated statistically. Here we are interested in the system properties as we vary θ, the degree of correlation, and the variation is always in the entire range $0° < \theta > 360°$.

The questions addressed here include the following: To what class of walks does this new model belong? What are the differences from the well-known lattice models? What is the detailed behavior of the usual random walk quantities? The numerical model that is used to answer these questions is described in detail in Sec. II. Our results are given in Sec. III, and finally a summary and conclusions in Sec. IV.

II. MODEL AND METHOD OF CALCULATIONS

Our model pertains to a random walk in continuous space in two dimensions. No lattice periodicity is used, thus all x and y positions are possible. A particle is allowed to perform a random walk, by choosing at random the direction of motion at each step. The length of each step is constant and always the same, say equal to one length unit. The correlation parameter is introduced via the angle θ. The direction of motion for each step is limited inside this angle as follows: When the next step is to be made, first we draw the extension of the direction of motion of the previous step. This exten-

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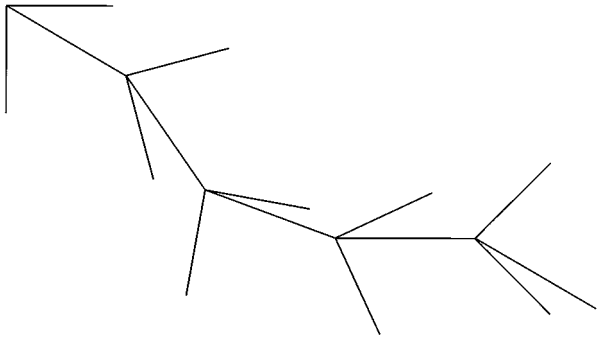

FIG. 1. A pictorial of correlated motion in continuous space. For a given angle θ (here $\theta=90^o$) random directions of motion are chosen for each step, as given by a random angle, which is formed by using the extension of the previous step and the interval $-\theta/2$ to $+\theta/2$, as shown here.

sion is considered to be the dichotomy of the new angle θ (or, an angle $\theta/2$ is formed above it, and $\theta/2$ below it). Then the full angle θ is constructed, and a random direction is chosen inside this angle. This is the direction of the next step. An example is shown in a pictorial in Fig. 1, where $\theta=90°$. Subsequent steps are also performed using the same mechanism. It is obvious that the smaller the θ, the larger is the correlation. Also, $\theta=0$ corresponds to motion on a straight line (totally correlated walk), while $\theta=360°$ is the case for totally uncorrelated motion (stochastic random walk). Similar considerations would apply to three-dimensional space, where a solid angle θ would be used, with the same principles as here.

To monitor the mean-square displacement we use no lattice (i.e., we have free space), but keep the values of the x and y coordinates, as a function of time, for a fixed value of θ. We vary θ in the interval $0-360°$, and consider about 30 different θ values. The advantage of this algorithm is that one never has finite-size effects, regardless of the length of time. We thus go routinely to 10^7 steps, and if necessary it is feasible to extend this realistically to 10^9 steps.

In order to monitor the regions of space that are visited by such a correlated process we use a boxing technique. Here it is necessary to use an underlying lattice. We divide the available space in a large number of boxes (squares), typically 3000×3000 for the two-dimensional case. For simplicity we keep the length of the box equal to the length of the step. We trace the particle motion and monitor the number of boxes that are visited in a random walk as a function of time. During the walk cyclic boundary conditions are used, so that the particle is never ''forced'' to stay in a limited size area. The number of boxes visited at least once corresponds to the well-known S_N property in lattices. Additionally, we monitor the number of visits for each box, a quantity that leads to the ''entropy'' function of the system. However there is a new element in the continuous space case: A trajectory traced by a single step may go over and visit two boxes in one step (instead of the lattice case, where only one site can be visited in one step). Thus, one can either count the initial and final boxes only (case I), which corresponds to the lattice case, or can additionally count the intermediate boxes (case II). We treat both cases.

III. RESULTS

In Fig. 2 the mean-square displacement is shown as a function of time (number of steps) for several different θ values. The case of $\theta=360°$ corresponds to totally stochastic random walk, and gives a straight line with slope equal to 1.00, as expected. Several curves are shown with varying correlation parameter θ, in the range $2°<\theta>360°$. As θ is

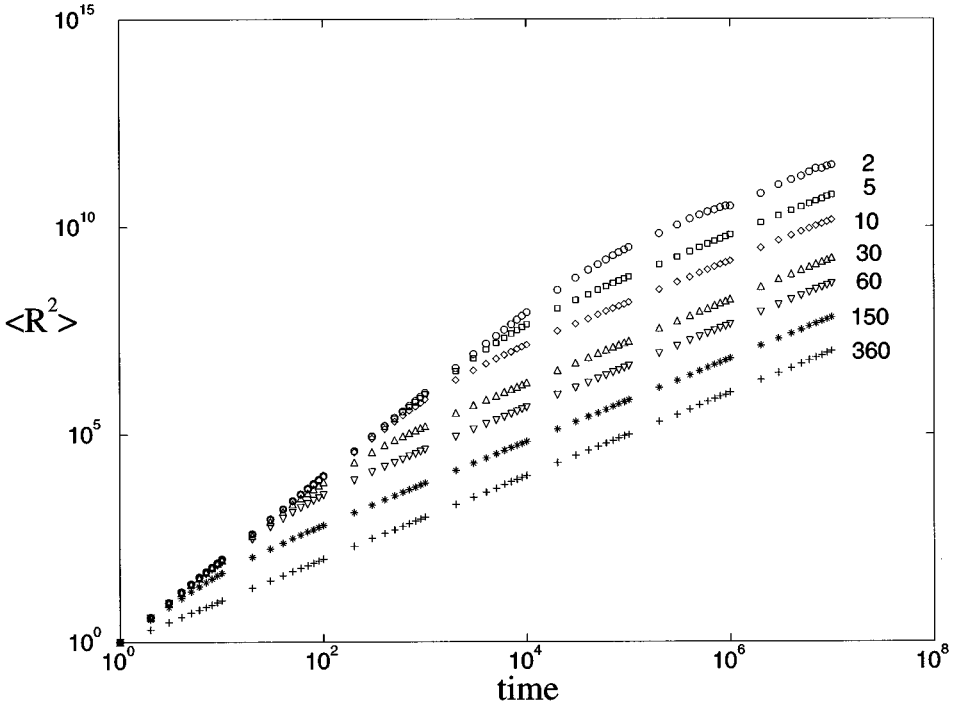

FIG. 2. $\langle R^2\rangle$ vs N (number of steps) for several different scattering angles θ. The calculation was carried over continuous space with no boundaries. Several different θ values are shown: 360, 150, 60, 30, 10, 5, 2. These data are averages of 5 000 realizations.

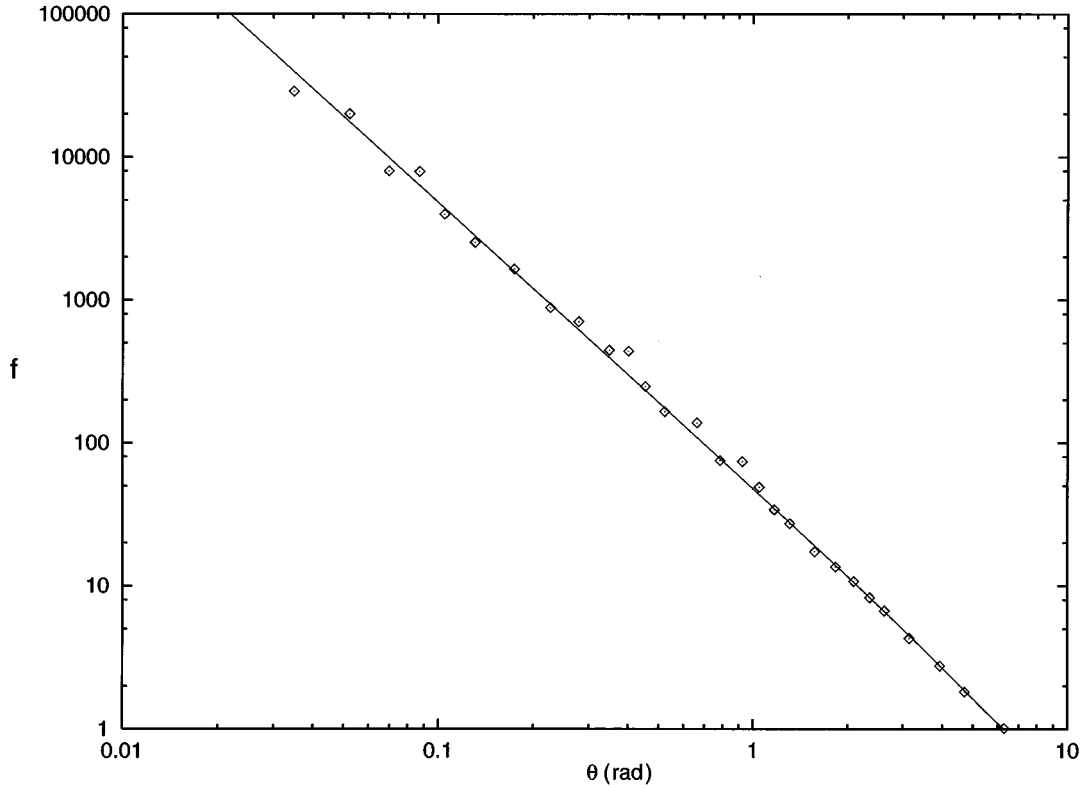

FIG. 3. The intercept f vs the correlation angle θ. The points correspond to the intercept on the y axis of the lines of Fig. 2, and the straight line represents Eq. (4).

decreased and the motion becomes correlated we observe that initially the slope is larger than the stochastic case. The smaller the θ, the larger the initial slope. This early-time increase manifests the fact that the particle, due to the correlation, is able to get further away from the point of origin, producing a larger $\langle R^2 \rangle$, as compared to the uncorrelated walk. At longer times, however, we observe that there is a crossing over to the same slope as the normal stochastic walk. This means that all slopes, for all θ values, become parallel to the $\theta = 360^o$ case. This is in agreement to the well-known result for lattices [4]:

$$\langle R_N^2 \rangle = fN \quad N \to \infty. \tag{1}$$

This shows that for N approaching infinity, for a finite correlation, the mean-square displacement is proportional to N, with a proportionality constant f. Thus, correlated walks belong to the same universality class as the simple random walks. It is realized that the factor f is indeed the actual correlation factor, which is, of course, related to θ. As it has been previously [7,8] shown from the field of polymers, f is given by

$$f = \frac{1 + \langle \cos\vartheta \rangle}{1 - \langle \cos\vartheta \rangle}. \tag{2}$$

The angle ϑ is the angle between two consecutive jumps, and $\langle \cos\vartheta \rangle$ is the average over all possible jump directions, properly weighted. We see that this result is identical for chain molecules as well as for correlated walks. Upon integrating the term $\cos\vartheta$ from $-\theta/2$ to $\theta/2$ (due to the definition of our model), and considering all possible θ angles, we arrive at

$$\langle \cos\vartheta \rangle = \frac{\sin(\theta/2)}{\theta/2}. \tag{3}$$

Then

$$f = \frac{\theta/2 + \sin(\theta/2)}{\theta/2 - \sin(\theta/2)}, \tag{4}$$

which can directly be used in Eq. (1). For the regular, uncorrelated walk, where $\theta = 360$, we get the expected result that $f = 1$. For any other values of θ different than 0 or 360, $f \neq 1$. We can now proceed to use the data of Fig. 2 to calculate numerically the f values. By extrapolating the portion of the straight line with slope equal to 1 (the long time portion), we find the intercept on the y axis, and the corresponding value of f as a function of θ. A plot of f vs θ in log-log form is given in Fig. 3. The straight line represents Eq. (4), and we see that we get very good agreement. The slope of the straight line is -2.

In Fig. 2 we observe additionally that the crossover to the asymptotic behavior is a strong function of θ. For each θ value we estimate t_c, the crossover time. This is given by the intersection of the two straight lines: the early-time and the late-time parts of each curve. In Fig. 4 we plot t_c as a function of θ in log-log form. We observe that we get a straight line with a slope of about -1.88. This implies an expression of the form

$$t_c \sim \theta^h, \tag{5}$$

where we find that the exponent $h = -1.88$.

The next property we look at is the measure of the visitation efficiency of the undelying space during the random

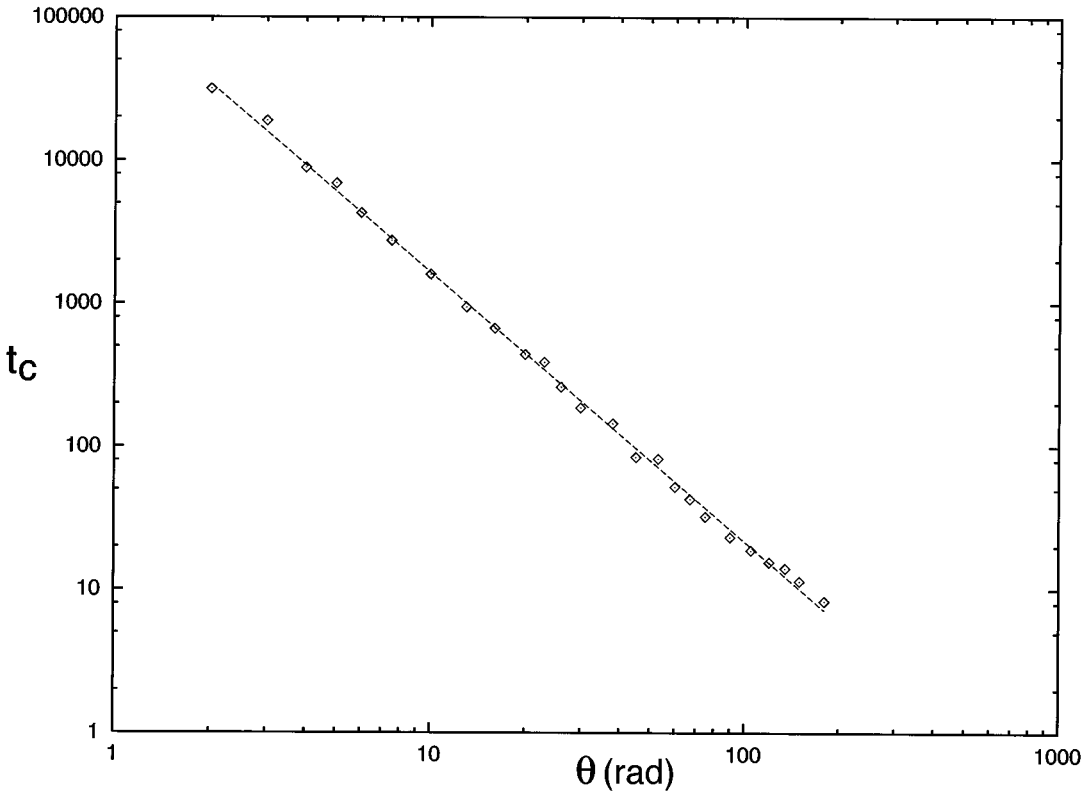

FIG. 4. The crossover time t_c vs the correlation angle θ. The points are calculated from the data of Fig. 2, while the straight line is the best fit. The slope of the straight line is h=−1.88.

walk process, as a function of time. Fig. 5 shows the number of boxes visited at least once, for both cases, as explained in Sec. II. Case I corresponds to the lattice walk, and thus in the same figure we also plot the lattice S_N quantity, as it has been reported in the literature [9], for the case of $\theta = 360$ (stochastic walk). We see that it is in excellent agreement with the continuous space walk data, again showing that the two processes belong to the same class, and in fact are identical. Several values of the correlation parameter are shown in this figure. We notice a considerable difference in the numerical data between case I and case II, and also observe that this difference increases with increasing correlation. This trend is rather simple to understand: As correlation increases and S_N also increases, the situation arises much more frequently where intervening boxes are visited by the particle path. With increasing correlation, the revisitation rate decreases, and more boxes are visited less frequently (see also the I_N property below). This results in more visits of intervening boxes at higher values of the correlation parameter, producing this difference between the two cases, as shown in Fig. 5.

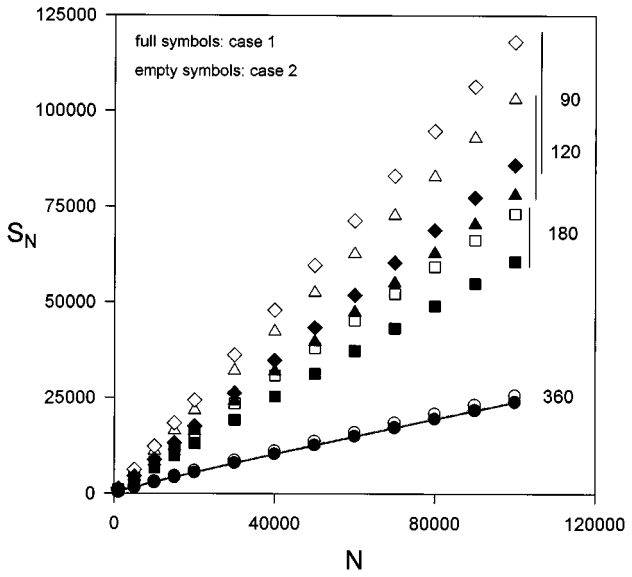

FIG. 5. $\langle S_N \rangle$ vs N (number of steps) for several different scattering angles θ, as marked. The solid line is the result of the Henyey-Seshadri formalism. The full symbols pertain to case I, the empty symbols to case II. Symbols are marked as follows: θ=360, circles; θ=180, squares; θ=120, triangles; θ=90, diamonds.

Comparing the S_N curves for the different values of θ we see that the trend goes as expected, i.e., S_N increases with increasing correlation. The analytical solution to this problem is rather intractable, even for lattices, but some attempt has been made in the past [5] to derive numerically a fitted equation for lattice correlated walks. We will relate the data of the present work in continuous space to the reported equation for the lattice case. A proposed solution for the lattice correlated S_N was [9]

$$\langle S_N \rangle = \frac{\pi f N}{\ln(\beta N)} \sum_{j=0}^{\infty} c_j (\ln BN)^{-j}, \tag{6}$$

where f is a function of p_f, p_f is the probability for scattering in the forward direction for the lattice model (the correlation parameter of the lattice model), B is a fitted constant, which was derived numerically, and $\beta = 8fe^B$. Using these B values (found in Table I of Ref. [5]), we find a correspon-

TABLE I. The correspondence of the models in the lattice case (where the correlation parameter is given by the probability p_f), and in the continuous space (given by the angle θ), together with the corresponding $\langle\cos\vartheta\rangle$.

p_f	θ	$\langle\cos\vartheta\rangle$ lattice model	$\langle\cos\vartheta\rangle$ continuous space model
0.4	308	0.200	0.163
0.5	270	0.333	0.300
0.6	240	0.466	0.413
0.7	209	0.600	0.531
0.8	178	0.733	0.644
0.9	142	0.866	0.763
0.95	122	0.933	0.821

dence between p_f and θ, which is given in Table I. This correspondence is found by simply matching the S_N values produced by the different p_f [Eq. (6)] and θ (present simulation data) calculations. No additional fitting is performed here. We can also now directly compare the $\langle\cos\vartheta\rangle$ term of the lattice model (of Ref. [5]) with that of Eq. (3). For the lattice model the parameter f is

$$f=\frac{p_f+1/2}{1-p_f} \tag{7}$$

resulting in

$$\langle\cos\vartheta\rangle=\tfrac{1}{3}(4p_f-1). \tag{8}$$

The values of $\langle\cos\vartheta\rangle$ are also given in Table I for both cases. We notice that they have the same trend, but differ by about 10–20% in all cases. The conclusion, therefore, can be drawn that the influence of S_N is qualitatively similar, but there remains a quantitative difference which might be caused by the arbitrariness of the box subdivision.

The quantity S_N gives an overall measure of the spread of the particle motion, but it gives no information about the revisitation properties of the motion. This information is given through the probability $P_{k,N}$ that box k has been visited after N steps. This quantity is given by

$$P_{k,N}=\frac{W_{k,N}}{\Sigma_k W_{k,N}}=\frac{W_{k,N}}{N}, \tag{9}$$

where $W_{k,N}$ is the number of times box k has actually been visited in N steps. In the above equation, strictly speaking, the second equality is valid only for case I. As in the case of discrete lattices this quantity leads to the ''entropy'' function

$$\langle I_N\rangle=-\sum_{\mathbf{k=1}}^{S_N} P_{k,N}\ln P_{k,N}, \tag{10}$$

which in turn produces the information dimension D_I of the process

$$D_I=\frac{I_N}{\ln N}. \tag{11}$$

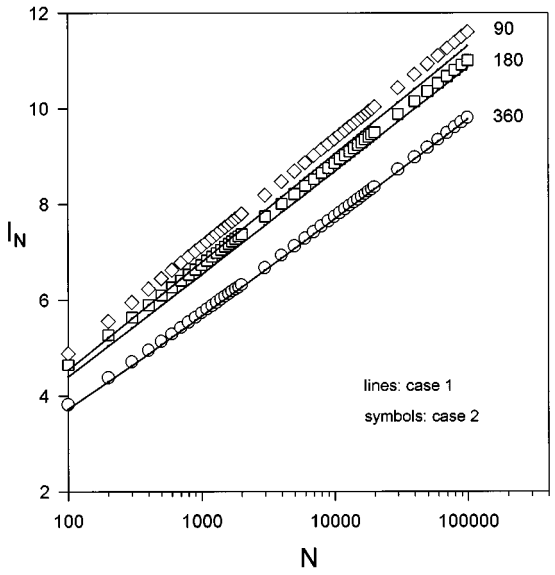

FIG. 6. $\langle I_N\rangle$ vs N (number of steps) for several different scattering angles θ, as marked. The lines pertain to case I, while the symbols to case II.

A plot of the $\langle I_N\rangle$ function vs time (number of steps) is given in Fig. 6, for both models, for uncorrelated and correlated walks. In this figure we observe a trend similar to the $\langle S_N\rangle$ behavior, as follows: (1) Case II data are always larger than case I, for the same reason as previously explained. (2) As correlation increases the entropy increases also. (3) The data in Fig. 6 give an almost linear relationship, but upon closer inspection one sees that there are more than one regimes. We consider, however, this latter point not to be in the interests of the present work, and we will not address it here any further. However, comparison with the same quantities for the lattice walks shows once again complete agreement between the two cases.

Another direct way of comparing the behavior of $\langle S_N\rangle$ for

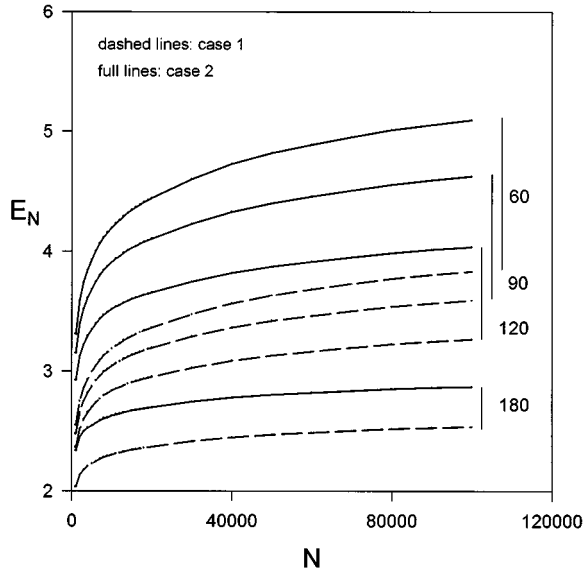

FIG. 7. The efficiency $\langle E_N\rangle$ vs N (number of steps) for several different scattering angles θ, as marked.

correlated walk in continuous space with that of uncorrelated random walk is to define the efficiency E_N as (similar to the definition of the lattice case)

$$E_N = \frac{\langle S_N \rangle_{\text{corr}}}{\langle S_N \rangle_{\text{uncorr}}}. \tag{12}$$

Figure 7 shows the data for E_N for various values of the correlation parameter θ. We observe a behavior similar to that in the lattice walks [5]. The number of boxes visited increases less strongly than the number of steps, due to the logarithmic correction in the denominator of Eq. 5. Thus, for small θ (large correlation) we have an effective proportionality of $\langle S_N \rangle$ with N, since a constant correction term appears in the denominator. Thus the ratio E_N increases with N. This is less visible in large values of θ, as expected.

IV. CONCLUSIONS

In the present work we extended the ideas on correlation processes from lattices to continuous space. The usual properties of random walks were calculated numerically and they were found to behave in an analogous way. Due to the nature of the process, correlation was introduced by the use of an algorithm that employes an angle θ that limits the direction of motion. This is a simple model borrowed from the polymer science for the construction of the algorithm that performs the correlated steps of the walk. It is found that the mean-square displacement initially increases faster, as a function of the correlation parameter, but after a certain time t_c the increase is the same, as uncorrelated walks. This shows that correlated walks, in the long time limit, belong to the same class of processes as the uncorrelated walks, only with different prefactors that denote the extent of correlation. This prefactor is derived similarly, as in the case of chain molecules, in Eq. (4), and it is valid in the long time limit. For the short time limit a crossover time t_c to the universal behavior is found. This crossover time also obeys a scaling relationship with the correlation parameter θ with an exponent $h=-1.88$. We conclude that from the simulation data we are able to provide simple formulae for the walk properties and the crossover behavior, and also provide the numerical values of the coefficients.

The visitation efficiency of the walk is described by the $\langle S_N \rangle$ and $\langle I_N \rangle$ properties, which were also calculated numerically in the simulation procedure. The results were compared to the equivalent properties in lattice walks and their correspondence was established. In all cases studied in the present work we found complete equivalence between the lattice walk and the continuous space walk, both for the uncorrelated and for the correlated case.

ACKNOWLEDGMENT

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