Self-avoiding random walkers with steps along eight possible directions (octopus walkers)

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Abstract: *Different types of random walkers are studied by assuming that they have eight different possibilities to make steps in pre-determined directions. The walkers are not allowed to step on already visited places in the plane (self-avoiding walkers). The main variables chosen to depict their behavior are the number of steps and the distance they reach before they are trapped. A measure of how the walkers are diffused, an index of how the paths of the walkers are folded and the effect of restricting the region where the walkers may walk are also studied.*

Key words: *random walkers, diffusion, octupus walkers, Brownian motion*

Resumo: *Diferentes tipos de caminhadas aleatórias são estudados assumindo que há oito diferentes possibilidades para caminhar em direções pré-determinadas. Aos caminhantes não é permitido andar em lugares já visitados no plano (caminhantes auto-controlados). As principais variáveis escolhidas para descrever seu comportamento são o número de passos e a distância que eles alcançam antes de serem capturados. Uma medida da difusão, um índice de como as suas trajetórias são desdobradas e o efeito de restringir a região onde eles podem andar também são estudados.*

Palavras-chave: *caminhadas aleatórias, difusão, caminhantes* octupus*, movimento browniano*

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1 Introduction

Random walkers have been, and still are, a very powerful tool in pure and applied mathematics to study problems in physics, chemistry and biology in general [1, 2, 3]. Diverse aspects of the configuration and structure of polymer have also successfully used self-avoiding random walkers. In general the studies are based upon walkers which can choose at random among four possible orthogonal directions [4, 5, 6]. The purpose of the present study is to present results from numerical experiments of self-avoiding random walkers who have additional possibilities to choose in order to make a new step.

2 The octopus walker

It is defined as a walker who may take steps in eight different directions, each one of them inclined at an angle of 45^o with respect to the neighboring directions. One of these directions is chosen at random in order to take a step. The possibilities, set as initial conditions for any site in space, for any time and for every walker, sketched in figure 1, are the following: *p(1)* (in the East direction), *p(2)* (North-East), *p(3)* (North), *p(4)* (North-West), *p(5)* (West), *p(6)* (South-West), *p(7)* (South) and *p(8)* (in the South-East direction), with the condition that

$$\sum_{I=1}^{8} p(I) = 1 \tag{1}$$

The length of each step is equal to unity in directions $I = 1, 3, 5$ and 7, and equal to $\sqrt{2}$ for $I = 2, 4, 6$ and 8.

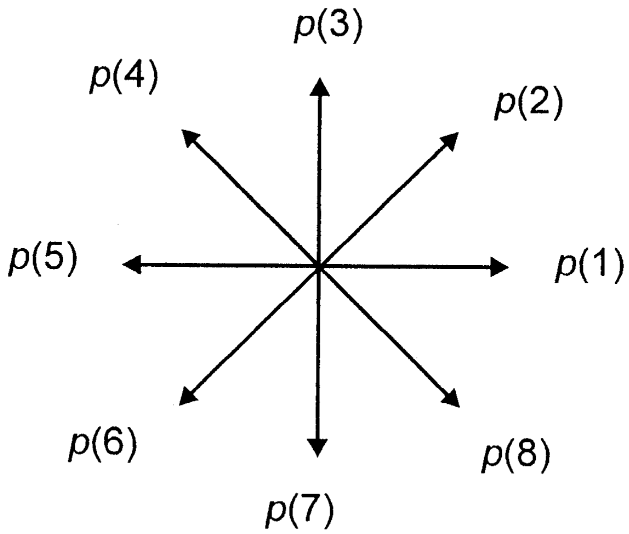

Figure 1. The eight possible directions the octopus walker may take during one of his steps, according with the possibilities, $p(I)$, with I =1 to 8, assigned to each of the directions. The length of steps is either unity or $\sqrt{2}$.

The plane where the walker roams is a grid composed of square cells of sides equal to unity. There are J_F cells along the horizontal and K_F cells along the vertical frontiers of the region, and walks start at the geometrical center of the lattice. A single step always consists of a displacement from the current lattice site to one of the eight nearest-neighbor cells. A periodic boundary condition is set to the space, thus transforming the plane into a torus. However, in the first part of this study the space is sufficiently large so that walkers never reach the boundaries. In the second part of the study we will reduce the size of the space in order to see the effect of confinement.

3 Self-avoiding walkers

Provided a random walker is given enough time, and with the characteristics pointed out in the above paragraphs, he will step on each and every cell of the region, no matter its dimensions. With this eternal walk, some of the sites may be visited more than once (overlapping). In order to limit this capacity to walk forever we will impose to the walker the condition that he will never step on a cell already visited.

When the walker decides to make a new step, he looks for all the free sites surrounding him; he apportions the possibilities he has been assigned to (as initial conditions) among the free neighboring sites and chooses one of them at random. If he fails to find a free site, it is considered that he has been trapped and, therefore, his random walk is terminated.

If we denote with (J_0, K_0) and (J_i, K_i) the initial and final positions of the walker, respectively, the distance reached when he is trapped is

$$D_i = \sqrt{(J_i - J_0)^2 + (K_i - K_0)^2} \tag{2}$$

When one walker has ended his walk, the number of steps, NS_i , and the distance, D_i , are recorded. The grid is cleared and a new walk starts. When a certain number of walkers, NW, have been studied, a mean number of steps, NS_{mean}, and a mean distance, D_{mean}, are computed as

$$NS_{\text{mean}} = \frac{1}{NW} \sum_{i=1}^{NW} NS_i \quad \text{and} \quad D_{\text{mean}} = \frac{1}{NW} \sum_{i=1}^{NW} D_i \tag{3}$$

In all our numerical experiments we have taken $NW = 10000$ random octopus walkers in order to have reasonable mean results.

4 Possibility p(3) chosen as the independent variable

When any of the possibilities $p(I)$ prevail with respect to the rest, the mean orientation of the random walk will be in that particular direction. However, the introductory nature of the notes we are dealing with should start with a more basic study: We will use the possibility $p(3)$ as an independent variable in order to study the properties of the octopus walker. The rest of possibilities will be given by

$$p(1) = p(3) = p(5) = p(7) \tag{4}$$

and

$$p(2) = p(4) = p(6) = p(8) = \frac{1 - 4p(3)}{4} \tag{5}$$

When $p(3) = 0.25$, from the above equations, then $p(1) = p(5) = p(7) = 0.25$, and $p(2) = p(4) = p(6) = p(8) = 0$. The random walkers taking steps with these possibilities will be herein called "cross walkers"; these walkers were the ones studied by Hemmer and Hemmer [4]. The literature on this subject deals in general with cross walkers [7]; many variations on this matter may be found in 1. When $p(3) = 0$, then $p(1) = p(5) = p(7) = 0$, and $p(2) = p(4) = p(6) = p(8) = 0.25$. These walkers will be herein called "diagonal walkers". For any other value of $p(3)$ in the range $0 < p(3) < 0.25$ the random walker will be of the octopus type.

5 Mean behavior of a large number of walkers

An example case of the type of results we will be dealing with is the number of steps, NS_i, performed by each of the $NW = 10000$ self-avoiding octopus random walkers, all of them with $p(3) = 0.125$. Equation (4) and (5) give the same possibilities for the rest of directions. Figure 2 gives the results of the probabilistic distribution of NS_i; this typical example shows that the number of steps may be found in the range, $NS_{\min} \leq NS_i \leq NS_{\max}$; for this particular case we have found $NS_{\min} = 9$ and $NS_{\max} = 1528$, with a mean value of $NS_{\text{mean}} = 213.91$.

Noteworthy are four facts:

a) the relatively high dispersion of the number of steps, if compared with the mean;

b) NS_{mean} is greater that the number of steps of maximum frequency, $NS_{\max\,\text{freq}}$;

c) the condition that $NS_{\text{mean}}/NS_{\max\,\text{freq}} \approx 2$; and

d) the distribution of probabilities is far from smooth, denoted by the presence of peaks and valleys.

These properties are common to all frequency distributions of the number of steps for any value of $p(3)$ in the range $0 \leq p(3) \leq 0.25$. Hemmer and Hemmer [4] show a similar frequency distribution of NS_i for $p(3) = 0.25$ (the cross walker). Their results are $NS_{\text{mean}} = 70.7 \pm 0.2$ and $D_{\text{mean}} = 11.87 \pm 0.05$, for $NW = 60000$ random cross walkers; they found $NS_{\max\,\text{freq}} = 33$, i.e., $NS_{\text{mean}}/NS_{\max\,\text{freq}} \approx 2.1$. Our numerical results for this particular case are $NS_{\text{mean}} = 70.93$ and $D_{\text{mean}} = 11.95$, with $NS_{\max\,\text{freq}} = 35$, i.e., $NS_{\text{mean}}/NS_{\max\,\text{freq}} \approx 2.0$. Except for small differences, most likely due to the random nature of the phenomenon, both results may be considered as equal.

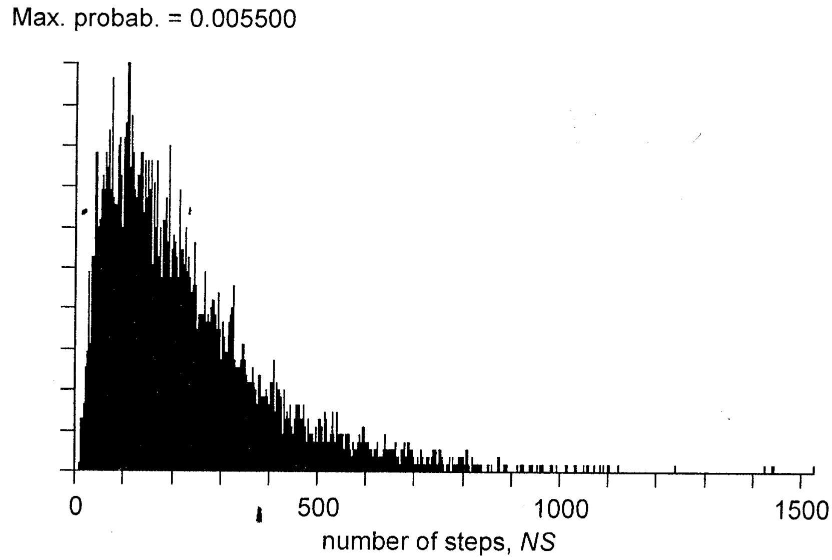

Figure 2 - Probability distribution of the number of steps, NS_i, for $i = 1, 2, 3, \ldots, NW$, performed by $NW = 10000$ self-avoiding random walkers, resulting from a particular numerical experiment in which the possibilities for choosing directions, set as initial conditions, are: $p(I) = 1/8$, for $I = 1$ through 8. Note that some of the walkers are trapped with a few steps, while others require nearly 1500 steps. Also notice that the probability distribution is far from smooth. The mean value of steps, NS_{mean}, for this case is 213.9, about twice the number of steps of maximum frequency (107.5). Probability distributions similar to the one herein shown are obtained when $p(3)$ is varied according to the rules of Eqs. (4) and (5).

For the case of diagonal walkers, identified by $p(3) = 0$, we obviously found the same value for NS_{mean}, and $D_{\text{mean}} = 11.95\sqrt{2} = 16.90$. This means that cross walkers and diagonal walkers are the same type of self-avoiding walkers, except that distances are multiplied by $\sqrt{2}$ for the latter.

Frequency distributions of mean distances, as defined in Eq. (2), are similar to the one just presented.

We now turn our attention to the influence of $p(3)$ upon the mean number of steps and mean distances, i.e., the functions $NS_{\text{mean}} = f_{NS}[p(3)]$ and $D_{\text{mean}} = f_D[p(3)]$, in figures 3 and 4, respectively. Numerical results (represented with full circles) correspond to a lattice of $J_F = K_F = 800$; this region may be considered as infinite since no walker ever reached the boundaries.

We have just described the results at both ends of the functions, i.e., when $p(3) = 0$ and $p(3) = 0.25$. When we are in the range $0 < p(3) < 0.25$ (note that inequalities are "smaller than", and not "smaller or equal than") the values of NS_{mean} as well as those of D_{mean} are greater than those corresponding to $p(3) = 0$ or $p(3) = 0.25$.

This means that the octopus walker performs more steps and reaches longer distances when $0 < p(3) < 0.25$.

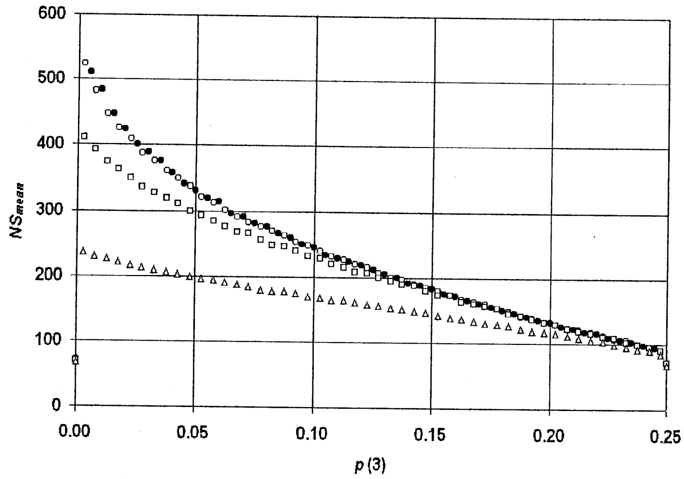

Figure 3. Mean number of steps, NS_{mean}, as a function of $p(3)$, for $NW = 10000$ random walkers. When $p(3)$ is equal to $1/4$ or zero, cross and diagonal walkers, respectively, $NS_{\text{mean}} \simeq 71$ steps. When $p(3)$ is in the range $0 < p(3) < 1/4$, NS_{mean} increases when $p(3)$ decreases. The results corresponding to an "unrestricted" region, $J_F = K_F = 800$ cells along the horizontal and vertical, respectively, are shown with full circles; in these cases none of the 10000 walkers has reached the frontiers of the region. When the region is restricted, the mean number of steps decreases for a constant $p(3)$; results are shown for $J_F = K_F = 100$ (open circles), 50 (squares) and 25 (triangles); in these cases a torus-like shape is given to the region and a periodic boundary condition is set. The decrease of NS_{mean} may be attributed to the premature trapping of the walkers when he invades its own previous path. The same symbols for unrestricted or restricted regions are used in the rest of figure.

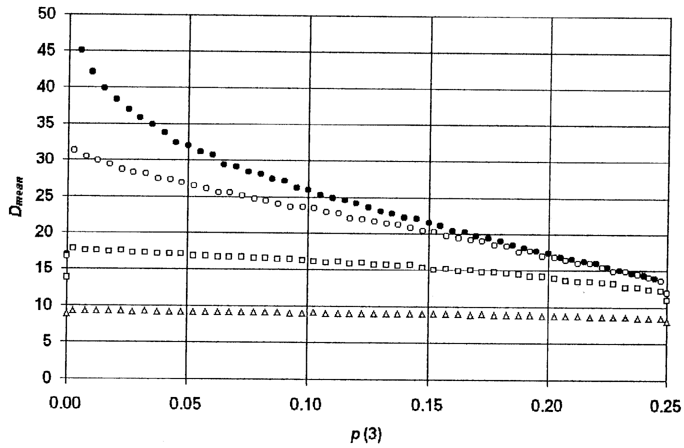

Figure 4. Same as in figure 3, in this case dealing with mean distances D_{mean}; D_i is measured from the starting point of the random walk to its final position (where the octopus walker is trapped.)

The reason for this lies in the fact that he is able to cross its own path, thus opening new regions where he can ramble. The octopus walker postpones its own trapping. Neither cross walkers nor diagonal walkers are able to cross their paths.

It may be clearly seen that NS_{mean}, as well as D_{mean}, increase when $p(3)$ decreases.

With extremely low possibilities for the cross directions, namely $p(3) = p(1) = p(5) = p(7) = 0.000001$, and extremely high possibilities along the four diagonals, namely, $p(2) = p(4) = p(6) = p(8) = 0.249999$, we have an octopus walker with almost all its possibilities along the diagonals and a few, insignificant chances for cross steps. The number of steps increase from $NS_{\text{mean}} = 70.93$ (diagonal walker) to $NS_{\text{mean}} = 568.44$. Such small "perturbations" are sufficient to make an 8-fold increase in the mean number of steps. Mean distances also increase, from $D_{\text{mean}} = 16.91$ to $D_{\text{mean}} = 49.23$, i.e., almost three times greater.

It should be noticed the large dispersion of the number of steps; for the previous case of an octopus walker with small perturbations we found a maximum of $NS_{\text{max}} = 4877$ and a minimum of $NS_{\text{min}} = 27$; when the walker is purely in diagonal directions the results were $NS_{\text{max}} = 509$ and $NS_{\text{min}} = 7$.

We may have an approximate relation between $p(3)$ and mean values by means of

$$NS_{\text{mean}} \cong 474.08\, e^{-6.518 p(3)} \text{ and } D_{\text{mean}} \cong 40.81\, e^{-4.350 p(3)} \tag{6}$$

in the range $0.025 \leq p(3) \leq 0.249$.

5.1 A measure of the diffusion of the octopus walker

The self-avoiding random walker we are dealing with struggles to find a free site where he can step on and continue his walk; we may think of this effort as a "diffusion". Its measure, which could be based upon the ratio of the square of a distance and the number of steps he made to reach this distance, is given by

$$\nu = \frac{1}{2}\frac{1}{NW}\sum_{i=1}^{NW}\frac{D_i^2}{NS_i} \tag{7}$$

where D_i^2, from Eq. (2), is the squared displacement. If one step is assimilated to a unit of time, this coefficient has the dimensions of a kinematic viscosity in Fluid Mechanics.

Figure 5 (full circles) shows the function $\nu = f_\nu[p(3)]$ for an unlimited space with $J_F = K_F = 800$. It clearly shows the two-fold decrease in the coefficient when $p(3)$ goes from 0 to 0.25. The octopus walker who has the greatest capacity to diffuse himself is a diagonal walker with small components (small as they may be) along the cross directions. The walkers who have the smallest diffusion are the cross walkers, i.e., the most widely used in the current literature.

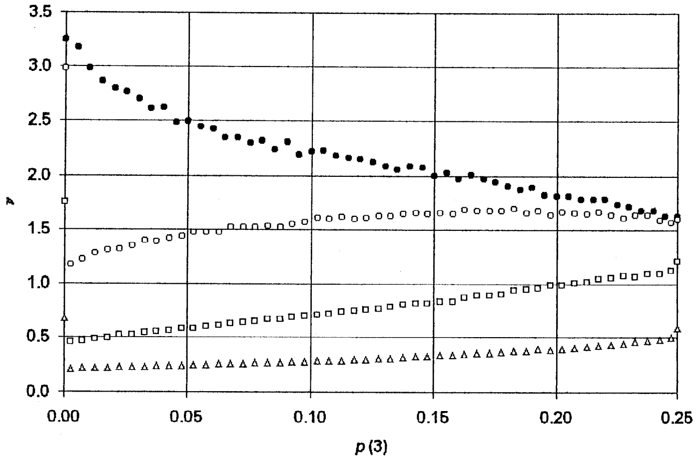

Figure 5. The ratio of a squared distance D_i^2 and the number of steps NS_i the octopus walker needed to reach its final position may be used as a measure of how the walker diffuses when he struggles to find a free site to step on. This figure shows how the measure of diffusion, [illegible], given in Eq. (7), varies in the range $0 \le p(3) \le 1/4$: [illegible] decreases when $p(3)$ increases in an otherwise unrestricted region. The opposite effect, i.e., [illegible] increases with $p(3)$, may be observed when the region allowed for the walker to ambulate is restricted.

5.2 Folding of the path of walkers

The visual aspect of the path of random walkers is in general a broken line in which, most of the times, it is impossible to distinguish its origin and its end. In order to have a measure of how twisted a path is, we may define an index of folding by

$$I_{fo} = 1 - \frac{1}{NW} \sum_{i=1}^{NW} \frac{D_i}{D_{i,s}} \tag{8}$$

where D_i is the distance from the origin to the end of the path, as mentioned above, and $D_{i,s}$ is the "stretched distance", i.e., the sum of all steps of unit length and those of length $\sqrt{2}$. $I_{fo} = 0$ means a walker without folding; this case is highly improbable since his path is a straight line. $I_{fo} = 1$ is a case (impossible event due to the condition of self-avoidance) in which there is a perfect or complete folding.

Figure 6 represents the numerical results for the function $I_{fo} = f[p(3)]$. They show that, for a pure diagonal walker, with $p(3) = 0$, $I_{fo} = 0.832$; however, when $p(3)$ is slightly greater than zero, for instance $p(3) = 0.005$, the index of folding increases to $I_{fo} = 0.937$. When $p(3)$ increases towards 0.25, I_{fo} decreases smoothly to its minimum, which corresponds to $I_{fo} = 0.832$ for $p(3) = 0.25$. The lowest folding is for the pure diagonal and for pure cross walkers, while the highest folding come from an octopus walker with most of its probabilities along the diagonal directions and very low chances along the cross directions.

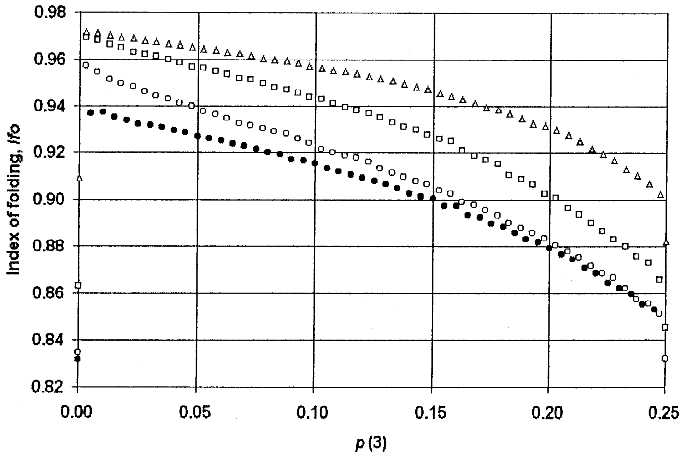

Figure 6. The distance D_i referred to the "stretched" distance $D_{i,s}$ (i.e., the sum of all steps of unit length plus those of length $\sqrt{2}$), leads to the definition of I_{fo}, a coefficient of folding given in Eq. (8); it measures how wrinkled the path of the walker is. This figure shows how I_{fo} varies with $p(3)$.

Based upon probability distributions of the number of steps for walkers with and without the condition of self-avoidance, Hemmer [8] has proposed

$$I_{fo} = 1 - \sqrt{\frac{2}{NS_{\text{mean}}}} \tag{9}$$

which fits more than reasonably well with numerical experiments, even for the extremes of the curve at $p(3) = 0$ and $p(3) = 0.25$.

5.3 Entropy

The probabilities of the distances reached by each walker and the number of steps they make to reach that distance can be used to compute their entropies. We have analyzed how they behave with $p(3)$ but they do not show significant variations. Suffice to say that entropies for the number of steps and for distances are almost constant (of the order of 0.80 and 0.65, respectively). Though the study of chaoticity goes beyond the scope of the present study, the existence of particular values of $p(3)$ with peaks of order and disorder can not be disregarded at the present moment.

5.4 Confinement of octopus walkers

It has already been pointed out that all octopus walkers as yet studied could walk freely along an unlimited region, without ever reaching its boundaries; this condition was satisfied with a plane composed of $J_F = K_F = 800$ cells. However, some of the octopii may reach one of the four boundaries when the space is restricted and, therefore, due to the torus-like shape of the region, the octopus may invade its own previous path. The limitation of space may cause his premature trapping. This is clearly seen in figure 3 with open triangles when the space is reduced to $J_F = K_F = 25$. However, even with such a small place to walk around, the increase of NS_{min} with the decrease of $p(3)$ is still noticeable. A torus with $J_F = K_F = 100$ (open circles in figure 3), much smaller than 800 (full circles), show almost the same function $NS_{\mathrm{mean}} = f_{NS}[p(3)]$.

Figure 4 shows the results of confinement for the function $D_{\mathrm{mean}} = f_D[p(3)]$; its general behavior is similar to the one just seen, though the effects of reducing the size of the region are more pronounced. In this respect, note that for $J_F = K_F = 25$, D_{mean} is independent of $p(3)$ and equal to about 9 units.

It was shown before in figure 5 with full circles that [illegible] decreases when $p(3)$ increases from 0 to 0.25, when the octopus walker has an unlimited region to walk. Open circles, squares and triangles in figure 5 show the effect of confinement upon [illegible] with the opposite behavior: diffusion increases when $p(3)$ increases and when the available space to roam is restricted.

Restriction of the area causes an increase in the index of folding, as shown in figure 6.

5.5 The octopus walker without the condition of self-avoidance

This paper contains information, mainly about NS_{mean} and D_{mean}, of an octopus walking until he is trapped in his own path. If we eliminate the condition of self-avoidance, for the number of steps limited by Eq. (6), the distance reached, D^{*}_{mean}, is smaller than D_{mean}. An approximate value is $D^{*}_{\mathrm{mean}}/D_{\mathrm{mean}} \approx 0.7$ for the range $0.005 < p(3) < 0.25$.

The index of folding for octopus walkers without self-avoidance is slightly greater (by a factor of 1.02) than those with self-avoidance in the vicinity of $p(3) = 0$; for $p(3)$ near 0.25 the factor increases to 1.05. For both ends of the curve, at $p(3) = 0$ and $p(3) = 0.25$, the factor is 1.08.

6 Conclusions

The behavior of random walkers which are not allowed to step on any site they have previously visited (self-avoiding random walkers) are studied by means of the number of steps they make before being trapped at some distance from the origin of their walks. Mean values of the number of steps and distances show that there is a wide variety of behaviors, depending upon the possibilities they have to choose one from eight different directions (octopus walkers). The common random walker has only four possible orthogonal directions, each one with equal chances to be chosen; under these circumstances he may last only 71 steps before being trapped. The main property of octopus random walkers is that they may last much more than that. With a suitable election of the eight possible directions it may take almost

600 steps. If the octopus walker is allowed to ambulate over a torus-like surface, he is prematurely trapped.

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