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Self-directed walk: a Monte Carlo study in three dimensions

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Abstract. The self-directed walk is studied in three dimensions. Monte Carlo simulations on the simple cubic lattice provide an estimate of the radius of gyration exponent $\nu = 0.67 \pm 0.01$ in agreement with our recent Flory-like theory leading to $\nu = 2/d$ when $2 \leqslant d \leqslant 4$.

1. Introduction

In a recent work (Turban and Debierre 1987, hereafter referred to as I) we introduced a new type of growing random walk in which the walker is allowed to jump with the same probability in any direction where the path is open. An open path is defined as a lattice direction in which no site has already been visited by the walker. The probability of an allowed step i is

$$p_i = 1/\text{number of open paths}. \tag{1.1}$$

This walk is self-avoiding and indefinitely growing since the walker is always at least allowed to continue in the direction of the last step.

In two dimensions, the walk is built up of long directed parts, the radius of gyration exponent $\nu = 1$ so that we called it the self-directed walk (SDW). In I a self-consistent Flory-type argument was developed, similar to that used for the true self-avoiding walk (Pietronero 1983), leading to the following values of the radius of gyration exponent:

$$\begin{aligned} \nu &= 1 && 1 \leqslant d \leqslant 2 \\ \nu &= 2/d && 2 \leqslant d \leqslant 4 \\ \nu &= 1/2 && d \geqslant 4. \end{aligned} \tag{1.2}$$

The upper critical dimension is $d_c = 4$ and $\nu = 1$ at and below two dimensions, a result which is in agreement with our 2D simulations.

The purpose of the present work is to test the 3D prediction $\nu = \frac{2}{3}$. In § 2 the Monte Carlo procedure used to grow the SDW is described and the numerical results are presented and discussed in § 3.

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2. The Monte Carlo procedure

The Monte Carlo method which is used to grow the SDW has been presented in I. The walks are generated on a $180 \times 180 \times 180$ simple cubic lattice. At each step N, the radius of gyration

$$R_g^2(N) = \frac{1}{N^2} \sum_{i<j} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2 \tag{2.1}$$

is stored. A step is chosen at random from among the five possible directions since a backstep is forbidden. When a site has been visited in the chosen direction, the jump is rejected and a new one is attempted. In order to spare computer time, one stores for each direction the maximum and minimum coordinates of the visited sites. Walks of up to 600 steps were generated. The value of the radius of gyration was averaged over 10 000 samples. For larger N values the statistics is affected by finite-size effects since the more extended walks which are larger than the cubic box are systematically eliminated. For $N = 600$ this occurs only for 1% of the walks and one has to go down to N around 400 to keep the 10 000 walks inside the box. The three projections of a typical SDW are shown on figure 1.

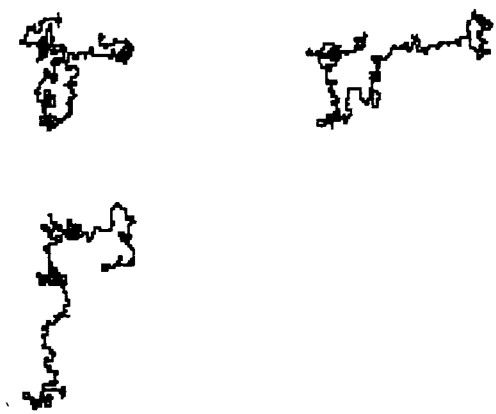

Figure 1. Projections of a typical SDW of 900 steps on the simple cubic lattice.

3. Numerical results and discussion

The radius of gyration is expected to grow with N like

$$\langle R_g^2(N) \rangle = AN^{2\nu}(1 + BN^{-\Delta} + CN^{-1} + \ldots) \tag{3.1}$$

where Δ is a non-analytic correction to scaling exponent and the last term is the analytic correction.

Figure 2 gives a plot of $\frac{1}{2}\ln\langle R_g^2(N)\rangle$ against $\ln(N)$, where the slope of the broken line corresponds to $\nu = 0.67$. The exponent ν is estimated using (Lyklema 1986)

$$\nu(N) = \tfrac{1}{2}\ln(\langle R_g^2(N+i)\rangle / \langle R_g^2(N-i)\rangle) / \ln[(N+i)/(N-i)]. \tag{3.2}$$

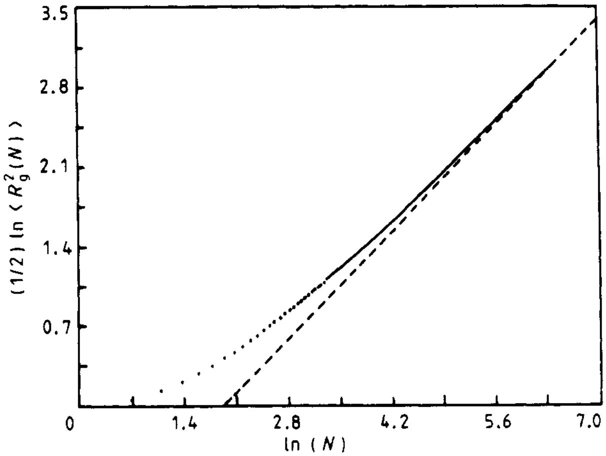

Figure 2. Plot of $\frac{1}{2}\ln\langle R_g^2(N)\rangle$ against $\ln(N)$. The broken line has a slope $\nu = 0.67$.

The results are shown on figure 3 with $i = 10$. Equations (3.1) and (3.2) lead to the following corrections to scaling:

$$\nu(N) = \nu - \tfrac{1}{2}B\Delta N^{-\Delta} - \tfrac{1}{2}CN^{-1} + \ldots \tag{3.3}$$

but the statistical fluctuations for large N values are too large to detect an eventual non-analytic correction term. The results were fitted by assuming that the leading correction is the analytic one (i.e. equation (3.3) with $B = 0$).

A least-squares fit of $\nu(N)$ against N^{-1} in the range $N = 30$-600 gives

$$\nu = 0.666 \pm 0.010 \tag{3.4}$$

where the error indicated is the RMS deviation. When the fit is restricted to the range $N = 30$-480 where the statistical fluctuations are not so large one obtains

$$\nu = 0.672 \pm 0.009 \tag{3.5}$$

in good agreement with the preceding estimate. The coefficient of the N^{-1} correction is

$$C = 8.0 \pm 0.8. \tag{3.6}$$

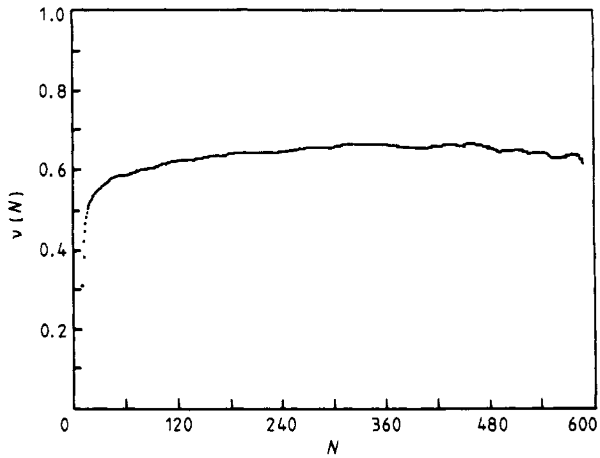

Figure 3. Plot of $\nu(N)$ against N for $i = 10$.

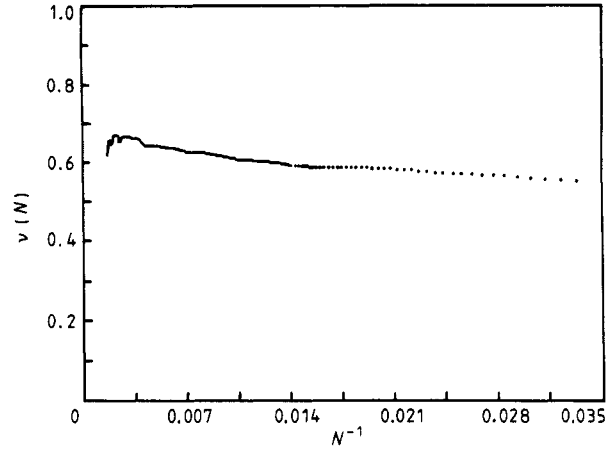

Figure 4. Plot of $\nu(N)$ against N for $i = 10$ and $N = 30$–600.

A plot of $\nu(N)$ against N^{-1} is given in figure 4 for $N = 30$–600. The amplitude A has been obtained through a least-squares fit of $N^{-2\nu}\langle R_g^2(N)\rangle$ against N^{-1}:

$$A = 0.0816 \pm 0.0004. \tag{3.7}$$

The main result of this study is the confirmation of the self-consistent theory for the self-directed walk proposed in I. The predicted value $\nu = \frac{2}{3}$ is quite close to the numerical result $\nu = 0.67 \pm 0.01$.

Finally let us mention that the SDW may also be viewed as a ballistic particle cluster linear aggregation process in which the particles are launched at random along the three principal lattice directions and stick only when they hit the tip of the chain.

References

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