The winding angle of planar self-avoiding walks

1984 J. Phys. A: Math. Gen. 17 L569

(http://iopscience.iop.org/0305-4470/17/11/003)

J. Phys. A: Math. Gen. 17 (1984) L569–L578. Printed in Great Britain

LETTER TO THE EDITOR

The winding angle of planar self-avoiding walks

Michael E Fisher†, Vladimir Privman† and Sidney Redner‡

† Baker Laboratory, Cornell University, Ithaca, New York 14853, USA

‡ Department of Physics and Center for Polymer Studies, Boston University, Boston, Massachusetts 02215, USA

Received 25 April 1984

Abstract. The problem of understanding the asymptotic statistical behaviour of the winding angle, θ_N, of a self-avoiding walk of N steps on a planar lattice is posed. Exact series expansion data for the square lattice up to $N=21$ are reported. These data and Monte Carlo estimates up to $N \leq 170$ steps are fitted well by a logarithmic growth law for $\langle\theta_N^2\rangle$. The ratio $\langle\theta_N^4\rangle/\langle\theta_N^2\rangle^2$ appears to approach a limit of 2.9 to 3.2, which is close to the Gaussian value, 3. Heuristic scaling arguments are consistent with simple logarithmic growth (and also illuminate the logarithmic behaviour known rigorously for free Brownian motion).

In recent years there has been an increasing interest in the geometrical interpretation of cluster growth properties on space lattices. In both the 'classical' problems, such as percolation clusters, lattice animals, self-avoiding walks (see Stauffer 1981 and McKenzie 1972 for reviews), and in the newer class of dynamic aggregation models (see e.g. Stanley *et al* 1983), one usually studies the 'size' of an object as a function of the number N of constituent 'monomers'. The radius of gyration is the most natural measure of mean cluster size (see e.g. Peters *et al* 1979 and Grassberger 1982a); for self-avoiding walks an appropriate quantity is the root-mean-square end-to-origin distance of N-step walks, which grows asymptotically according to $R_N = \sqrt{\langle r_N^2\rangle} \sim N^{\nu}$, with, it is believed, $\nu = \frac{3}{4}$ in $d=2$ spatial dimensions (Nienhuis 1982).

In this note we consider another geometrical property of *two-dimensional* self-avoiding walks, namely, the *winding angle*, θ, measured with respect to the direction of the first step. It is convenient to introduce a polar coordinate system with the origin at the starting point of the walk and the positive x axis directed along the first step. On the nth step the walk arrives at (r_n, θ_n) and θ_n changes by increments, $\Delta\theta_n = \theta_n - \theta_{n-1}$, each less than $\frac{1}{2}\pi$ in magnitude. The final value after N steps, θ_N, may be positive or negative, and is unrestricted in magnitude. However, it is worth noting that for a *free* walk which does not revisit the origin on, say, the plane square lattice, $|\theta_N|$ is bounded by $\frac{1}{4}\pi N$ while for a self-avoiding walk one obtains a bound close to $\pi N^{1/2}$ (by considering a close-packed walk which spirals around the origin).

By symmetry, the odd moments $\langle\theta_N^{2k-1}\rangle$ $(k=1,2,3,\ldots)$ vanish identically. However, the even moments, $\langle\theta_N^{2k}\rangle$, are positive and their asymptotic behaviour is the focus of this note. In table 1 we list the values of $c_N\langle\theta_N^2\rangle$ and $c_N\langle\theta_N^4\rangle$ for $N \leq 21$ on the square lattice as found by direct enumeration of all walks by established methods (Redner 1982 and references therein). Here c_N is the total number of N-step self-avoiding walks, given by Sykes *et al* (1972); these are believed to vary asymptotically as

0305-4470/84/110569+10$02.25

Table 1. Values of $c_N\langle\theta_N^2\rangle\times10^{-k}$ and $c_N\langle\theta_N^4\rangle\times10^{-k}$ for the square lattice correct to 15 decimal places.

N	$\frac{1}{4}c_N\langle\theta_N^2\rangle$	k	$\frac{1}{4}c_N\langle\theta_N^4\rangle$	k
2	1.233 700 550 136 17	0	7.610 085 237 031 44	−1
3	8.246 235 188 499 53	0	1.536 604 804 392 36	1
4	2.964 908 275 147 87	1	9.397 021 962 112 68	1
5	1.105 575 468 731 20	2	4.887 465 204 442 50	2
6	3.441 587 467 011 97	2	1.843 647 644 022 20	3
7	1.119 881 129 856 37	3	7.220 567 962 561 04	3
8	3.301 262 906 043 03	3	2.385 130 875 731 57	4
9	1.002 157 092 174 98	4	7.953 307 275 941 86	4
10	2.882 014 071 486 29	4	2.483 969 437 085 23	5
11	8.424 207 855 257 78	4	7.697 343 548 208 59	5
12	2.383 894 186 066 11	5	2.316 247 352 743 40	6
13	6.812 280 327 107 98	5	6.902 367 602 289 42	6
14	1.905 714 518 863 43	6	2.024 231 697 584 31	7
15	5.366 500 290 277 61	6	5.890 711 369 044 07	7
16	1.488 506 221 881 86	7	1.696 477 942 983 41	8
17	4.148 659 638 543 12	7	4.857 467 697 099 09	8
18	1.143 283 847 346 96	8	1.380 625 805 079 22	9
19	3.162 262 736 780 55	8	3.906 657 682 640 31	9
20	8.670 491 624 998 57	8	1.099 412 605 153 97	10
21	2.384 214 713 678 27	9	3.083 171 262 458 56	10

$C_\infty N^{\gamma-1}\mu^N$ when $N\to\infty$, where

$$\mu\equiv 1/z_c\simeq 2.6381\pm0.0002 \qquad \text{and} \qquad \gamma=1\tfrac{11}{32}=1.34375 \tag{1}$$

(Guttmann 1984, Nienhuis 1982).

In analysing these data to estimate their asymptotic behaviour, it is natural, at first, to postulate a power law behaviour, say,

$$\langle\theta_N^{2k}\rangle\sim N^{\omega_k}, \tag{2}$$

since power laws characterise many properties of both free and restricted random walks. However, Spitzer (1958) has analysed rigorously the winding angle distribution of Brownian motion on the plane, in continuous time t: he proves that the cumulative probability distribution satisfies

$$\lim_{t\to\infty}\Pr[\theta(t)<\chi\ln t]=\pi^{-1}\int_{-\infty}^{2\chi}\mathrm{d}x/(1+x^2), \tag{3}$$

so that $\chi=\theta(t)/\ln t$ is described asymptotically by a Cauchy distribution. It follows that the moments $\langle|\theta(t)|^\lambda\rangle$ vary like $(\ln t)^\lambda$ although, owing to the long tail of the Cauchy distribution, they exist only for $|\lambda|<1$.

Although the behaviour of free random walks on a *lattice* seems not to have been answered analytically, Spitzer's result suggests that a purely logarithmic behaviour of the moments should be considered so that the exponents ω_k vanish. Indeed, if one contemplates some sort of real-space renormalisation group transformation, say of decimation type (see e.g. Shapiro 1978), being performed on a self-avoiding chain, one concludes that angular coordinates will rescale only as marginal variables since they remain unchanged under simple changes of length scale. This heuristic argument, which is supported by a more detailed scaling-type argument presented below, again suggests $\omega_k \equiv 0$ (all $k \geq 1$).

We have tested the conjecture (2) by studying the series $\langle\theta_N^2\rangle$ and $\langle\theta_N^4\rangle$ by the usual two-point-fit extrapolation and Padé approximant techniques. A clear downward trend of the exponent estimates, $\omega_k^{\text{eff}}(N)$, which represent *effective* exponents, is observed as N increases and a vanishing limit as $N \to \infty$ is indicated. A negative exponent, associated with *finite* limiting values, $\langle\theta_\infty^2\rangle$ and $\langle\theta_\infty^4\rangle$, seems somewhat implausible on physical grounds (see further below) and is also in contradiction with the steadily increasing values observed, particularly in the Monte Carlo simulations reported below which run up to $N \simeq 170$: see figure 1.

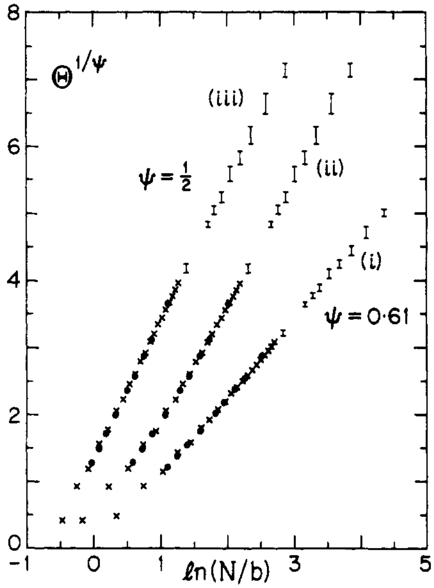

Figure 1. Plots suggesting that the mean square of the winding angle, θ_N, for self-avoiding walks of N steps on a square lattice is asymptotically proportional to $(\ln N)^{2\psi}$ with (i) $\psi \simeq 0.61$ or, (ii) and (iii), $\psi = \frac{1}{2}$. The exact enumeration data for $N = 2, 3, \ldots, 21$, with $\Theta^2 = \langle\theta_N^2\rangle$, are shown by crosses. The error limit symbols and full circles represent Monte Carlo results for $\Theta^2 = \overline{\theta^2}(z)$ from constant fugacity simulations which extend up to $\bar{N}(z) \leq 170$. The values selected for b are (i) 1.40, (ii) 2.35 and (iii) $2.35e \simeq 6.39$ with, in addition, N replaced by $N + 2$.

Accordingly, we have tested fits to the forms

$$\langle\theta_N^{2k}\rangle \approx a_k[\ln(N/b_k)]^{2k\psi_k}, \tag{4}$$

which are suggested by analogy with the Brownian motion results and which represent some of the simplest divergences weaker than a power law. Note that the parameter b_k is vital if a logarithmic form is contemplated; if $2k\psi_k$ is not close to unity one might wish also to add a 'background' term, say e_k, but this is not feasible for data analysis with a restricted range of data. (Corrections representable by replacing N by $N + n_0$ are also important for small N: see figure 1 and below.) Indeed, it is clear that in order to validate such a logarithmic growth law with reasonable certainty one really needs data over *several decades* of N. Nevertheless, we will demonstrate that the relation (4) for $k=1$ with ψ_1 and b_1 determined from the series data for $N \leqslant 21$ provides a very good fit to the Monte Carlo results up to $N \simeq 170$. Even so, it must be pointed out that the moments grow very slowly with N and, even for the longest walks simulated, we find $\langle\theta_N^2\rangle < \pi^2$. Thus we cannot rule out some qualitative change in behaviour setting in when a typical walk has a winding angle of order π at which stage one might be tempted to speculate that the angular self-avoiding constraint becomes more important: however, see the further theoretical discussion below.

With these reservations in mind, we report briefly on our procedure for fitting the data of table 1 to the logarithmic law (4). For a trial exponent value ψ we calculate

$$T_N^{(k)}(\psi) = \langle\theta_N^{2k}\rangle^{1/2k\psi} \approx A_k \ln(N/b_k), \tag{5}$$

where the expected variation indicated entails $A_k = a_k^{1/2k\psi}$. Then we form the approximants

$$A_k^{(N)}(\psi) \equiv (T_N - T_{N-2})/\ln[N/(N-2)], \tag{6}$$

$$B_k^{(N)}(\psi) \equiv [T_N \ln(N-2) - T_{N-2} \ln N]/\ln[N/(N-2)], \tag{7}$$

which should approach A_k and $B_k = A_k \ln b_k$, respectively, as $N \to \infty$. Note that the use of index $N-2$, in place of $N-1$, serves to cancel some of the odd–even oscillation present for both $k=1$ and 2; this is a general characteristic of configurational data for loose-packed lattices like the square lattice. Plots of $A_k^{(N)}(\psi)$ and of $B_k^{(N)}(\psi)$ against ψ for increasing values of N should both display intersections close to one definite value of ψ if the fits are consistent. Figure 2 shows how this analysis proceeds for

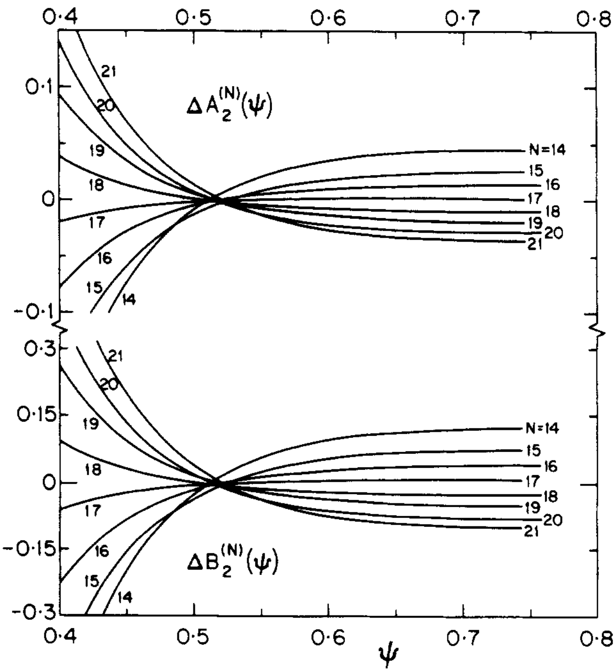

Figure 2. Plots of the fitting deviations, $\Delta A_2^{(N)}(\psi)$ and $\Delta B_2^{(N)}(\psi)$ (see equation (8)), for the mean fourth power of the winding angle for $N = 14$ to 21 in order to determine the optimum value of the exponent ψ_2 in the asymptotic form (4).

$\langle \theta_N^4 \rangle$ $(k=2)$. The range $N=14$ to 21 is displayed and, for sensitivity, the deviations

$$\Delta A_k^{(N)} = A_k^{(N)} - \bar{A}_k, \qquad \Delta B_k^{(N)} = B_k^{(N)} - \bar{B}_k, \tag{8}$$

are plotted where, for convenience, the mean values are defined by

$$\bar{A}_k(\psi) = \tfrac{1}{8} \sum_{N=14}^{21} A_k^{(N)}(\psi), \tag{9}$$

and, similarly, for $\bar{B}_k(\psi)$. These mean values vary strongly with ψ, decreasing monotonically and roughly exponentially with, e.g., $\bar{A}_2 \simeq 6.4$, $\bar{B}_2 \simeq 7.9$ at $\psi = 0.40$, and $\bar{A}_2 \simeq 0$, $\bar{B}_2 \simeq 1.3$ at $\psi = 0.72$.

The location of intersection regions of $\Delta A_2^{(N)}$ and $\Delta B_2^{(N)}$ in figure 2 appears to be internally consistent and suggests the exponent estimate

$$\psi_2 = 0.52 \pm 0.04, \tag{10}$$

where the confidence limits represent a necessarily somewhat subjective estimate based on the analyses described as well as on two-point fits of $\langle \theta_N^4 \rangle$ to the more primitive form $a(\ln N)^{2k\psi}$. In a study of the second moment series similar results are found. However, the spread of the intersection regions is somewhat larger and yields the estimate

$$\psi_1 = 0.61 \pm 0.07. \tag{11}$$

The corresponding coefficient estimates are not very precise: thus we quote only the central values,

$$b_1 \simeq 1.4 \qquad \text{and} \qquad b_2 \simeq 2.3. \tag{12}$$

Both these satisfy $b_k \ll 21$ so that there is a reasonable hope that the onset of asymptotic behaviour is visible in the data.

The estimates (10) and (11) do not exclude the possibility $\psi_1 = \psi_2$ which it is natural to expect on scaling grounds: on the contrary, they actually *suggest* the equality as the following argument shows!

Consider the 'dimensionless' ratio

$$\mathscr{R}_N^{(4)} = \langle \theta_N^4 \rangle / \langle \theta_N^2 \rangle^2. \tag{13}$$

By the Cauchy–Schwartz inequality this cannot be less than unity. Hence, if (4) is accepted with $\psi_1 > 0$ one must have $\psi_2 \geqslant \psi_1$. However, the estimates (10) and (11) alone would suggest the reverse inequality: hence *equality* seems likely. To test this we have examined the ratios, $\mathscr{R}_N^{(4)}$, directly. They pass through a maximum value of about 3.3 at $N=12$ and thereafter, allowing for a small, damped oscillation, decrease monotonically. Extrapolation against $1/N$ or $1/N^{1/2}$ suggests a limit satisfying

$$2.9 \leqslant \mathscr{R}_\infty^{(4)} \leqslant 3.2. \tag{14}$$

In the light of this estimate it is worth recalling that for a Gaussian distribution one has the exact result $\mathscr{R}_G^{(4)} = 3$. The apparent finiteness of $\mathscr{R}_\infty^{(4)}$ again supports the equality and the natural speculation

$$\psi_1 = \psi_2 = \tfrac{1}{2} \tag{15}$$

then seems quite plausible. The quality of the resultant fits for $\psi_1 = 0.50$ and 0.61 can be gauged from figure 1, which includes also the Monte Carlo data to be described below. Note that one should take $b_1 \simeq 2.35$ if one accepts $\psi_1 = \frac{1}{2}$. Plot (iii) in figure 1 embodies the shift from N to $N + n_0$ mentioned previously: see further below.

In order to probe the validity of the asymptotic relation (4) for higher values of N, a constant-fugacity Monte Carlo simulation was performed (Redner and Reynolds 1981, Redner unpublished). A grand ensemble of self-avoiding walks is generated with a constant fugacity, z, per step. Thus the number of steps of a given walk in the ensemble is not fixed, but the average value, $\bar{N}(z)$, should approach

$$N_0(z) = \sum_N c_N N z^N \Big/ \sum_N c_N z^N. \tag{16}$$

The reason for selecting this method of simulation lies in the delicate nature of the quantity being estimated. The variation of $\langle \theta_N^2 \rangle$ with N is sufficiently weak that any uncontrolled bias introduced into the simulation could easily yield seriously misleading results. On the other hand, some sort of systematic biasing procedures are necessary in order to extend a 'canonical' or fixed-N simulation to obtain samples with $N \gtrsim 100$. The constant fugacity approach has the advantage of being free of uncontrolled bias while being able to reach significantly larger values of N within a reasonable expenditure of computing time.

Now, when z increases towards the critical value $z_c = 1/\mu$ (see equation (1)) the ideal mean value behaves as

$$N_0(z) \approx \gamma z_c/(z_c - z). \tag{17}$$

In table 2 the observed values of $\bar{N}(z)$ are compared with this asymptotic prediction for $z \to z_c$. We conclude that the asymptotic form for $\bar{N}(z)$ suffices to describe the Monte Carlo data for $\bar{N} \gtrsim 20$. (Recall that $N = 21$ is the largest N value reached in the exact enumerations.)

In table 2 we also report the observed values of $\overline{\theta^2}(z)$ which should approach

$$\theta_0^2(z) = \sum_N c_N \langle \theta_N^2 \rangle z^N \Big/ \sum_N c_N z^N. \tag{18}$$

If one assumes the validity of the asymptotic expression (4) and approximates the sums by integrals one is led to

$$\theta_0^2(z) \approx a_1 [\ln(N_0/\tilde{b}_1)]^{2\psi_1}, \tag{19}$$

Table 2. Results of the Monte Carlo simulation at fugacity z for $\bar{N}(z)$ and $\overline{\theta^2}(z)$. The values displayed for $N_0(z)$ have been calculated from the *asymptotic form* (17) by using the values for z_c and γ given in (1).

z	$\bar{N}(z)$	$N_0(z)$	$\overline{\theta^2}(z)$	z	$\bar{N}(z)$	$N_0(z)$	$\overline{\theta^2}(z)$
0.300	5.09 ± 0.04	6.4	1.283 ± 0.016	0.365	34.7 ± 0.3	36.2	4.183 ± 0.068
0.310	6.00 ± 0.04	7.4	1.488 ± 0.015	0.369	49.0 ± 0.5	50.6	4.84 ± 0.04
0.320	7.28 ± 0.05	8.6	1.712 ± 0.014	0.370	54.8 ± 0.6	56.2	5.06 ± 0.06
0.330	8.95 ± 0.08	10.4	1.992 ± 0.008	0.371	61.3 ± 0.8	63.2	5.25 ± 0.08
0.340	11.63 ± 0.06	13.0	2.366 ± 0.019	0.372	70.4 ± 0.8	72.1	5.60 ± 0.11
0.345	13.44 ± 0.09	15.0	2.587 ± 0.024	0.373	82 ± 1	84.0	5.84 ± 0.10
0.350	16.1 ± 0.1	17.5	2.882 ± 0.035	0.374	100 ± 2	100.7	6.18 ± 0.12
0.354	18.9 ± 0.1	20.3	3.122 ± 0.036	0.375	121 ± 3	125.4	6.65 ± 0.15
0.360	25.1 ± 0.1	26.7	3.657 ± 0.042	0.376	163 ± 2	166.4	7.15 ± 0.10

as $z \to z_c$ (or $N_0 \to \infty$), where the leading corrections may be of relative order $1/(\ln N_0)^2$, while the modified scale is given by

$$\tilde{b}_1 = \gamma b_1 \exp[-\Gamma'(\gamma)/\Gamma(\gamma)], \tag{20}$$

in which $\Gamma(x)$ is the standard gamma function and the prime denotes differentiation.

Now the Monte Carlo data may be compared usefully with the exact enumeration results as shown in figure 1. For the latter $\langle \theta_N^2 \rangle^{1/2\psi}$ is plotted against $\ln(N/b)$ for $N = 2, 3, \ldots, 21$ with (i) ψ taken as the central estimate $\psi_1 = 0.61$, from (11), and $b = b_1 = 1.4$, from (12), and, (ii) with $\psi = \frac{1}{2}$ and $b = 2.35$. The first choice yields a plot which is close to linear for $N \geq 5$ while, to graphical accuracy, the choice $\psi = \frac{1}{2}$ yields linearity only for $N \geq 9$. The Monte Carlo data have been represented in similar fashion but with $\langle \theta_N^2 \rangle$ replaced by $\overline{\theta^2}(z)$, N replaced by the asymptotic form (17) for $N_0(z)$, and b set equal to $\tilde{b}_1$ as given by (20). The Monte Carlo results track the exact enumeration data, as far as they go, surprisingly well. For higher values of $N \sim N_0$ they display no significant deviation from a straight line with the assignment $\psi = 0.61$ and, at most, suggest only a slight upward curvature with $\psi = \frac{1}{2}$. Thus it appears that the second moment of the winding angle is well described by a logarithmic growth law at least up to $N \leq 170$.

As a further check on the plausibility of the simple value $\psi_1 = \frac{1}{2}$ in the relation (4), we have allowed, in plot (iii) on figure 1, for a shift in the value of N to $N + n_0$: by scanning one discovers that $n_0 = 2$ yields a remarkably linear plot for the full accessible range of N! (For consistency, the shift in the Monte Carlo data is made by adding $\tilde{n}_0 = n_0 \tilde{b}_1 / b_1$ to $N_0(z)$; to avoid overlap of the plots, the value of b_1 has been replaced by $b_1 \mathrm{e}$, which merely results in a shift of unity along the horizontal axis.)

We present, finally, some heuristic considerations which, we believe, throw light on the observed logarithmic behaviour of $\Theta_N^2 \equiv \langle \theta_N^2 \rangle$ and which support the conjecture $\psi_1 = \frac{1}{2}$. Let

$$\boldsymbol{r}_n \equiv (r_n, \theta_n) = \sum_{m=1}^{n} \boldsymbol{s}_m, \tag{21}$$

be the position vector after n steps in a walk of a total of N steps and let $\boldsymbol{s}_m$, with $|\boldsymbol{s}_m| = a$, be the nearest-neighbour step vector which brings the walk to $\boldsymbol{r}_m$. If $R_N^2 \equiv \langle r_N^2 \rangle$ is the square end-to-end distance averaged over all allowed walks, one then has

$$\Delta R_N^2 \equiv R_N^2 - R_{N-1}^2 = a^2 \left[1 + 2 \sum_{l=1}^{N-1} g_N^s(l) \right], \tag{22}$$

where the step–step correlation function is defined by

$$g_N^s(l) = \langle \boldsymbol{s}_N \cdot \boldsymbol{s}_{N-l} \rangle / \langle \boldsymbol{s}_N^2 \rangle. \tag{23}$$

If ρ_n and τ_n are the *radial* and *tangential* components of the (reduced) step vector $\boldsymbol{s}_n / a$, this may be rewritten as

$$g_N^s(l) = \langle \rho_N \rho_{N-l} \rangle + \langle \tau_N \tau_{N-l} \rangle \equiv g_N^\rho(l) + g_N^\tau(l). \tag{24}$$

In a free (or unrestricted) random walk one has $g_N^s(l) \equiv 0$ for $l \geq 1$ and the standard result $R_N^2 \approx AN$ (or $\nu = \frac{1}{2}$) then follows immediately from (22). More generally, in a walk with only short-range restrictions which, e.g., allow self-intersections provided any polygons formed are of order exceeding k (Fisher and Sykes 1959), the correlations will decay exponentially with l so that the sum in (22) remains bounded as $N \to \infty$; consequently, $\nu = \frac{1}{2}$ again follows. On the other hand, in a self-avoiding walk with

$\frac{1}{2} < \nu < 1$ the step–step correlation function must decay more slowly; however, a long walk forgets its origin eventually so that one expects $g_N^s(l)$ to approach a definite limit for fixed l as $N \to \infty$. A natural ansatz is thus

$$g_N^s(l) \approx G/l^\sigma, \qquad \text{as } N \to \infty, \tag{25}$$

where G is a positive constant or, more realistically, a *scaling function*, $G(w)$, of argument $w = l/N$. If this is accepted, the sum in (22) dominates when $\sigma \leq 1$ and, for consistency, one must have

$$\sigma = 2(1-\nu); \tag{26}$$

then $\sigma = \frac{1}{2}$ if $\nu = \frac{3}{4}$ is correct (Nienhuis 1982).

Now the separate radial and tangential correlation functions, $g_N^\rho(l)$ and $g_N^\tau(l)$ in (24), are unlikely to be equal (since the statistics of sub-classes of walk will depend on the winding angle). Nonetheless it seems plausible that both will exhibit similar scaling behaviour with, moreover, the *same* exponent $\sigma_\rho = \sigma_\tau = 2(1-\nu)$. Even should this equality fail, however, it seems *unlikely* that one could have $\sigma_\tau < 2(1-\nu)$ since that would imply a cancellation between $g_N^\rho(l)$ and $g_N^\tau(l)$ in the sum yielding $g_N^s(l)$.

Let us now explore a similar line of reasoning for the mean square winding angle $\Theta_N^2 \equiv \langle \theta_N^2 \rangle$. We have, as before,

$$\Delta\Theta_N^2 \equiv \Theta_N^2 - \Theta_{N-1}^2 = \langle \Delta\theta_N^2 \rangle + 2 \sum_{l=1}^{N-1} g_N^\theta(l), \tag{27}$$

where the angular correlation function is

$$g_N^\theta(l) = \langle \Delta\theta_N \Delta\theta_{N-l} \rangle. \tag{28}$$

Note also that when $r_n \geq 3a$ one has, to good precision,

$$\Delta\theta_n \simeq \tau_n a / r_n, \tag{29}$$

where $a\tau_n$ is the tangential step component; the bound $|\Delta\theta_n| \leq a/r_n$ follows.

Owing to the 'mismatch' between a polar coordinate system and a translationally invariant lattice, the angular correlation function does not, in general, vanish even for a free walk. However, it should decay exponentially rapidly for any walk with restrictions of finite range. In that case the behaviour of $\Delta\Theta_N^2$ should be dominated by $\langle \Delta\theta_N^2 \rangle$ which, recalling (29), should be close to $c\langle a^2/r_N^2 \rangle$ with, roughly, $c \simeq \frac{1}{2}$. Now, accepting asymptotic Gaussian behaviour for a free walk we can write

$$\left\langle \frac{a^2}{r_N^2} \right\rangle \approx \int_a^\infty \frac{2\pi r\, \mathrm{d}r}{r^2} \frac{\exp(-\frac{1}{2}r^2/Na^2)}{2\pi N} = \tfrac{1}{2}N^{-1}\ln(2N/e_{\mathrm{E}}) + \mathrm{O}(N^{-2}), \tag{30}$$

where the lattice structure has been recognised by the imposition of a lower cut-off: this evidently dominates the behaviour for large N. Note that $\ln e_{\mathrm{E}} \simeq 0.5772$ is Euler's constant although the true coefficient here will be sensitive to the exact form of lattice cut-off. If one accepts (30) as characterising the behaviour of $\langle \Delta\theta_N^2 \rangle$ one concludes, via (27), that

$$\Theta_N^2 \approx a_0[\ln(N/b_0)]^2 \tag{31}$$

as $N \to \infty$ with, roughly, $a_0 \simeq \frac{1}{8}$ and $b_0 \simeq \frac{1}{2}e_{\mathrm{E}}$. If, in order to examine the continuum limit, one sets $N = t/a^2$ one thus sees the scaling of $\theta(t)$ with $\ln t$, as established rigorously by Spitzer (1958). But notice *also* the (logarithmic) divergence of the second moment at fixed t when $a \to 0$: this seems to reflect the Cauchy distribution of $\theta(t)/\ln t$, found by Spitzer, which has a divergent second moment.

For a self-avoiding walk the calculation of $\langle a^2/r_N^2 \rangle$ goes differently. First, the exponential factor in the integrand in (30) should be replaced by the corresponding self-avoiding scaling form, $N^{-d\nu}X(r/aN^{\nu})$, with $d=2$. It is recognised, however, that the scaling function $X(x)$ vanishes like a positive power as $x \to 0$ when $d<4$ (see e.g. McKenzie 1972). Accordingly, the integral remains bounded when one removes the lattice cut-off by taking $a \to 0$. More generally, in a self-avoiding walk of N steps the positions of intermediate locations, m steps along the chain, scale in similar fashion. We may thus anticipate the result

$$\langle a^2/r_N r_{N-l} \rangle \approx D(l/N)N^{-2\nu}, \tag{32}$$

as $N \to \infty$.

If one accepts this and *assumes also* that the reduced angular correlation function, $g_N^{\theta}(l)/g_N^{\theta}(0)$, decays rapidly, say faster than $1/l^{1+\varepsilon}$ with $\varepsilon > 0$, one is led, via (27), to

$$\Theta_N^2 \approx \Theta_\infty^2 - D_\infty/N^{2\nu-1} + \ldots, \tag{33}$$

where Θ_∞^2 is finite! This is a surprising result and one which is scarcely consistent with the numerical evidence (although one cannot actually rule out a large value, say, $\Theta_\infty^2 > 15$). It implies a long-range directional correlation that, in effect, remembers forever the direction of the first step! But, in essence, that amounts to a self-contradiction since, to obtain (33), a *rapid* decay of angular correlations was postulated. Clearly, then, such a rapid decay is *not* plausible and the conjecture (33) is poorly founded†.

To estimate the angular correlation function let us recall (29) and then suppose that the tangential step and overall radial distributions may, to sufficient accuracy, be factorised: this yields

$$g_N^{\theta}(l) \approx a^2 \langle \tau_N \tau_{N-l}/r_N r_{N-l} \rangle \approx g_N^{\tau}(l) \langle a^2/r_N r_{N-l} \rangle, \tag{34}$$

where the tangential step–step correlation function was introduced in (24). Now we may adopt (32) for the radial expectation and, as discussed before, postulate a scaling form like (25) for $g_N^{\tau}(l)$ with $\sigma_\tau = \sigma = 2(1-\nu)$ by (26). By this route we arrive at

$$\Delta\Theta_N^2 \approx \frac{2}{N} \int_0^1 \frac{\mathrm{d}w}{w^{2(1-\nu)}} G_\tau(w) D(w), \tag{35}$$

where it is to be noted that the factors N^{ν} have cancelled out! There seem no grounds for doubting that the integral over the scaling functions converges. Thus we finally conclude that Θ_N^2 diverges precisely like $a_1 \ln(N/b_1)$ i.e. $\psi_1 = \frac{1}{2}$ (see (4) and (15)).

Physically, this result may be understood by realising, from (25), that the predominant effect of the self-avoiding constraint is to bias a walk to keep growing in the same direction as the last step. (Compare with Grassberger (1982b).) If that step happens to have a significant tangential component, the bias translates into a growth of the winding angle: the step sizes must be rescaled by radial distance to obtain angles but no new process (or new exponent) is involved. By the same token, a deviation of σ_τ from σ seems implausible; but note that if $\Delta\sigma = \sigma_\tau - 2(1-\nu)$ were positive, so that $g_N^{\tau}(l)$ decays *more* rapidly than $g_N^{\rho}(l)$, the exponent of N in (36) would exceed unity

† Attention should be drawn, in this context, to the study of the 'persistence length' of self-avoiding walks by Grassberger (1982b). In $d=2$ dimensions, if the first step is directed along the positive x axis the mean end-coordinate $\langle x_N \rangle$ appears to diverge weakly as $N \to \infty$.

and one would be back to a result like (33) (although with $2\nu - 1$ replaced by $\Delta\sigma$): but, as argued before, this seems to be almost self-contradictory!

Finally, notice that our detailed heuristic analysis has mainly served to confirm the surmise stated originally on the basis of renormalisation group rescaling ideas, namely, that angles, being dimensionless, should behave as marginal variables with vanishing power-law exponents. Our detailed arguments suggest $\psi_1 = \frac{1}{2}$, so that $\langle\theta_N^2\rangle \approx a_1 \ln(N/b_1)$, but one knows from renormalisation group analyses in critical phenomena (see e.g. Wegner 1976) that more subtle powers of logarithms may appear in a marginal variable when nonlinear couplings to other variables are fully accounted for. It may, indeed, be possible to carry out such calculations here to lend further strength to the conjecture $\psi_1 = \psi_2 = \frac{1}{2}$ or, perhaps, to modify it.

We have enjoyed helpful discussions with M Barma, F Family, F Spitzer and H E Stanley. The financial support of the National Science Foundation through grant DMR-81-17011 and, in part, through the Material Science Center at Cornell University is gratefully acknowledged. The Center for Polymer Studies at Boston University is supported, in part, by grants from the ARO, NSF and ONR.

References

Fisher M E and Sykes M F 1959 *Phys. Rev.* **114** 45
Grassberger P 1982a *Z. Phys.* B **48** 255
—— 1982b *Phys. Lett.* **89A** 381
Guttmann A J 1984 *J. Phys. A: Math. Gen.* **17** 455
McKenzie D S 1972 *Phys. Rep.* **27C** 35
Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
Peters H P, Stauffer D, Hölters H P and Loewenich K 1979 *Z. Phys.* B **34** 399
Redner S 1982 *J. Stat. Phys.* **29** 309
Redner S and Reynolds P 1981 *J. Phys. A: Math. Gen.* **14** 2679
Shapiro B 1978 *J. Phys. C: Solid State Phys.* **11** 2829
Spitzer F 1958 *Am. Math. Soc. Trans.* **87** 187
Stanley H E, Family F and Gould H 1983 *J. Polymer Sci.* in press
Stauffer D 1981 in *Disordered Systems and Localization, Lecture Notes in Physics* vol 149 (Berlin: Springer)
Sykes M F, Guttmann A J, Watts M G and Roberts P D 1972 *J. Phys. A: Gen. Phys.* **5** 653
Wegner F J 1976 in *Phase Transitions and Critical Phenomena* vol 6, ed C Domb and M S Green (London: Academic)