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A unifying model of generalised random walks

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Abstract. We propose a unifying model for generalised static random walks, in which each walk has a weight $\exp(-g\Sigma(n_i)^\alpha)$, where n_i is the occupation number of a site and α and g are variable parameters. Special cases of this general walk include the ordinary (Brownian) random walk, the self-avoiding walk, the lattice Domb-Joyce model and the interacting random walk model recently introduced by Stanley *et al.* The asymptotic properties of the walk are studied in one dimension by effective medium arguments and exact enumeration methods. For repulsive correlations we find SAW behaviour, while for attractive correlations the model is self trapping for $1 < \alpha \leq 2$ and exhibits anomalous diffusion, with continuously varying exponents, for $0 \leq \alpha < 1$. In higher dimensions comments are made about effective medium predictions, and their relationship to other generalised random walk models.

1. Introduction

Very recently, a number of generalised random walk models have made their way into the literature. The reasons for the introduction of each problem vary widely, from the study of superuniversal (dimension independent) properties (the interacting random walk of Stanley *et al* 1983) to the description of polymer growth (the kinetic growth walk of Majid *et al* 1983), and the discussion of novel critical properties in their own right (the generalised self-avoiding walk of Turban (1983) and the true self-avoiding walk (TSAW) of Amit *et al* (1983)). Although all the above models are similar in the sense that they incorporate correlations between steps, each of them exhibits quite distinct asymptotic properties. Accordingly, emphasis has been mainly given to the differences between the models, rather than to whether it is possible to build a unified picture of the mechanisms underlying the several distinct features displayed by them. A first step in this latter direction was the study of Duxbury *et al* (1984), where the qualitative features of the one-dimensional versions of the TSAW and of the interacting random walk of Stanley *et al* (1983) were analysed and compared to those of the Domb-Joyce model (Domb and Joyce 1972), and of a model based on the weighting of turning points, whose behaviour is related to that of an Ising spin chain. In the present work we make use of effective medium arguments and exact enumeration methods in order to discuss quantitatively the role played by a density dependent weighting function in the determination of asymptotic properties of generalised random walks. Apart from setting general conditions for the existence anomalous diffusion in one-dimensional systems, our results enable us to proceed one step further towards a unified view of the basic features of interacting random walks. More precisely, we

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show how the model of Stanley *et al* (1983) and the Domb–Joyce model can both be obtained by the variation of a single parameter in a generalised weighting function. In higher dimensions we discuss whether our particular weighting function (and its approximate expression as given by an effective medium approach) may, or may not, represent a reduced excluded volume constraint in generalised self-avoiding walks. In order to do so, we make contact with the recent work of Turban (1983), Shapir and Oono (1984) and Guttmann *et al* (1984) on the k-tolerant self-avoiding walk.

In what follows, we first define a generalised random walk model where the energy scales as the αth power of the density, and make use of an asymptotic expression for the density distribution of one-dimensional random walks, recently derived by Redner and Kang (1983) (see also Chan and Hughes 1984, Anlauf 1984), together with effective medium arguments (Flory 1971, de Gennes 1979), and obtain predictions for the asymptotic behaviour of the one-dimensional version of the model. There is then a short section on effective medium arguments for the model in higher dimensions and with repulsive correlations. The resulting expressions have recently appeared in the literature in two different contexts (Turban 1983 and Majid *et al* 1984) and we comment on the relationship between those models and ours.

Section 4 contains the results of exact enumerations of one-dimensional walks of up to 21 steps. In the series generation, series for any g and α are generated from a set of weighted partitions which are generated once and stored, and in the series analysis some peculiar effects occur due to finite size and crossover effects. The results however confirm the predictions of the one-dimensional effective medium arguments. The paper concludes in § 5 with a summary and discussion.

2. Effective medium arguments in one dimension

Consider a generalised random walk in which each configuration with N steps is weighted according to the αth power of the number of times n_i a site i is visited:

$$W = \exp\left(-g \sum_{i=1}^{S} (n_i)^{\alpha}\right). \qquad (1)$$

The sum spans all $S(S \leq N+1)$ visited sites, and the factor g is a parameter which varies the 'strength' of the correlations between steps, and can be attractive or repulsive (see below). The case $\alpha = 0$ is the interacting random walk of Stanley *et al* (1983), while $\alpha = 2$ corresponds to the lattice Domb–Joyce (DJ) model (Domb and Joyce 1972). The factor in the DJ model is $\frac{1}{2}n_i(n_i - 1)$, but this is irrelevant, since it amounts to adding the same weight $\exp(gN/2)$ to all N step walks. The present model allows us to study the changeover between the (rather distinct) characteristics of the two models which takes place as α is varied from 0 to 2. More precisely, the model of Stanley *et al* (1983) displays anomalous diffusion, with exponent $\frac{1}{3}$, in the attractive one-dimensional case (Redner and Kang 1983), whereas the attractive one-dimensional DJ model traps itself (Duxbury *et al* 1984, see also below). The question then arises as to what the conditions are for the onset of anomalous diffusion, and whether the characteristic exponent is always the same (as long as diffusion occurs) or changes continuously as the driving mechanisms vary. Apart from being of possible relevance in the context of diffusion problems, a proper understanding of this question will help to clarify the role played by density correlations in establishing the different types of asymptotic behaviour of generalised random walks.

We begin by considering the asymptotic probability distribution for a one-dimensional random walk with N steps which visits S distinct sites (Redner and Kang 1983):

$$P(N, S) \simeq [\cos(\pi/(S+1))]^N \times \exp(-S^2/2N). \tag{2}$$

If we attribute a weight given by (1) above as the intrinsic probability of an N step walk, which visits S sites and is characterised by the set of occupation numbers $\{n_i\}$, and interaction parameters g and α, we have

$$P(N, S, \{n_i\}, g) = P(N, S) \times \exp\left(-g \sum_{i=1}^{S} (n_i)^\alpha\right). \tag{3}$$

We note that for $\alpha < 1$, 'stretched' configurations are favoured if $g < 0$, whereas multiple visits to the same site are favoured if $g > 0$. The situation is reversed $\alpha > 1$. For $g = 0$ and/or $\alpha = 1$ one has the ordinary unbiased random walk.

If we now assume that (i) the average end-to-end distance $\langle R_N^2\rangle^{1/2}$ is proportional to the average span of the walk $\langle S_N\rangle$ (which is sensible in one dimension) and (ii) the average span scales with the same power of N as the most probable value of S, S_{max}, (which is in agreement with general scaling ideas, and does not necessarily imply a very narrowly peaked distribution function), we can find the asymptotic behaviour by requiring that the logarithm of (3) above be stationary with respect to S (Redner and Kang 1983).

The problem now is how to find the S dependence of (1). At this point we make the effective medium replacement $n_i \to N/S$, that is, n_i is replaced by an average number of visits to a site. Now write

$$\sum_{i=1}^{S} (n_i)^\alpha \to S(N/S)^\alpha = S^{1-\alpha} N^\alpha. \tag{4}$$

With the help of (4), and using (2), the steepest descents condition for S_{max} becomes

$$\frac{d}{dS}\left\{ N \ln\left[\cos\left(\frac{\pi}{S+1}\right)\right] - \frac{S^2}{2N} - gS^{1-\alpha}N^\alpha \right\} = 0 \tag{5}$$

which in the limit $N, S \to \infty$ gives,

$$N\pi^2/S^3 - S/N - g(1-\alpha)S^{-\alpha}N^\alpha = 0. \tag{6}$$

If S grows faster than $N^{1/2}$, it is consistent to neglect the first term on the LHS of (6), and one has

$$S_{max} = g(\alpha - 1)N, \tag{7}$$

provided that (a) if $\alpha > 1$, $g > 0$; or (b) if $\alpha < 1$, $g < 0$. The result (7) is consistent with the favourable conditions for 'stretched' configurations noted above, and we see that the asymptotic behaviour is always that of a one-dimensional self-avoiding walk. On the other hand, if S_{max} grows slower than $N^{1/2}$, it is consistent to neglect the second term on the LHS of (6). We then have two cases: (i) for $\alpha < 1$ and $g > 0$,

$$S_{max} = \left(\frac{\pi^2}{g(1-\alpha)}\right)^{1/(3-\alpha)} N^{(1-\alpha)/(3-\alpha)}. \tag{8}$$

Which besides reproducing the known results for $\alpha = 0$ (Redner and Kang 1983), shows that anomalous diffusion is expected for all $0 \leq \alpha < 1$, with the α dependent exponent $(1-\alpha)/(3-\alpha)$. At $\alpha = 1$ one should jump discontinuously to the ordinary random walk behaviour. In the second case: (ii) for $\alpha > 1$ and $g < 0$, the formal expression is the same as (8) above. If interpreted literally, this means that S_{max} scales with a negative power of N. We see this as signalling self-trapping behaviour, a regime in which there is no longer a diverging length as $N \to \infty$, therefore the scaling assumptions mentioned earlier should break down.

From the preceding arguments, we deduce the 'phase diagram' of figure 1, where ordinary random walk behaviour occurs along the broken lines. In order to check whether these predictions are correct, we have proceeded to exact enumeration work, which is reported in § 4. However before going into this analysis, we comment on the application of effective medium arguments to the random walk with weights (1) in higher dimensions.

3. Flory-like arguments in higher dimensions

Recently, Turban (1983) has discussed a generalised self-avoiding walk, called the k tolerant self-avoiding walk, in which only k and higher multiple visits to a site ($k \geq 2$) are forbidden (the first mention of this class of walks appears to have been by Malakis (1975, 1976)). In general space dimensionality and from a Flory argument with a repulsive energy term similar to (4) above (where his k is substituted for our α), Turban obtains k dependent exponents (which approach mean field values as $k \to \infty$) and upper critical dimensionalities. An argument based on fractal theory is used to support the values found for the upper critical dimensionalities, and in one dimension the problem is shown to be equivalent to the SAW (which corresponds to $k = 2$) for any finite k. In two and three dimensions, however Turban's findings have been criticised by Guttman *et al* (1984), who give numerical evidence from exact enumeration of k tolerant SAWs to support the view that the exponents remain the same as for the SAW for any finite k. This view is supported by the momentum space RG work of Shapir and Oono (1984).

The Flory results found by Turban (1983) in fact seem to apply more naturally to the generalised random walk introduced here. Before showing how this arises, we make some comments on what might be a suitable form for the Flory energy for the k tolerant SAW. Our view is that however natural it seems to think of a generalised excluded volume condition, which becomes effective at the kth time a site is visited, as being represented by a k body interaction, the correspondence can not be seen as more than plausible. An equally plausible Flory energy, that gives predictions in agreement with the calculations of Guttmann *et al* (1984) and Shapir and Oono (1984), is $E_{rep} \simeq (\rho - c)^2$; where c is a constant less than or equal to ρ. For any $c < \rho$ this form predicts that the behaviour is like a SAW. On the other hand, the existence of a k body interaction, has deeper consequences, as is well known for spin systems (see e.g. Toulouse and Pfeuty 1975), and it is not surprising that in that case the exponents and critical dimensionalities turn out to be k dependent.

To perform a Flory approximation for the generalised weights introduced in (1) in higher dimensions, one needs a relationship between the S used in the Flory enegy (4) and the average end-to-end distance measure R. If we take $S = R^d$ (as is reasonable within a mean field approximation), and make the usual scaling comparison with the entropy term R^2/N, we get the same results as found by Turban (1984) (and also Majid *et al* 1984), that is, the upper critical dimension is given by $d_c = 2\alpha/(\alpha-1)$, and the end-to-end distance exponent below this dimension is given by $\nu = (\alpha+1)/(2-d+\alpha d)$.

It is interesting to note that the higher-dimensional Flory arguments discussed above are only applicable to the case of repulsive correlations. This is in contrast to the results of § 2 where both repulsive and attractive correlations were discussed within effective medium arguments. For a proper treatment of the attractive region in higher-dimensional cases, one would need the higher-dimensional version of the probability distribution close to the origin, which in one dimension is given by the cosine term of (2) (Redner and Kang 1983). To our knowledge, such an asymptotic form is not as yet available for general d, and we shall not pursue this point further.

4. Results of exact enumerations in one dimension

We have enumerated all walks of up to 21 steps in one dimension. With the weights given by (1), a computationally convenient procedure is (for a given N) to classify the walks according to which partition of $N+1$, into non-negative integers, is realised by the set $\{n_i\}$ of site occupation numbers of each walk. All walks that have the same partition have the same weight (given by (1)), and not all partitions occur due to connectivity constraints. An example is the $N=8$ step generalised walks in one dimension, where the full 256 walks possible are grouped into just 17 partition classes. With the multiplicity and cumulative end-to-end squared distance for each class, one can proceed directly to the evaluation of $\langle R_N^2\rangle$ and $\langle S_N\rangle$ for any values of the parameters α and g. A table of partition data is generated for each N up to 21, the number of distinct partitions which occur in a 21 step walk being 455. This procedure can also be used in higher dimensions; the number of distinct partitions (for fixed N) will increase somewhat with dimension due to weakening connectivity constraints, but is still easily manageable on a medium sized computer. Some sample series for the one-dimensional case are given in table 1.

Assuming

$$\langle R_N^2\rangle \simeq N^{2\nu}, \qquad \langle S_N\rangle \simeq N^s \tag{9}$$

one can extract finite lattice estimates of ν and s via the standard ratio method

$$2\nu_N = \ln\{\langle R_N^2\rangle/\langle R_{N-2}^2\rangle\}/\ln\{N/(N-2)\} \tag{10a}$$

$$s_N = \ln\{\langle S_N\rangle/\langle S_{N-2}\rangle\}/\ln\{N/(N-2)\}. \tag{10b}$$

It is expected that the estimates for ν and s will converge to the same limit as $N\to\infty$. In the present case we have to deal both with finite lattice and crossover effects; the latter being due to the fact that for a given α one has distinct asymptotic behaviour respectively for $g=0$, g positive and g negative. In addition there is a variation in the expected asymptotic behaviour with α, as can be seen from figure 1.

In figure 2 we plot our finite lattice estimates for the exponent s against $\tanh(g)$ as compared with the effective medium predictions (7) and (8) for $\alpha = 1.4$, 1.0 and 0 and two different values of N, respectively 13 and 21. A similar picture holds for the estimates of ν. We can see that undoubtedly the general qualitative trend obtained from the effective medium predictions is followed. On the other hand, crossover effects

Table 1. Enumeration data at $g = 1.0$, for $\alpha = 0$, 0.2, 0.4 and 0.6.

(a) $\langle S_N \rangle$ series

N	$\alpha = 0$	0.2	0.4	0.6
1	2.000 000 00	2.000 000 00	2.000 000 00	2.000 000 00
2	2.268 941 42	2.299 159 88	2.336 151 48	2.381 241 17
3	2.537 882 85	2.598 319 76	2.672 302 96	2.762 482 33
4	2.774 440 96	2.834 727 34	2.916 277 38	3.026 774 21
5	3.015 978 74	3.077 656 38	3.167 142 12	3.296 700 04
6	3.201 628 28	3.259 538 65	3.350 770 35	3.493 596 16
7	3.404 368 78	3.457 509 69	3.548 838 36	3.701 915 38
8	3.552 216 07	3.602 488 83	3.694 563 93	3.857 728 25
9	3.724 806 70	3.768 762 83	3.858 001 72	4.026 929 65
10	3.850 712 23	3.891 220 28	3.979 890 02	4.156 079 93
11	4.001 936 17	4.035 298 54	4.119 422 14	4.298 347 72
12	4.115 133 45	4.143 650 57	4.225 502 56	4.408 982 19
13	4.250 327 09	4.271 286 52	4.347 519 90	4.531 554 58
14	4.355 006 70	4.369 878 09	4.442 296 88	4.628 534 66
15	4.477 364 19	4.484 606 85	4.550 811 73	4.736 054 01
16	4.575 333 58	4.575 688 19	4.636 923 82	4.822 481 57
17	4.687 115 01	4.679 926 26	4.734 658 47	4.918 127 93
18	4.779 292 95	4.764 795 57	4.813 781 10	4.996 115 70
19	4.882 324 61	4.860 374 65	4.902 719 14	5.082 182 32
20	4.969 343 80	4.939 907 59	4.976 013 86	5.153 250 38
21	5.065 145 53	5.028 289 93	5.057 671 34	5.231 453 12

(b) $\langle R_N^2 \rangle$ series

N	$\alpha = 0$	0.2	0.4	0.6
1	1.000 000 00	1.000 000 00	1.000 000 00	1.000 000 00
2	1.075 765 69	1.196 639 52	1.344 605 93	1.524 964 66
3	1.578 635 91	1.715 973 07	1.903 982 55	2.162 758 62
4	1.727 203 93	1.896 568 13	2.149 512 07	2.531 822 34
5	2.083 882 56	2.260 705 26	2.540 064 24	2.992 872 03
6	2.260 781 70	2.434 454 67	2.736 393 10	3.268 439 52
7	2.532 900 69	2.709 965 53	3.029 164 71	3.617 660 17
8	2.702 247 65	2.865 681 73	3.188 316 99	3.827 462 29
9	2.933 940 27	3.092 669 44	3.422 186 56	4.101 775 25
10	3.085 724 37	3.228 271 93	3.552 326 91	4.263 418 32
11	3.298 075 69	3.427 597 23	3.748 714 31	4.485 490 58
12	3.433 781 91	3.546 007 54	3.856 817 79	4.611 734 38
13	3.634 041 47	3.727 321 45	4.027 527 84	4.795 733 67
14	3.757 733 83	3.832 430 60	4.119 126 47	4.895 702 51
15	3.947 570 42	4.000 031 83	4.270 901 84	5.051 118 09
16	4.062 925 77	4.095 241 35	4.350 163 09	5.131 424 33
17	4.242 602 58	4.251 246 82	4.487 135 22	5.264 845 47
18	4.352 303 83	4.339 178 09	4.557 136 39	5.330 320 15
19	4.522 161 49	4.484 938 40	4.682 067 31	5.446 491 77
20	4.627 971 91	4.567 499 59	4.745 067 15	5.500 697 41
21	4.788 706 28	4.704 128 24	4.859 959 84	5.603 135 57

are strongly felt in the smoothing out of the finite lattice data (although such effects do become less pronounced as N increases). We discuss quantitative extrapolations of finite N data (via Neville tables) further on in this section. As concerns figure 2, we wish to recall the following.

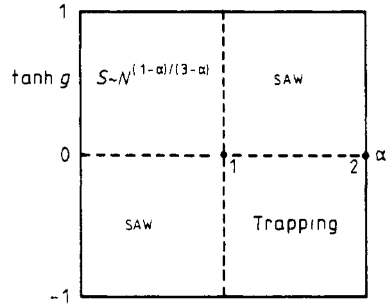

Figure 1. 'Phase diagram' for the generalised random walk in one dimension as predicted by the Flory approach. Pure random walk behaviour occurs along the broken lines.

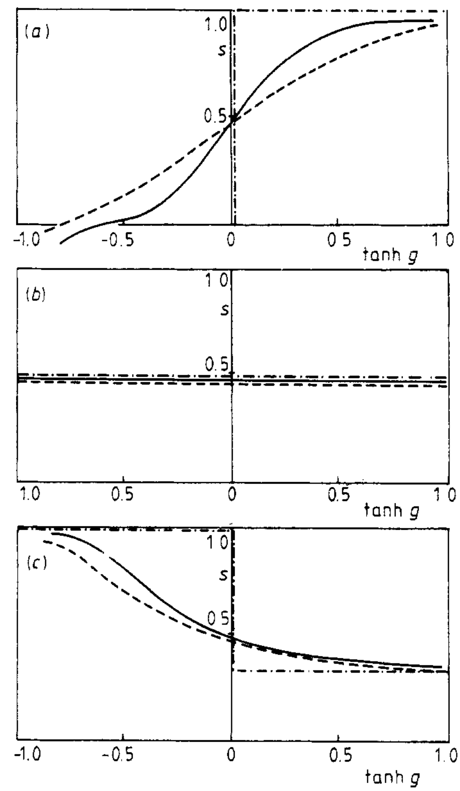

Figure 2. Plots of estimates of the exponent s (in 1D) found from (10b) for (a) $\alpha = 1.4$, (b) $\alpha = 1.0$ and (c) $\alpha = 0$ as a function of tanh(g). The full line denotes the $N = 21$ result, the broken curve the $N = 13$ results and the chain curve indicates the effective medium prediction (at $g = 0$ this always gives $s = \frac{1}{2}$).

(i) In figure 2(a) for $g < 0$, the apparently negative value of ν is due to the fact that expression (10b) was used in a region where one already has $\langle S_N \rangle < \langle S_{N-2} \rangle$, which signals the onset of the trapping region, in which the walk extent actually decreases for N larger than a certain critical value.

(ii) For the special case $\alpha = 1$, the finite lattice estimates for s are slightly off the exact value $\frac{1}{2}$, whereas for the $\langle R_N^2 \rangle$ series the exact value $\nu = \frac{1}{2}$ is reproduced for any finite N.

At this point we can state that all the exponent predictions from the effective medium arguments regarding trapping ($\alpha > 1$, $g < 0$) and self-avoiding walk behaviour ($\alpha > 1, g > 0$ and $\alpha < 1, g < 0$) have been found to hold from our exact enumeration data. Accordingly, we now concentrate on the $0 \leqslant \alpha \leqslant 1$, $g > 0$ region where anomalous diffusion is predicted.

In this region we find that the finite lattice estimates of ν against g exhibit a non-monotonic variation as a function of g. In fact the estimates consistently show a trough at a certain value of g before tending to the expected large g behaviour. For the $\langle R_N^2 \rangle$ series using odd–odd ratios this trough occurs at around $g \simeq 1.5$. This effect is probably due to the finite length of the series, but is still strong at $N = 21$ and $\alpha = 0$. This effect is not displayed in figure 2(c) as the value $\tanh(g) = 0.9$ ($g = 1.47$) is not yet in the region where the effect occurs for the span series.

In attempting to find the asymptotic exponents from the series data, it is important to choose values of g that minimise the finite lattice and crossover effects. This choice is somewhat arbitrary, but we found that values of g near the trough described above tended to give the best results. The results of series analysis at a sample value of g are described below.

Series extrapolations were peformed for various α at fixed $g = 1.0$, using Neville tables (see e.g. Gaunt and Guttman 1974). As can be expected from the variety of effects present in the problem, the Neville tables show considerable scatter. In general, the series for $\langle S \rangle$ behave better that those for $\langle R^2 \rangle$. Also note that for $N = 21$, $\langle R^2 \rangle$ series at $\alpha = 0$ are larger than $\langle R^2 \rangle$ series at $\alpha = 0.2$, reversing the behaviour at small N (see table 1), and a similar effect occurs in the $\langle S \rangle$ series. This can be explained from (8) by noting that a small value of α means a larger exponent but a smaller amplitude, thus, for small N the amplitude effect dominates and we see the ordering as in the first rows of table 1. At larger N, it is the largest exponent which matters and the ordering is eventually reversed. It is easy to show from (3) that indeed the first crossing, as N grows, is between the $\alpha = 0$ and $\alpha = 0.2$ walk.

In table 2 we show our estimates of the exponents s and ν obtained from Neville tables and for $g = 1.0$, as compared to the effective medium prediction (8). This table shows that although there is considerable scatter, the general trend predicted by (8) is clearly followed. In particular, the non-trivial feature that the exponents vary from $\frac{1}{3}$ to zero as α goes from zero to one (see figure 1), is explicitly shown. In addition the results are consistent with the scaling prediction $s = \nu$ for fixed α.

Table 2. Estimates of the exponents s and ν (see text) found from Neville tables, compared with the values predicted from the effective medium approximation (8).

α	s	ν	$(1-\alpha)/(3-\alpha)$
0	0.34 ± 0.04	0.32 ± 0.06	0.333
0.1	0.32 ± 0.04	0.27 ± 0.06	0.310
0.2	0.30 ± 0.03	0.23 ± 0.06	0.286
0.3	0.27 ± 0.03	0.20 ± 0.07	0.259
0.4	0.24 ± 0.03	0.19 ± 0.08	0.231
0.5	0.22 ± 0.03	0.15 ± 0.09	0.200
0.6	0.19 ± 0.03	0.10 ± 0.10	0.167
0.7	0.15 ± 0.03	small	0.130
0.8	0.09 ± 0.04	small	0.091
0.9	small	small	0.048

5. Summary and conclusions

We have discussed the asymptotic behaviour of one-dimensional correlated random walks in which configurations with multiple occupancy of sites are weighted by a factor proportional to the integral over the span of the αth power of the number of times each site is visited. Varying α between zero and two, and for attractive and repulsive correlations between repeated visits to a site, we have been able to explore the region between the interacting random walk of Stanley *et al* (1983) ($\alpha = 0$), and the Domb-Joyce model for a polymer chain ($\alpha = 2.0$). Both effective medium and exact enumeration results have been used and for one dimension we reach the following conclusions.

(i) For repulsive correlations and $0 \leq \alpha \leq 2$ (except at the special points $g = 0$ and/or $\alpha = 1$) one always has the asymptotic behaviour of the self-avoiding walk, with end-to-end distance exponent $\nu = 1$.

(ii) For attractive correlations and $1 < \alpha \leq 2$ the walks always collapse upon the origin, which we denote by 'trapping' behaviour.

(iii) For attractive correlations and $0 \leq \alpha < 1$ we find anomalous diffusion, with exponents which vary continuously with α.

Thus, while enabling us to proceed one step further towards a unified picture of the relevant features of correlated random walks, our results also set some general conditions for the existence of anomalous diffusion in one-dimensional systems.

The general agreement between exact enumeration results and the picture emerging from the peculiar phase diagram of figure 1 adds weight to the simple effective medium ideas used in the derivation of the latter. However, we are still far from understanding why Flory-like approximations usually work (apart from the usual general arguments about a fortuitous cancellation of errors); we are just faced with the fact that they do work in one more, and a particularly complicated, case.

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Note added in proof. A generalisation similar to the one described here for static random walks, may be considered for dynamic random walks. That is, generalisations of the 'true self-avoiding walk', to walks with weights given by equation (1) *and* having the local normalisation condition. These generalised walks have been studied in a recent preprint by Ottinger and he finds that the exponent ν depends continuously on α in this case also. We thank Professor Ottinger for sending us a preprint of his work.

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