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LETTER TO THE EDITOR

On a random process interpolating between Markovian and non-Markovian random walks

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Abstract. We give the exact solution in one dimension of the continuum analogue of a model of Stanley *et al* which interpolates between Markovian (Pólya) and self-avoiding random walks on lattices, and make some heuristic comments on the nature of phase transitions in the model in higher dimensions.

Probabilistic lattice models are gaining increasing importance in a wide variety of problems in physics, with perhaps the most important such models being the *Markovian random walk* (Weiss and Rubin 1983, Hughes and Prager 1983), the *self-avoiding walk* (Barber and Ninham 1970, Hughes and Prager 1983), and *percolation theory* (Deutscher *et al* 1983, Hughes and Ninham 1983). It has been shown by Domb and Joyce (1972) that if multiple visits to individual sites are assigned an energy penalty, a model may be constructed which interpolates between the ordinary Markovian walk of Pólya type (unbiased motion, with only nearest-neighbour transitions) and the self-avoiding walk. Recently, Stanley *et al* (1983) have proposed an alternative scheme for interpolation between Pólya walks and self-avoiding of self-attracting walks. They give numerical evidence (drawn from series analyses and Monte Carlo simulations) which suggests that their model possesses 'super-universal' lattice- and dimension-independent properties, and that it is related to percolation theory. In this letter we give the exact solution of the continuum analogue of their model in one dimension, and make some general observations about their model in higher dimensions.

The model of Stanley *et al* is defined as follows. For Pólya's walk on a periodic lattice of coordination number z, let (the random variable) S_N denote the number of distinct sites visited in a walk of duration N steps. In the model of Stanley *et al*, each realisation of the walk is assigned a statistical weight $p^{S_N} = \exp(-KS_N)$. When $K>0$ (i.e. $p<1$), walks in which few distinct sites are visited are favoured, while if $K<0$ (i.e. $p>1$), walks with many distinct sites visited receive the greatest weight. The limit $K\to-\infty$ corresponds to a self-avoiding walk, while $K\to\infty$ returns a self-attracting walk; the ordinary Pólya walk is obtained by setting $K=0$. If one defines a partition function

$$Z(N,K) = \sum_{\text{all } z^N \text{ walks}} \exp(-KS_N), \tag{1}$$

the ensemble average of any function $f(S_N)$ of S_N becomes

$$\langle f(S_N)\rangle_K = \left(\sum_{\text{all } z^N \text{ walks}} \exp(-KS_N) f(S_N)\right)\Big/ Z(N,K). \tag{2}$$

In particular,

$$\langle S_N\rangle_K = -Z(N, K)^{-1}\, \partial Z(N, K)/\partial K = -\partial \log Z(N, K)/\partial K \tag{3}$$

and

$$\langle S_N^2\rangle_K = Z(N, K)^{-1}\, \partial^2 Z(N, K)/\partial K^2. \tag{4}$$

Stanley *et al* have sought the asymptotic values of $Z(N, K)$, $\langle S_N\rangle_K$ and $\langle S_N^2\rangle_K$ in the limit of large N. In particular, when $\exp(-K) = p_c$, the percolation threshold of the lattice, they find *dimension-independent* growth exponents for the ensemble-averaged mean and variance of S_N (for lattices of dimension $\geqslant 2$):

$$\langle S_N\rangle_{-\log p_c} \sim N^{2/3}, \qquad \langle S_N^2\rangle_{-\log p_c} - \langle S_N\rangle^2_{-\log p_c} \sim N^{4/3}. \tag{5}$$

They also find that the *connective constant*

$$\lambda(K) = \lim_{N\to\infty} N^{-1} \log Z(N, K) \tag{6}$$

is approximately 3.4, independent of dimension.

For a *one-dimensional* Pólya walk, the number of distinct sites visited, S_N, differs by 1 from the span R_N of the walk, defined as the difference in coordinates of the left-most and right-most sites visited after N steps: $S_N = R_N + 1$. Thus

$$Z(N, K) = \left(\sum_{\text{all walks}} \exp(-KR_N)\right) \exp(-K) \tag{7}$$

$$= Z^N \langle \exp(-KR_N)\rangle_0 \exp(-K) \tag{8}$$

where $\langle\ \rangle_0$ denotes the average with respect to the ordinary Pólya walk, i.e., in the case $K = 0$. Since the Pólya walk has the diffusion equation as its continuum limit, it is of interest to examine in place of $\langle \exp(-KR_N)\rangle_0$ the expected value of $\exp(-KR_t)$, with R_t the span at time t of the continuum diffusion process generated by the equation $(\partial/\partial t)p = \frac{1}{2}(\partial^2/\partial x^2)p$. (We have set the value of the diffusion constant to $\frac{1}{2}$ without loss of generality.) Darling and Siegert (1953) have determined the probability density function $\phi(r, t)$ for the span R_t:

$$\phi(r, t) = \frac{8}{\sqrt{2\pi t}} \sum_{j=1}^{\infty} (-1)^{j-1} j^2 \exp\left(-\frac{j^2 r^2}{2t}\right) \tag{9}$$

$$= \frac{2}{\pi^2} \frac{\partial^2}{\partial r^2}\left[r \sum_{j=0}^{\infty} \frac{1}{(j+\frac{1}{2})^2} \exp\left(-\frac{2\pi^2 t (j+\frac{1}{2})^2}{r^2}\right)\right]. \tag{10}$$

These two everywhere convergent expansions for $\phi(r, t)$, useful for $r > \sqrt{(2t)}$ and $r < \sqrt{(2t)}$ respectively, are related by theta function identities. We shall use them to determine the large t value of

$$\Phi(K, t) \equiv \int_0^\infty e^{-Kr} \phi(r, t)\, dr \tag{11}$$

and thereby determine the limiting 'connective constant'

$$\Lambda(K) \equiv \lim_{t\to\infty} t^{-1} \log \Phi(K, t) \tag{12}$$

and also the mean $\langle R_t\rangle_K$ and variance $\sigma_t^2=\langle R_t^2\rangle_K-\langle R_t^2\rangle_K$ via the equations

$$\langle R_t\rangle_K=-\Phi(K,t)^{-1}\,\partial\Phi(K,t)/\partial K=-\partial\log\Phi(K,t)/\partial K, \tag{13}$$

$$\langle R_t^2\rangle_K=\Phi(K,t)^{-1}\,\partial^2\Phi(K,t)/\partial K^2. \tag{14}$$

(We note the classical results for $K=0$: $\langle R_t\rangle_0\sim\{8t/\pi\}^{1/2}$, $\langle R_t^2\rangle_0\sim 4t\log 2$.) To analyse the large t behaviour of $\Phi(K,t)$ we split the integral in (11) into two parts, an 'inner' part $\Phi_{\rm I}$ which emphasises the behaviour of the integrand near $r=0$, and an 'outer' part $\Phi_{\rm O}$ which emphasises the large r behaviour:

$$\Phi_{\rm I}(K,t)=\int_0^{\sqrt{(2t)}}\mathrm{e}^{-Kr}\phi(r,t)\,\mathrm{d}r,\qquad \Phi_{\rm O}(K,t)=\int_{\sqrt{(2t)}}^{\infty}\mathrm{e}^{-Kr}\phi(r,t)\,\mathrm{d}r. \tag{15}$$

The 'self-repelling' case ($K<0$). The magnitude of $\Phi_{\rm I}$ is easily estimated:

$$\Phi_{\rm I}(K,t)\leqslant\exp(|K|\sqrt{(2t)})\int_0^{\sqrt{(2t)}}\phi(r,t)\,\mathrm{d}r<\exp(|K|\sqrt{(2t)}). \tag{16}$$

We estimate $\Phi_{\rm O}$ by using the alternating series (9). For each fixed $r\geqslant\sqrt{(2t)}$, the sequence $a_j\equiv j^2\exp\{-j^2r^2/(2t)\}$ is strictly decreasing. The sum $\phi(r,t)$ of the alternating series $\Sigma_{j=1}^{\infty}(-1)^{j-1}a_j$ can be bounded rigorously using a well known theorem (Apostol 1974):

$$0<(-1)^n\left(\phi(r,t)-\sum_{j=1}^{n}(-1)^{j-1}a_j\right)<a_{n+1}. \tag{17}$$

In particular, taking $n=1$, we have

$$-a_2\phi(r,t)-a_1<0 \tag{18}$$

and so

$$-\frac{32}{\sqrt{(2\pi t)}}\int_{\sqrt{(2t)}}^{\infty}\exp\left(-\frac{2r^2}{t}+|K|r\right)\mathrm{d}r$$
$$<\Phi_{\rm O}(r,t)-\frac{8}{\sqrt{(2\pi t)}}\int_{\sqrt{(2t)}}^{\infty}\exp\left(-\frac{r^2}{2t}+|K|r\right)\mathrm{d}r<0. \tag{19}$$

Making the changes of variable $r=\frac{1}{2}\xi\sqrt{(2t)}$ and $r=\xi\sqrt{(2t)}$ in the left and right integrals respectively and completing the square in the argument of the exponential, we find that

$$-\frac{16}{\sqrt{\pi}}\exp(\tfrac{1}{8}K^2t)\int_2^{\infty}\exp\left[-\left(\xi-\frac{|K|\sqrt{t}}{2\sqrt{2}}\right)^2\right]\mathrm{d}\xi$$
$$<\Phi_{\rm O}(r,t)-\frac{8}{\sqrt{\pi}}\exp(\tfrac{1}{2}K^2t)\int_1^{\infty}\exp\left[-\left(\xi-\frac{|K|\sqrt{t}}{\sqrt{2}}\right)^2\right]\mathrm{d}\xi<0 \tag{20}$$

and so as $t\to\infty$,

$$\Phi_{\rm O}(r,t)=8\exp(\tfrac{1}{2}K^2t)[1+\varepsilon(t)] \tag{21}$$

where $\varepsilon(t)$ vanishes exponentially with t. Since $\Phi_{\rm O}$ dominates $\Phi_{\rm I}$, we have established rigorously that

$$\Phi(K,t)\sim 8\exp(\tfrac{1}{2}K^2t),\qquad t\to\infty,\qquad K<0, \tag{22}$$

and so the 'connective constant' (equation (12)) is

$$\Lambda(K)=\tfrac{1}{2}K^2, \qquad K<0. \tag{23}$$

While it is not in general permissible to differentiate asymptotic equalities, the evident absence of oscillations in $\Phi(K, t)$ enables us to differentiate (22) as often as we please, giving for the ensemble-averaged mean and variance of the span

$$\langle R_t\rangle_K \sim |K|t, \qquad \sigma_t^2 \sim t. \tag{24}$$

At fixed large time, the mean increases with $|K|$, but the variance is independent of $|K|$.

The 'self-attracting' case ($K>0$). The magnitude of Φ_{O} is easily estimated:

$$\Phi_{\mathrm{O}}(K, t) \leqslant \exp[-K\sqrt{(2t)}] \int_{\sqrt{(2t)}}^{\infty} \phi(r, t)\,\mathrm{d}r = o(\exp[-K\sqrt{(2t)}]. \tag{25}$$

To estimate Φ_{I}, we use the series (10), make the change of variables $r=\xi\sqrt{(2t)}$, and integrate by parts twice, giving

$$\Phi_{\mathrm{I}}(K, t) = \frac{2}{\pi^2}\exp\{-K\sqrt{(2t)}\}\Theta'(1) + \frac{2K\sqrt{(2t)}}{\pi^2}\exp\{-K\sqrt{(2t)}\}\Theta(1) + \frac{4K^2t}{\pi^2}\int_0^1 \exp(-K\sqrt{(2t)}\xi)\Theta(\xi)\,\mathrm{d}\xi, \tag{26}$$

where

$$\Theta(\xi) \equiv \xi \sum_{j=0}^{\infty} (j+\tfrac{1}{2})^{-2} \exp[-\pi^2(j+\tfrac{1}{2})^2/\xi^2]. \tag{27}$$

Appealing to absolute convergence, we may interchange the orders of summation and integration in equation (27) and deduce that

$$\int_0^1 \exp(-K\sqrt{(2t)}\xi)\Theta(\xi)\,\mathrm{d}\xi = \sum_{j=0}^{\infty} \frac{1}{(j+\frac{1}{2})^2}\int_0^1 \xi \exp(-f_j(\xi))\,\mathrm{d}\xi \tag{28}$$

where we have written $f_j(\xi)=K\sqrt{(2t)}\xi+\pi^2(j+\frac{1}{2})^2/\xi^2$.

Since $f_j(\xi)$ attains its minimum at $\xi_j=\{2\pi^2(j+\frac{1}{2})^2\}^{1/3}\{K\sqrt{(2t)}\}^{-1/3}$, we see that

$$0<\sum_{j=1}^{\infty}\frac{1}{(j+\frac{1}{2})^2}\int_0^1 \xi\exp[-f_j(\xi)]\,\mathrm{d}\xi < \sum_{j=1}^{\infty}\frac{1}{(j+\frac{1}{2})^2}\exp[-f_j(\xi_j)]\int_0^1 \xi\,\mathrm{d}\xi$$
$$=\tfrac{1}{2}\sum_{j=1}^{\infty}\frac{1}{(j+\frac{1}{2})^2}\exp\{-\tfrac{3}{2}[2\pi^2(j+\tfrac{1}{2})^2]^{1/3}\{K\sqrt{(2t)}\}^{2/3}\}. \tag{29}$$

The large t behaviour of the integral in (28) is dominated by the behaviour of the $j=0$ term in the sum, which is easily extracted via Laplace's method (Olver 1974) after making the change of variables $\xi=(\pi^{2/4})^{1/3}(K\sqrt{(2t)})^{-1/3}$

$$\int_0^1 \xi\exp[-f_0(\xi)]\,\mathrm{d}\xi \sim \frac{\pi^{3/2}}{K\sqrt{(6t)}}\exp\left[-\tfrac{3}{2}\left(\frac{\pi^2}{2}\right)^{1/3}(K\sqrt{(2t)})^{2/3}\right]. \tag{30}$$

Inspecting equations (25), (26), (29) and (30), we see that

$$\Phi(K, t) \sim \frac{8K\sqrt{(2t)}}{\sqrt{(3\pi)}}\exp\left[-\frac{3}{2}\left(\frac{\pi^2}{2}\right)^{1/3}\{K\sqrt{(2t)}\}^{2/3}\right] \tag{31}$$

and so

$$\log \Phi(K, t) \sim -\tfrac{3}{2}(\pi^2 t)^{1/3} K^{2/3}. \tag{32}$$

The *connective constant vanishes*: $\Lambda(K) = 0$ for $K > 0$; $\Lambda(K)$ is therefore continuous for $-\infty < K < \infty$, but has a discontinuous first derivative at $K = 0$. Differentiating equation (32) with respect to K, we find the ensemble-averaged mean range to be

$$\langle R_t \rangle_K \sim (\pi^2 t/K)^{1/3}. \tag{33}$$

Although $\langle R_t \rangle_K$ is $O(t^{1/3})$ for all $K > 0$, the asymptotic relation is not uniform in K, and $\lim_{t\to\infty} \langle R_t \rangle_K / t^{1/3} = (\pi^2/K)^{1/3}$ diverges as $K \to 0$.

We conclude with a few remarks on the relation between the continuum problem we have analysed and the discrete model of Stanley *et al* (1983), and on the qualitative features of the latter model. In the discrete model, since $2 \leqslant S_N \leqslant N + 1$, we have the inequality $z^N \exp(-2K) > Z(N, K) > z^N \exp[-(N-1)K]$ for $K > 0$, and the same relation with the signs reversed for $K < 0$, so that

$$\begin{aligned} &-K + \log z \leqslant \lambda(K) \leqslant \log z, \qquad && K > 0, \\ &\log z \leqslant \lambda(K) \leqslant \log z + |K|, \qquad && K < 0. \end{aligned} \tag{34}$$

The continuous and discrete models differ in their behaviour for $K \to -\infty$, since the former gives a connective constant proportional to K^2, while the latter gives a connective constant proportional to $|K|$. This deviation can be attributed to the continuous model's allowing rare excursions of order exceeding t in time t; no excursions exceeding $N+1$ are possible in the discrete model. There is no such inconsistency between the continuous and discrete models for $K > 0$, so it is likely that in one dimension $\lambda(K) \equiv \log 2$, and $\langle S_N \rangle_K \propto N^{1/3}$.

The prospects for exact analysis of problems of the type considered by Stanley *et al* in higher dimensions seem remote, for the distribution of S_N in Pólya's walk is inadequately known. It has long been established (see, e.g. Montroll and Weiss 1965) that for d-dimensional hypercubic lattices,

$$\langle S_N \rangle_0 \sim \begin{cases} (8N/\pi)^{1/2} & d = 1 \\ \pi N / \log N & d = 2 \\ (1 - R) N & d \geqslant 3 \end{cases} \tag{35}$$

with R the probability of eventual return of the walker to the starting site. It is also known (Jain and Orey 1968, Jain and Pruitt 1971, Darling and Siegert 1953, Weiss and Rubin 1983) that

$$\sigma_N^2 \equiv \langle S_N^2 \rangle_0 - \langle S_N \rangle_0^2 \sim \begin{cases} \sigma^2 N & d = 1 \\ \sigma^2 N^2 / \log^4 N & d = 1 \\ \sigma^2 N \log N & d = 3 \\ \sigma^2 N & d \geqslant 4 \end{cases} \tag{36}$$

with σ a lattice-dependent constant. The distribution of S_N is known to obey the central limit theorem for $d \geqslant 3$, so that within any finite interval $-C\sigma_N < S_N - \langle S_N \rangle_0 < C\sigma_N$, it is permissible to replace the distribution of S_N by a Gaussian. However the asymptotic forms of the distribution of S_N near 0 and near N do not appear to have been well characterised yet. If one assumes that the distribution is everywhere Gaussian (and this may be a rather poor approximation), one arrives at the following simple expression for the partition function:

$$Z_N \sim \frac{z^N}{\sqrt{(2\pi\sigma_N}} \int_0^{N+1} \exp\left(-KS - \frac{\{S-\langle S_N\rangle_0\}^2}{2\sigma_N^2}\right) \mathrm{d}s. \tag{37}$$

Completing the square in the exponent, we see that the integrand attains its maximum at $S^* = \langle S_N\rangle_0 - K\sigma_N^2$. When $d \geqslant 4$, S^* lies well inside the integration interval when $|K|$ is sufficiently small, and we arrive at the following approximation for the connective constant:

$$\lambda(K) \sim \log z - (1-R)K + \tfrac{1}{2}\sigma^2 K^2.$$

The Gaussian ansatz also gives for the expected number of distinct sites visited

$$\lim_{N\to\infty} \frac{\langle S_N\rangle_K}{N} = -\frac{\mathrm{d}\lambda}{\mathrm{d}K} \sim (1-R) - \sigma^2 K, \tag{38}$$

i.e., it predicts a correction linear in K. These entirely heuristic arguments suggest that in sufficiently high dimensions, there is a finite range of values of K, encompassing the origin, in which there is no change in the qualitative structure of the ensemble-averaged properties. One may then reasonably ask if there are phase transitions at finite values of K, or whether the condensed or expanded states are attained only in the limits $K \to \infty$ and $K \to -\infty$ respectively.

After this letter was completed, the authors noticed a recent analysis by Redner and Kang (1983) of the one-dimensional discrete problem, using a transfer matrix formalism. They obtain expressions for the most probable value (in the ensemble) $S_{\max}$ of the number of distinct sites visited:

$$S_{\max} \sim |K|N \qquad K<0, \tag{39}$$

$$S_{\max} \sim \{N\pi^2/K\}^{1/3} \qquad K>0, \tag{40}$$

and they argue that $S_{\max} \sim \langle S_N\rangle_K$. Their results agree with our continuum analysis if we replace N by t. However, their analysis for the repulsive ($K<0$) discrete problem cannot be valid for large $|K|$ since, as we have remarked above, $S_N \leqslant N+1$; this constraint is violated by (39) when $K<-1$. It may require a somewhat careful and subtle analysis to see whether or not for the discrete problem there exists a phase transition at a finite, negative value of K, K_c (say). In other words, does $\langle S_N\rangle_K \sim N$ for $K<K_c$, or only in the limit $K\to-\infty$? Redner and Kang note that a result equivalent to equation (32) follows from a theorem on 'Wiener sausages' due to Donsker and Varadhan (1975).

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