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LETTER TO THE EDITOR

Spiral growing self-avoiding walk: A new universality class

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Abstract. We introduce the concept of a spiral growing self-avoiding walk (SGSAW) by imposing Privman's spiralling constraint on the growing self-avoiding walk introduced by Majid *et al* and Lyklema and Kremer. We study the critical properties of the SGSAW using Monte Carlo simulation. The exponent ν associated with the average radius of gyration, $\langle S_N \rangle$, is 0.8. On the other hand, the critical exponent ν_R associated with the end-to-end distance, $\langle R_N \rangle$, is much less than ν. The latter is in sharp contrast to the result $\nu = \nu_R$ for the usual SAW. Directed GSAWs are shown to behave like directed usual SAWs.

Recent advances in the theory of self-avoiding walks (SAW) have taken place along two complementary lines. Firstly, the underlying mysteries of usual SAW (USAW) have been unveiled and, secondly, several new types of SAW, for example directed SAW (Chakrabarti and Manna 1983, Cardy 1983, Redner and Majid 1983, Szpilka 1983), spiral SAW (Privman 1983, Redner and de Arcangelis 1983, Joyce 1984, Blöte and Hilhorst 1984, Whittington 1984, Guttman and Wormald 1984), true SAW (Amit *et al* 1983, Obukhov and Peliti 1983, Pietronero 1983, Obukhov 1984, Family and Daoud 1984), growing SAW (Majid *et al* 1984, Lyklema and Kremer 1984), have been introduced. Some of these walks are yet to be realised experimentally. However, their study remains interesting and worthwhile because each of these walks exhibits universality. This letter is a step along the latter line of development.

It is usually believed that both the end-to-end distance, R_N, and the radius of gyration, S_N, of an N-step SAW exhibit identical critical behaviour. This has also been proved by Monte Carlo simulation of USAW (Rapaport 1985a, b). However, we shall show in this letter that for the new type of walk introduced here the exponents for R_N and S_N are quite different from each other. The exponent associated with S_N, rather than that associated with R_N, is a measure of the compactness of the walk.

Imposing a spiralling constraint (Privman 1983) on a USAW on a square lattice leads to a spiral SAW whose critical behaviour turns out to be quite different from that of the USAW. In this letter we show analogously that the imposition of the same spiralling constraint on a growing SAW (GSAW) on a square lattice leads to a critical behaviour different from those of both GSAW and sprial SAW. For obvious reasons, the new type of walk introduced in this letter will be called a spiral growing self-avoiding walk (SGSAW). Its critical behaviour is studied using Monte Carlo simulation of N-step walks up to $N = 100$ and averaging over a large number of configurations for each fixed value of N on a CDC Cyber 76 scalar computer.

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First we explain GSAW, the spiralling constraint and SGSAW in more detail. In a GSAW the walker distinguishes between the sites already visited and those not visited so far in choosing his next host site. Let us call the sites already visited the 'closed sites' (the doors of these hosts are closed to the walker) and those not already visited the 'open sites'. Then the probability, p_i, to jump onto the ith nearest-neighbour open site is given by $p_i = 1/(\text{number of nearest-neighbour open sites})$. However, if the walker falls into a trap where he is surrounded by closed sites the walk is to be terminated. Thus a GSAW apparently looks very similar to an USAW; in fact, the same configurations appear in both. However, USAW and GSAW have drastically different critical behaviours because of the difference in the statistics of the corresponding configurations. The spiralling constraint is a constraint on the bond angles—the walker can either proceed along the same direction as that of the preceding step or can take a left turn, but a right turn is forbidden. The imposition of the latter constraint on the GSAW on a square lattice leads to the SGSAW.

Now we summarise the method of computation. On a square lattice one of the four nearest neighbours of the current site is chosen randomly. If the site so chosen turns out to be one of the closed sites a new random number is called. This procedure takes the property of GSAW into account. Using this procedure we thus generate a large number of GSAW configurations (more than 10^5 configurations for each N up to $N = 160$). Then averaging the square of the end-to-end distance ρ_N^2 over all these configurations and assuming the simple scaling form

$$\langle \rho_N^2 \rangle \propto N^{2\nu_g} \tag{1}$$

for large N, we estimate $\nu_g = 0.67$ for GSAW. This value is in good agreement with $\nu_g = 0{\cdot}67$ obtained by Majid *et al* (1984) from Flory-type arguments as well as Monte Carlo simulation and also with $\nu_g = 0.68 \pm 0.01$ computed by Lyklema and Kremer (1984) from exact enumeration. Next, we impose the spiralling constraint on the GSAW. Moreover, the lattice sites are placed in a one-dimensional array by imposing a helical boundary condition on the square lattice. Each of the walks starts from the centre of the square and the distance of the end point of an N-step walk from the centre is measured in the same fashion as done by Pandey *et al* (1984) for a random walk on percolation clusters. For smaller walks (up to $N = 25$) 10^5 SGSAW configurations are generated for each N. For longer walks, we run the CDC Cyber computer for two hours of CP time for each N. Then we average the quantity of interest, namely the end-to-end distance squared, R_N^2, over all those configurations, thereby obtaining $\langle R_N^2 \rangle$. The radius of gyration, S_N, of any walk is defined by

$$S_N^2 = \sum_i (\boldsymbol{r}_i - \boldsymbol{r}_{\mathrm{CM}})^2$$

where $\boldsymbol{r}_i$ are the positions of the lattice sites visited by the walker in an N-step walk and $\boldsymbol{r}_{\mathrm{CM}}$ is the position of the corresponding centre of mass. The average $\langle S_N \rangle$ for given N is computed in a manner very similar to that followed for the computation of $\langle R_N^2 \rangle$, except that the lattice sites are placed in a square array and the distance is measured in the usual way rather than in the manner of Pandey *et al* (1984).

It is well known that getting a USAW of, say, $N = 100$ in Monte Carlo simulations is very difficult because of attrition. In the course of the present work we found it much easier to generate GSAW than an equal number of USAW of the same length N. On the other hand, generating a SGSAW takes much longer than a GSAW of the same

N. For example, only about 100 configurations of a SGSAW with $N = 100$ compared with 2×10^5 configurations of a GSAW of $N = 160$ could be generated in two hours of CP time. Because of the bad statistics of the data beyond $N = 80$ we present only the data up to $N = 80$ in this letter.

Now we come to the analysis of the data. If the average radius of gyration $\langle S_N \rangle$ were simply proportional to N^ν, the gradient of the plot of $\ln \langle S_N \rangle$ against $\ln N$ would give the magnitude of the exponent ν. However, our data could not be fitted satisfactorily to such a simple scaling form over the whole range of N investigated; the plot of $\ln \langle S_N \rangle$ against $\ln N$ turns out to be curved (see figure 1(a)). We believe that the deviation of $\langle S_N \rangle$ from linearity for smaller values of N arises from finite-N effects. Plotting the gradient $\nu(N)$ of the latter curve for various values of N against $1/N$ (figure 1(b)) and extrapolating to $1/N \to 0$, we get $\nu = 0.8$. However, the gradient ν_R of the plot of $\ln \langle R_N \rangle$ against $\ln N$ (see figure 1(a)) is much smaller than ν. It is well known (Rapaport 1985a, b) that $\nu = \nu_R$ for USAW. Figure 1(a) clearly demonstrates the breakdown of the latter equality for SGSAW, at least for the size range studied here.

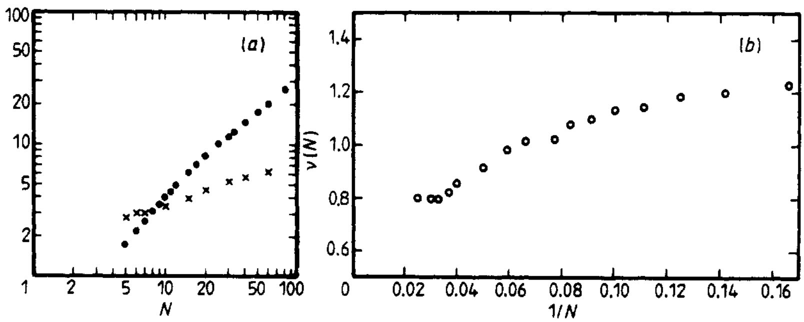

Figure 1. (a) Log-log plot of average radius of gyration, S_N (●), and the end-to-end distance, R_N (×), against the number of steps (N) of a SGSAW. The error bars for the data for all N are of the order of the symbol size, except for $N = 80$ where the error bar is twice as large. (b) Effective exponent $\nu(N)$ plotted against $1/N$.

We have also studied directed GSAW on a square lattice where the walker is allowed to move along both the $\pm x$ axes, but only along the $-y$ axis, motion along the $+y$ direction being forbidden. This walk is very similar to a directed SAW (Chakrabarti and Manna 1983); the directive contraint is imposed on USAW in the latter whereas the some constraint is imposed on GSAW in the former. The exponent ν of a directed GSAW turns out to be identical to that of a directed USAW, i.e., $\nu_x = \frac{1}{2}$ and $\nu_y = 1$. This equivalence arises because the motion along the y axis is nothing but a simple forward motion and that along the x axis is a simple unbiased random walk for the cases of both a directed SAW and a directed GSAW (Privman 1985).

In conclusion, we have introduced a new self-avoiding walk, namely the SGSAW, by imposing the spiralling constraint on the GSAW. Using Monte Carlo simulation, the SGSAW is shown to belong to a new universality class for which $\nu \neq \nu_R$.

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Note added in proof. Some error in our computation of the radius of gyration, S_N, came to our notice after the acceptance of this work for publication. However, the data for the end-to-end distance, R_N, were correct. First of all, now $\langle S_N\rangle < \langle R_N\rangle$ for all N investigated ($5 \leq N \leq 100$). Secondly, the correct slope of the $\ln\langle S_N\rangle$ against $\ln N$ curve is a decreasing function of N, with $\nu(N) \simeq 0.67$ at $N \simeq 5$ and $\simeq 0.38$ at $N \simeq 100$. Unfortunately, $N = 100$ seems to be not sufficiently large to reflect the true critical behaviour of SGSAW in the limit $N \to \infty$.

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