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Renormalisation group approaches to an interacting walk model

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Abstract. Renormalisation group techniques are developed to treat scaling behaviour and crossover in the configurational properties of a one-dimensional N -step interacting random walk (equivalent to the two-state rotational isomeric model in polymer theory). Three approximate methods are first given for the root-mean-square value $\mathcal{R} = \sqrt{\langle R^2 \rangle}$ of the end-to-end length R of the walk, resulting in a crossover form $\mathcal{R} = N^{\nu} F(N/N_c(K))$ in the scaling regime in which N and $N_c(K)$ are both large, where $N_c(K)$ is an effective value of the number of successive steps for which the walk continues in the same direction because of the effect of the interaction K . Exact scaling equations are then derived for the distribution function $P(R)$ for the end-to-end length and its scaling behaviour is obtained. The relationship of these results to work on block probability distributions in magnetic systems is discussed.

1. Introduction

Random and interacting walks have been of considerable interest as models of probabilistic and kinetic processes, particularly growth and generalised diffusion, and especially as models for polymer chains, where different segments of the chain are known to interact with each other. In many kinetic processes the 'interactions' (e.g. hopping) are of short range; an exception is the Levy flight process. In the polymer the interactions are of two sorts: those which are of short range along the chain (caused by chemical interactions between neighbouring monomers), and those which are of long range along the chain (which arise from the fact that no two polymer segments can occupy the same element of volume in space, the so-called 'excluded-volume effect' (Freed 1972)). While walks with long-range interactions are difficult to treat within the simple geometrical schemes that we present on account of their non-Markovian features, it is possible to treat walks with short-range interactions by our methods, and thus, for instance, to gain an understanding of many kinetic models and of the configurational properties of polymers at the Flory point (Freed 1972).

There are several models of interacting walks that interpolate between the pure random walk (RW) and the self-avoiding walk (SAW) limits, which correspond respectively to zero and infinite interaction strength. Of these, our model is one which bears a formal analogy to the Ising model and is one which has long been in use by polymer theorists, the so-called 'rotational isomeric' model (Volkenstein 1963, Birshtein and Ptitsyn 1966, Flory 1969). In essence, this is a model for polymers with hindered

internal rotation, in which a monomer is assumed to have r distinct possibilities of orientation with respect to the one that immediately precedes it, where r corresponds to the number of minima in the potential that governs this rotation. Each orientational state can be occupied with a certain probability, which is related to the depth of its corresponding minimum in the potential function. If we write $r = 2S + 1$, then there is a direct correspondence between the r -state rotational isomeric model and the $(2S + 1)$ Ising model; it turns out (Birshtein and Ptitsyn 1966) that for most cases of practical interest, r is small, and $r = 2$ or 3 are the cases most commonly treated in the literature (Volkenstein 1963, Birshtein and Ptitsyn 1966, Flory 1969). We deal therefore with the case $r = 2$; the case $r = 3$ is one to which our formalism can be trivially, if tediously, generalised.

In the absence of interactions, the kinetic process described by this model is simple diffusion, where the RMS end-to-end length \mathcal{R} of the N -step walk corresponds to the distance diffused in time N , and these variables are related by the non-interacting (random walk) result

$$\mathcal{R} \propto N^\nu \quad (1)$$

with exponent $\nu = \frac{1}{2}$. In interacting walks the relationship of \mathcal{R} to N involves non-trivial exponents and crossover between the behaviours they characterise. In polymers this crossover is between the different limiting configurational behaviours. In the kinetic processes the exponents are related to spectral dimensions and the crossover may be, for example, between diffusion and ballistic behaviour caused by interaction.

Such crossover in interacting walk models is described by a generalisation ('scaling form') of (1), given here. In addition to the RMS value $\mathcal{R} \equiv \sqrt{\langle R^2 \rangle}$ of the end-to-end length R , the full probability distribution $P(R)$ for R for an N -step interacting walk is of fundamental importance as it gives a much fuller characterisation of the configurations of the walk and thus of the polymer it represents, or alternatively, if one considers a growth process to be represented by the walk, of growth profiles. Moreover its Fourier transform is measured in diffraction experiments and is therefore of direct experimental significance. As will be shown in this paper, $P(R)$ and its Fourier transform are strongly affected by interactions, and they also show crossover between two limiting forms. The full crossover is obtained here in terms of two-variable scaling functions which completely describe the scaling regime where both the number of steps (N) and the interaction parameter (K) are large. In this regime, the distribution $P(R)$ is closely related to the universal distribution describing the block coordinate in the equivalent Ising model.

The methods used here to obtain these results are of the renormalisation group type. Some of the basic scaling and crossover behaviours can be obtained by simple approximate length scaling approaches. Three such schemes are developed, and provide generalisations of (1) to the interacting case. Next an exact transformation of the distribution $P(R)$ is derived from which the scaling and crossover properties of $P(R)$ and its Fourier transform are obtained.

The plan of the rest of the paper is as follows. Section 2 defines the model we use, and introduces the three approximate schemes devised to treat it. In § 3 we develop the exact scaling of the probability distribution $P(R)$ and obtain the other properties available from it. A discussion of our work, including its (formal) relationship to the de Gennes model of a polymer in a solvent (de Gennes 1979), and its contact with Bruce's results on asymptotic forms for probability distributions for block coordinates in Ising-like systems (Bruce 1981) is given in § 4.

2. The model: approximate scaling approaches

The two-state rotational isomeric model of a polymer can (together with biased diffusion and related growth models) be mapped onto the following interacting walk model. We consider a one-dimensional N -step walk in which a particular step is labelled by integer i (increasing along the chain) and its direction by a_i ($a_i = \pm 1$, where $+$ and $-$ correspond respectively to a right and left step) and where each step has a different probability according to whether it is in the same direction as or opposite to the immediately preceding one; the probability $P(a_i)$ for a step a_i can be expressed in terms of a_{i-1} as

$$P(a_i) = \exp(Ka_i a_{i-1}) (\exp(K) + \exp(-K))^{-1} \quad (2)$$

where K is a measure of bias in the walk or its related kinetic process, and where, in the polymer, K is the interaction strength divided by the thermal energy $k_B T$.

Our aim in this section is to determine, via scaling methods, the dependence of the RMS end-to-end length \mathcal{R} of the interacting walk on N , the number of steps, obtaining in particular the exponents characterising the asymptotic behaviours (cf (1)) and the crossover relationship that connects them.

We will describe here three approximate real space renormalisation group schemes that approach the problem from slightly different viewpoints. What unifies all of this is the following idea: as the quantity of interest to us is \mathcal{R} , we construct renormalisation group schemes that preserve \mathcal{R} exactly (cf § 2.1), or approximately (cf §§ 2.2 and 2.3) on a cluster, while decimating the number of steps (cf §§ 2.1 and 2.3) or the number of lattice sites (cf § 2.2) by a factor of two. The section concludes (§ 2.4) with an exact discussion of the crossover based on the exact length scaling statement from § 2.1 and the exact interaction scaling statement from § 2.3 (which is also obtainable from a magnetic analogue), a preliminary account of which has been given by Stinchcombe (1985).

2.1. 'de Gennes'-type decimation

The motivation for this scheme was found in the context of de Gennes' methods for applying renormalisation group concepts to the determination of ν for a polymer chain (de Gennes 1979).

His ideas, which were developed in the context of field theory, involved the grouping of successive chain subunits into renormalised subunits, subject to the preservation of the end-to-end length of the chain. In this spirit, we consider an N -step walk with step length a , where $x \equiv e^{-K}$ parametrises the interaction; we seek a renormalised a' such that the walker preserves \mathcal{R} by tracing out the same vectorial distance in a walk with half the number of steps. The resulting scaling equations are

$$a'^2 = 2a^2 [1 + (1 - x^2)/(1 + x^2)] \quad (3a)$$

$$N' = \frac{1}{2} N \quad (3b)$$

$$\mathcal{R}' = \mathcal{R}. \quad (3c)$$

The weight matching is obtained by stipulating (de Gennes 1979) that all interactions between two renormalised subunits must be taken into account for the determination of the renormalised interaction. Thus, to find the scaling of the interaction (i.e. x' in

terms of x) we use a majority rule that matches the weight of, e.g., an 'onward' step on the scaled walk to the net weight of all configurations on the original walk where 'onward' steps predominate. This results in

$$x'^2 = x^4(3 + x^2)/(1 + 3x^2). \quad (4)$$

This has fixed points $x^* = 1, 0$ related respectively to the random walk (rw) and the self-avoiding walk (SAW) (we ignore the unphysical $x^* = -1$, as $x \geq 0$ always). These two fixed points control the asymptotic scaling limits of the walk, in each of which a behaviour like (1) (but with different exponents $\nu, \tilde{\nu}$) occurs. With a scaling hypothesis of the form (de Gennes 1979)

$$R = af(N, x) \quad (5)$$

and the fact that R has been preserved under this scaling, we must have

$$R = af(N, x) = a'f(\frac{1}{2}N, x'). \quad (6)$$

At the fixed point $x^* = 1$, $f(N, x)$ then becomes $f(N, 1) \propto N^\nu$ where, from (3) and (6)

$$a/\sqrt{2a} = (N/2)^\nu / N^\nu \quad (7)$$

from which we see that $\nu = \frac{1}{2}$, as expected in this rw limit. As pointed out by de Gennes (1979) the recursive nature of the scaling technique imposes a power-law structure on $f(N, 1)$ and hence implies the existence of an exponent ν .

Similar considerations applied to the SAW fixed point $x^* = 0$ yield $f(N, 0) \propto N^{\tilde{\nu}}$ where

$$a/2a = (N/2)^{\tilde{\nu}} / N^{\tilde{\nu}} \quad (8)$$

and hence $\tilde{\nu} = 1$ as expected.

The crossover between these (exact) asymptotic behaviours which can be obtained from the scaling equations (3) and (4) is approximate because equation (4) is not exact. The transformation (4) of x was obtained by an approximate majority rule. It will be shown later that if one uses the (exact) interaction scaling from § 2.3, (4) can be replaced by an exact scaling equation which, with the use of (3), yields the exact crossover behaviour.

2.2. 'Series' method

With this method we make a direct comparison between walks on a lattice with lattice spacing l , and walks on a lattice with lattice spacing $l' = 2l$, subject to the approximate preservation of \mathcal{R} . Thus, unlike § 2.1, it is not the walk which is decimated but the lattice on which the walk is conducted. We look at this approach in two slightly different ways ((i) and (ii) below).

(i) A renormalised site (replacing a two-site cell of the original lattice) is said to be visited if an arbitrarily selected site, say the second site, in its generating cell is visited (cf Napiorkowski's 'centre rule' (Hoye and Napiorkowski 1980)). A renormalised nearest-neighbour step then corresponds to all possible walks that start on a selected site in one cell and terminate on the corresponding site in the neighbouring cell without visiting selected sites in other cells; as an approximation we consider walks with a maximum of four steps. The decimation can be described in terms of

figure 1, where + and ○ represent undecimated and decimated sites respectively. Let $S \equiv \kappa/(1+x^2)$, $T \equiv \kappa x^2/(1+x^2)$ be the weights attached to direct and reversed steps respectively, where $x \equiv e^{-\kappa}$ and κ is the fugacity attached to a step. The weight S' of the direct step spanning AB on the decimated lattice is then the combined weight of all two- and four-step walks on the original lattice that (assuming A was approached from the left) start at A and end at B, but are otherwise allowed to visit $0, A, 0_1, B, 0_2$ in an arbitrary fashion:

$$S' = S^2 + 3T^2S^2 + S^3T. \tag{9}$$

Similarly,

$$T' = TS + T^2S^2 + 2T^3S + S^3T. \tag{10}$$

At the SAW fixed point $x^* = 0$, these give

$$\kappa' = \kappa^2$$

so that the fixed point value of κ is $\kappa^* = 1$ and the linearised scaling equation (in terms of $\delta\kappa \equiv \kappa - \kappa^*$ and $\delta\kappa' = \kappa' - \kappa^*$) is

$$\delta\kappa'|_{\kappa^*=1} = 2\delta\kappa|_{\kappa^*=1}. \tag{11}$$

This, with the (approximate) preservation of \mathcal{R} , a scaling relation of the form $\mathcal{R}/l \sim (\delta\kappa)^{-\tilde{\nu}}$ and $l' = 2l$, implies

$$\frac{\mathcal{R}'/l'}{\mathcal{R}/l} = \frac{1}{2} = \frac{\delta\kappa^{\tilde{\nu}}}{\delta\kappa'^{\tilde{\nu}}} = \frac{1}{2^{\tilde{\nu}}} \tag{12}$$

so that $\tilde{\nu} = 1$, as expected.

Equations (9) and (10) also yield a RW fixed point $x^* = 1$ at which $T = S = \kappa/2 = \mu$ (which is the effective fugacity in this limit) satisfies

$$\mu' = \mu^2 + 4\mu^4. \tag{13}$$

The only real fixed point of this equation is at $\mu^* = 0.5$ which, with reasoning similar to that of (12), gives $\nu = 0.63$ (the exact values of μ^* and ν are both 0.5 in this limit).

(ii) We now choose a smaller cluster (Family and Gould 1984) and match the renormalised nearest-neighbour step on the new lattice to all walks that start at A and end at B (see figure 2), and are otherwise free to visit the sites A, 0_1 , B in an arbitrary fashion, provided they do not leave the chosen cluster. The notation is as in (i) above and the equations for S' and T' are

$$S' = S^2 + (2S^2T^2)/(1 - T^2) \tag{14}$$

$$T' = TS + (2T^3S)/(1 - T^2). \tag{15}$$

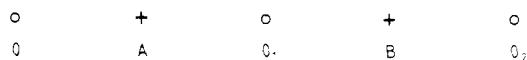


Figure 1. Chosen cluster for § 2.2(i).

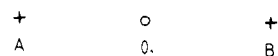


Figure 2. Chosen cluster for § 2.2(ii).

At the SAW fixed point $x^* = 0$, we recover (11), obtaining $\bar{\nu} = 1$, as before. At the RW fixed point $x^* = 1$, using $T = S = \mu$ as before, (14) and (15) reduce to

$$\mu' = \frac{\mu^2(1 + \mu^2)}{(1 - \mu^2)}. \tag{16}$$

The only real fixed point of this equation is at $\mu^* = 0.54$, which with reasoning along the lines of (12) gives $\nu = 0.58$.

Thus in both (i) and (ii) the asymptotic behaviour is exact in the SAW limit but approximate in the RW limit. Extensions of the method to overcome this limitation (which is a prerequisite for any adequate treatment of the full crossover) are very cumbersome so we return hereafter to scaling methods which decimate the walk rather than the lattice. The methods of this section are, however, simple and useful ways of investigating interacting walk problems as well as, e.g., problems involving random walks on random lattices.

2.3. Block distribution scaling (ternary approximation)

As in § 2.1, we decimate here the number of steps, but instead of considering just the root-mean-square value \mathcal{R} of the end-to-end distance R , we now consider its probability distribution $P(R)$. Since this provides a more detailed description of the configurational properties of the chain, its scaling properties are very important. The method of this subsection is based on a ‘blocking’ approximation to preserve \mathcal{R} under a decimation procedure that involves halving the number of steps at each stage of scaling. As will be evident, it is a ternary version of the exact scaling to be presented in § 3, and was the motivation for the latter: it also provides a useful exact scaling equation for the interaction parameter x . The consecutive steps of the walk are ‘blocked’ here into groups of two at each stage of scaling with the (approximate) blocking rules given by the majority rule illustrated in figure 3. This procedure is then used to obtain the scaling of the step length a and the interaction parameter x .

If $P_n(R)$ denotes the distribution for the end-to-end length R of a 2^n -step walk, it is straightforward to show that in terms of a (the step length), the first few distributions are given by

$$P_1(R; a, x) = (1 + x^2)^{-1} [\delta(R - 2a) + 2x^2\delta(R) + \delta(R + 2a)] \tag{17}$$

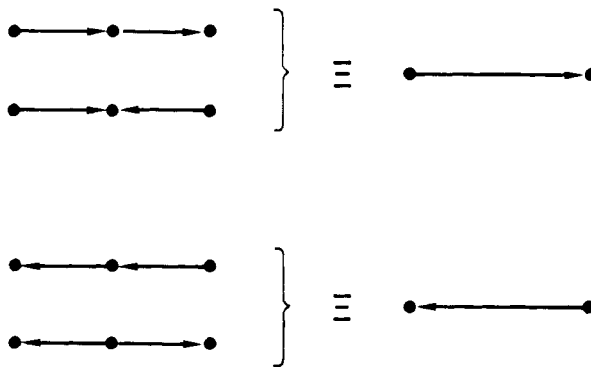


Figure 3. Schematic representation for ‘blocking’ rule in § 2.3.

$$\begin{aligned}
 P_2(R; a, x) = & (1+x^2)^{-3} \{ [\delta(R-4a) + (x^2+x^4)\delta(R-2a) + x^6\delta(R)] \\
 & + [(x^2+x^4)\delta(R-2a) + 2(x^2+x^4)\delta(R) + (x^2+x^4)\delta(R+2a)] \\
 & + [\delta(R+4a) + (x^2+x^4)\delta(R+2a) + x^6\delta(R)] \} \tag{18}
 \end{aligned}$$

etc. (The distributions P_n are normalised to 2 for convenience.) The two-step distribution P_1 has a ternary form, and the scaling procedure is to regard P_2 as a renormalised form of $P_1(R; a, x)$ (corresponding to a doubled number of steps), i.e. similar to (17) but with renormalised parameters x', a' . Unfortunately P_2 does not in general have the ternary form, so the matching of P_2 to P_1 is only approximate and involves a grouping of the terms on the right-hand side of (18) according to the blocking rules. This grouping has already been carried out in (18). From the matching of the weight of a blocked configuration to the combined weight of its component configurations we then have

$$\frac{x'^2}{(1+x'^2)} = \frac{2x^2}{(1+x^2)^2} \tag{19}$$

As will be discussed later, this equation is exact. From matching the contributions of a blocked configuration and its component configurations to the $(2m+1)$ th moments $\int R^{2m+1}P(R) dR$ of R we obtain

$$\frac{(a')^{2m+1}}{1+x'^2} = (a)^{2m+1} \left(\frac{2^{2m+1}}{(1+x^2)^3} + \frac{x^2}{(1+x^2)^2} \right) \tag{20}$$

which will be seen to be independent of m (and exact) only at the SAW limit. (19) has fixed points at $x^* = 1, 0$, corresponding respectively to the RW and SAW limits. Inserting $x^* = 0$ in (20), one obtains for the SAW limit

$$a' = 2a. \tag{21}$$

Using the scaling hypothesis (5) and the fact that we preserve \mathcal{R} (approximately) under this scaling, we obtain

$$\frac{\mathcal{R}'}{\mathcal{R}} = 1 = \frac{a'f(N/2, 0)}{af(N, 0)} \tag{22}$$

which, together with (21), implies $f(N, 0) \propto N^{\tilde{\nu}}$ with the exact value $\tilde{\nu} = 1$, as expected.

At the RW fixed point $x^* = 1$, (20) gives $a'^{2m+1} = \frac{1}{2}a^{2m+1}(2^{2m} + 1)$ and the m dependence reflects the fact that the real distribution P_2 is not ternary. The approximate nature of the RW treatment reflects the *approximate* matching of non-ternary distributions to ternary form. This does not affect the description of the SAW end because when there are no reversals the form of the distribution does not change under scaling (it is always binary). The evolution of the form of the distribution function in the general case strongly suggests the need to set up an exact scaling for the probability distributions $P(R)$. This is done in § 3, and not only leads to the exact scaling properties of \mathcal{R} but, which is more important, of the whole distribution.

2.4. Exact crossover and scaling forms

In this subsection we use results already derived to obtain the exact crossover and scaling behaviour of the RMS end-to-end distance \mathcal{R} . The approaches of §§ 2.1 and 2.3 both decimate the number of steps. While the scaling equations (3a)-(3c) for a ,

N and \mathcal{R} are exact in § 2.1, equation (4) for the scaling of the interaction parameter x is approximate. On the other hand the approach in § 2.3 provides the exact interaction scaling equation (19). This statement can be verified by comparison with the exact treatment given in § 3. Another way of seeing that (19) is exact is by using the relationship of the walk to an equivalent Ising problem in which, by the usual decimation by dilatation factor $b = 2$ preserving the correlation length, one has the exact scaling relation for the interaction

$$t' = t^2$$

with $t = \tanh K$ where K is the interaction parameter. This equation, which is also one of the results of § 3, is equivalent to (19). The exact scaling equations (3a)–(3c), and (19) written in terms of the variable t rather than x , can be used to show that each of the three quantities, \mathcal{R} , $N \ln 1/t$ and Na are invariant under scaling (in the scaling region $t \rightarrow 1$), and hence, using the fact that \mathcal{R} is proportional to a ,

$$\mathcal{R}^2 = N^2 a^2 F(N \ln t^{-1}). \quad (23)$$

This is an exact scaling form for the RMS end-to-end length of the N -step interacting walk. $N_c(K) \equiv 1/\ln t^{-1}$ can be interpreted as the average number of steps between reversals in the walk, which gives an understanding of the crossover variable $N/N_c(K) \equiv N \ln t^{-1}$ in (23). By considering the scaling equations at the fixed points of (19) one recovers the results $\nu = \frac{1}{2}$, $\tilde{\nu} = 1$ or (equivalently) the following statements concerning the asymptotic forms of the scaling function F in (23):

$$\begin{aligned} F(X) &\sim A & X &\ll 1 \\ &\sim BX^{-1} & X &\gg 1 \end{aligned} \quad (24)$$

where A, B are constants. (23) describes the exact crossover between the random walk ($\nu = \frac{1}{2}$, $N \gg N_c(K)$) and self-avoiding walk behaviour ($\tilde{\nu} = 1$, $N \ll N_c(K)$).

3. Exact scaling of block probability distributions

In this section we use methods first developed in connection with the conductivity of percolation clusters (Stinchcombe and Watson 1976) to investigate the exact scaling of the distribution $P(R)$ governing the end-to-end length R of our walk. The approach involves an exact generalisation of the viewpoint employed in § 2.3. The full distribution $P_n(R)$ for the 2^n -step walk is given by

$$P_n(R) = \frac{1}{2}[(1+t)P_{ns}(R) + (1-t)P_{nr}(R) + (1+t)P_{ns}(-R) + (1-t)P_{nr}(-R)] \quad (25)$$

where the $P_{ns}(\pm R)$ and $P_{nr}(\pm R)$ represent the 'onwards' and 'reversed' parts of the total distribution $P_n(R)$; for example $P_{ns}(+R)$ labels all walks which were entered from the left and go out to the right and $P_{nr}(-R)$ labels all walks which were entered from the right and go out to the right. The normalisation conditions are

$$\int_{-\infty}^{+\infty} P_{ns}(\pm R) dR = \int_{-\infty}^{+\infty} P_{nr}(\pm R) dR = 1 \quad (26a)$$

$$\int P_n(\pm R) dR = 2. \quad (26b)$$

The distribution $P_{n+1}(R)$ can be generated by combining two walks of half the number of steps (each described by $P_n(R)$) and continuing recursively. This process was already considered in the approximation of § 2.3, and is sufficient to give the full solution for the distribution and its scaling properties. The way in which this is done is by combining the constituent distributions $P_{ns}(\pm R)$ and $P_{nr}(\pm R)$ subject to the requirement that a walk going out to the right (left) can only combine serially with one coming in from the left (right). Furthermore, the resultant end-to-end length R' appearing in $P_{n+1}(R')$ is given by the sum of the end-to-end lengths R_1 and R_2 appearing in the original distributions $P_n(R_1)$ and $P_n(R_2)$. It follows that the scaling of P_n to P_{n+1} (or in more usual notation, of P to P') is described by integral equations of the following form:

$$\begin{aligned} & \frac{1}{2}(1+t')P'_s(R') \\ &= \iint_{-\infty}^{+\infty} dR_1 dR_2 \delta[R' - (R_1 + R_2)] \\ & \quad \times \left[\frac{1}{4}(1+t)^2 P_s(R_1)P_s(R_2) + \frac{1}{4}(1-t)^2 P_r(R_1)P_r(-R_2) \right] \end{aligned} \tag{27}$$

$$\begin{aligned} & \frac{1}{2}(1-t')P'_r(R') \\ &= \iint_{-\infty}^{+\infty} dR_1 dR_2 \delta[R' - (R_1 + R_2)] \\ & \quad \times \frac{1}{4}(1-t^2) [P_s(R_1)P_r(R_2) + P_r(R_1)P_s(-R_2)] \end{aligned} \tag{28}$$

and likewise for $R \rightarrow -R$. The $t \rightarrow t'$ recursion relation is obtained as usual (Stinchcombe and Watson 1976) by integrating (27) or (28) with respect to R' , and is easily seen to be

$$t' = t^2. \tag{29}$$

Equations (27), (28) and (29) are the basic scaling relations governing the exact evolution of $P(R)$ in our model.

The scaling equations can be used to obtain the scaling properties of the RMS value \mathcal{R} of the end-to-end length or of its full and constituent distributions. Because of their convolution form, Fourier transformation reduces the scaling equations to the following algebraic equations:

$$\frac{1}{2}(1+t')F'_s(\pm k) = \left[\frac{1}{2}(1+t) \right]^2 \sqrt{2\pi} F_s^2(\pm k) + \sqrt{2\pi} \left[\frac{1}{2}(1-t) \right]^2 F_r(\pm k) F_r(\mp k) \tag{30}$$

$$\frac{1}{2}(1-t')F'_r(\pm k) = \sqrt{2\pi} \frac{1}{4}(1-t^2) [F_s(\pm k)F_r(\pm k) + F_r(\pm k)F_s(\mp k)]. \tag{31}$$

Here $F_s(\pm k)$, $F_r(\pm k)$ are the Fourier transforms of $P_s(\pm R)$ and $P_r(\pm R)$ respectively and the $\sqrt{2\pi}$ appear as a consequence of our choice of symmetric normalisation in the Fourier transform integral (see the appendix) and its inverse. If we now define $G(k)$ as the Fourier transform of $P(R)$, then we have for the n th stage of iteration

$$G_n(k) = \frac{1}{2}(1+t)[F_{ns}(k) + F_{ns}(-k)] + \frac{1}{2}(1-t)[F_{nr}(k) + F_{nr}(-k)]. \tag{32}$$

Also, the mean square end-to-end length \mathcal{R}^2 is given by

$$\mathcal{R}^2 = -\frac{1}{2}\sqrt{2\pi} (d^2/dk^2) G(k)|_{k=0}. \tag{33}$$

After some algebra (see the appendix) it may be shown that, if we write $N \equiv 2^n$, the

mean square end-to-end length appropriate to the n th stage of iteration is given by

$$\mathcal{R}_n^2 \equiv \langle R_n^2 \rangle = Na^2 \left(\frac{1+t}{1-t} \right) - 2ta^2 \frac{(1-t^N)}{(1-t)^2} \tag{34}$$

in agreement with the result of Stanley (1971) derived from a different viewpoint.

In the scaling region (N large and t close to 1), we can write this as

$$\mathcal{R}_n^2 = 2N^2 a^2 \left(\frac{1}{X} - \frac{(1-e^{-X})}{X^2} \right) \tag{34'}$$

where $X \equiv N \ln t^{-1}$ ($\sim 2N e^{-2K}$ for $K \gg 1$) is our crossover variable. If we make the equivalence

$$F(X) \equiv 2 \left(\frac{1}{X} - \frac{(1-e^{-X})}{X^2} \right) \tag{35}$$

we have a result consistent with (23), with the explicit form of our crossover function given by (35). The asymptotic forms of (35) are

$$\begin{aligned} F(X) &\sim 1 && X \ll 1 \\ &\sim 2/X && X \gg 1 \end{aligned} \tag{36}$$

consistent with (24).

We now consider the asymptotic behaviours of (30) and (31) and associated ‘invariant’ distributions. If the interaction K is small, the walk is always of *rw* type, while if K is large, the walk has a *saw* nature until N becomes so large that crossover to *rw* behaviour occurs. The asymptotic dependences are governed by the fixed points $t^* = 0, 1$ of (29). At $t^* = 1$ (*saw* limit) only $P_s(\pm R)$ contribute to $P(R)$ and the scaling of the related Fourier transforms are, from (30),

$$F'_s(\pm k) = \sqrt{2\pi} F_s^2(\pm k). \tag{37}$$

It follows that $P_s(\pm R)$ retain their initial single delta function form (cf the appendix, equations (A16) and (A17)) under scaling with an effective step length that scales at each stage as

$$a' = 2a \tag{38}$$

and that the invariant distribution $P^*(R)$ remains of binary form under repeated iterations in this limit. Thus with the usual scaling arguments, we recover $\tilde{\nu} = 1$. The binary distribution just arrived at is one of the two ‘invariant’ distributions whose shape is unchanged on scaling, and only its scale (a in this case) changes.

By considering the other fixed point $t^* = 0$ (*rw* limit), we similarly find the other invariant distribution. In this case the symmetry of the zeroth-order distributions with respect to ‘direct’ and ‘reversed’ steps (cf equations (A16) and (A17) in the appendix) is maintained, and $P_s(\pm R)$ and $P_r(\pm R)$ contribute equally to $P(R)$, at all stages of scaling. The Fourier transform $G(k)$ then scales like

$$G'(k) = \frac{1}{2} \sqrt{2\pi} G^2(k) \tag{39}$$

from an initial form $(2/\sqrt{2\pi}) \cos ka$. It will be seen that after n iterations, the form of $G_n(k)$ is approximately Gaussian in the small k regime corresponding to our scaling

region: i.e. with $N \equiv 2^n$

$$\begin{aligned}
 G_n(k) &= (2/\sqrt{2\pi}) \cos^N ka \\
 &\sim (2/\sqrt{2\pi}) \exp[N \ln(1 - k^2 a^2/2 + \dots)] \\
 &\sim (2/\sqrt{2\pi}) \exp(-k^2 \Sigma_n^2/2)
 \end{aligned}
 \tag{40}$$

with $\Sigma_n \equiv \sqrt{Na} = \sqrt{2^n}a$.

Thus the invariant form of $P(R)$ describing the rw limit is also Gaussian to this approximation in the scaling region, with an effective step length Σ which scales as

$$\Sigma' = \sqrt{2}\Sigma
 \tag{41}$$

so that $\nu = \frac{1}{2}$, again using the usual scaling arguments.

The crossover from saw to rw behaviour in the scaling regime N and K both large can be discussed by considering the neighbourhood of the fixed point $t^* = 1$. Accordingly, the scaling equations (30) and (31) were iterated numerically for $t = 0.99$, and the distributions $P(R)$ and $G(k)$ determined at various stages of iteration. The scale of the R (or k) dependence of these distributions is set by \mathcal{R}_n/N^2 , while the dependence on N and K involves the crossover variable $N \ln t^{-1}$. Hence $P(R)$ and $G(k)$ have two-variable scaling forms

$$P(R; N, K) = \mathcal{P}(R(\mathcal{R}_n/N^2), N \ln t^{-1})
 \tag{42}$$

$$G(k; N, K) = \mathcal{G}(k(N^2/\mathcal{R}_n), N \ln t^{-1})
 \tag{43}$$

respectively, with \mathcal{R}_n given by (34').

Results of numerical iteration of the scaling equations are consistent with (42) and (43). Figures 4 and 5 show plots of $\mathcal{P}(R(\mathcal{R}_n/N^2), N \ln t^{-1})$ against $R(\mathcal{R}_n/N^2)$ for various values of the crossover variable $N \ln t^{-1}$. It can be seen that the dependence of the three variables R , N and K is properly represented by the two-variable scaling

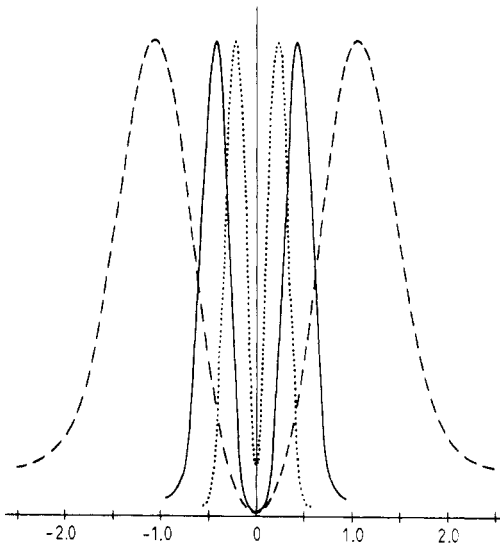


Figure 4. Plots of $\mathcal{P}(R(\mathcal{R}_n/N^2), X)$ against $R(\mathcal{R}_n/N^2)$ for values of $X \equiv 2^n \ln t^{-1} = 0.04$ (---), 10.29 (—) and 41.17 (···). Note the narrowing towards the origin of the distributions for increasing values of the crossover variable X .

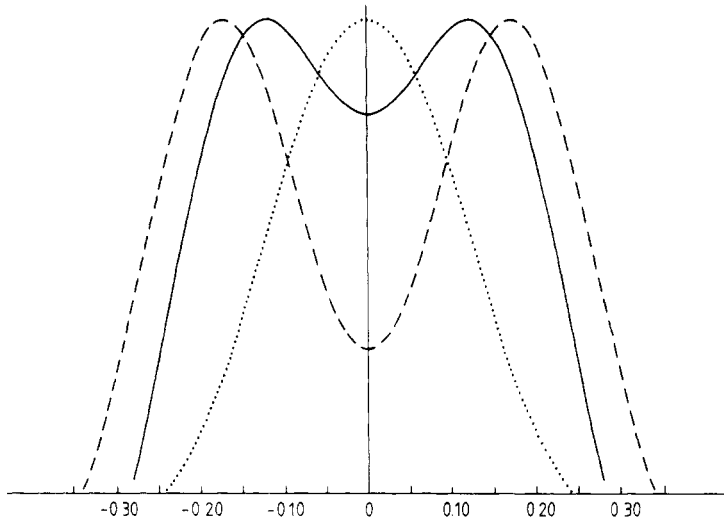


Figure 5. Plots of $\mathcal{P}(R(\mathcal{R}_n/N^2), X)$ against $R(\mathcal{R}_n/N^2)$ for values of $X \equiv 2^n \ln t^{-1} = 82.33$ (---), 164.66 (—) and 329.33 (···), showing the evolution towards a single-peaked distribution for increasing values of the crossover variable X .

form, and that the distribution crosses over from a binary to a ‘Gaussian’ form (i.e. from the SAW invariant distribution to the RW one) as the crossover variable varies from small to large values. The intermediate cases are of special interest.

Results are also displayed, in figures 6 and 7, for $G(k; N, K)$ —this quantity is of importance for scattering analyses. The plots are of $\mathcal{G}(k(N^2/\mathcal{R}_n), N \ln t^{-1})$ against $k(N^2/\mathcal{R}_n)$ for various values of $N \ln t^{-1}$. Once again, crossover is seen to occur between the oscillatory form of the invariant distribution corresponding to the SAW

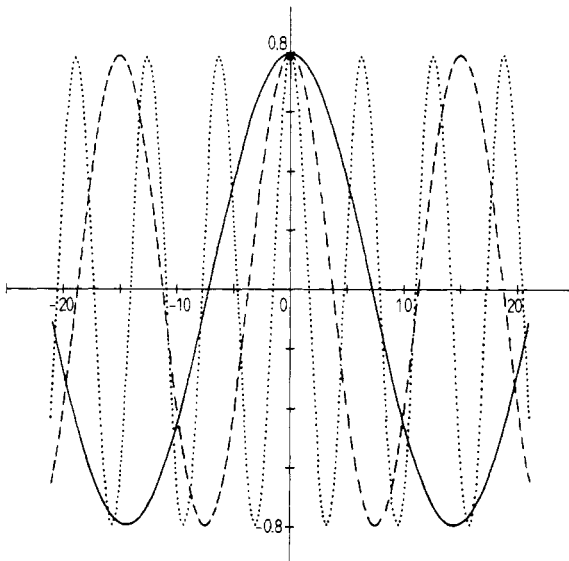


Figure 6. Plots of $\mathcal{G}(k(N^2/\mathcal{R}_n), X)$ against $k(N^2/\mathcal{R}_n)$ for values of $X \equiv 2^n \ln t^{-1} = 0.04$ (···), 10.29 (---) and 41.17 (—). Note the broadening of the distributions for increasing values of the crossover variable X .

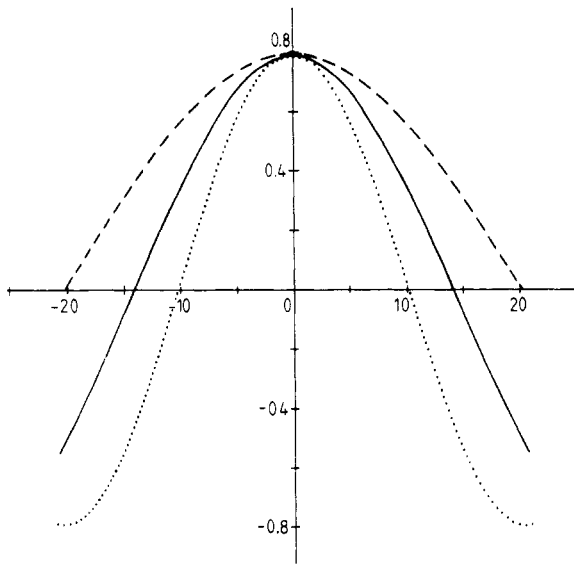


Figure 7. Plots of $\mathcal{G}(k(N^2/\mathcal{R}_n), X)$ against $k(N^2/\mathcal{R}_n)$ for values of $X \equiv 2^n \ln t^{-1} = 82.33$ (\cdots), 164.66 (—) and 329.33 (---). The distribution evolves towards a 'Gaussian-like' form for increasing values of the crossover variable X .

limit (small $N \ln t^{-1}$) and the 'Gaussian' form corresponding to the rw limit (large $N \ln t^{-1}$). Again the intermediate cases are of particular importance for comparison with real systems, as well as for the use of the scaling interpretation and the two-variable 'universal plots'.

4. Discussion

The main body of this paper has been concerned with applying real space renormalisation group techniques and associated scaling ideas to a specific interacting walk model. In § 2 we introduced three approximate decimation schemes to treat it, which are of considerable generality and can be used to look at different classes of problems, e.g. those involving random walks on random clusters, which are in turn related to problems of diffusion and aggregation. In § 3, we give for the first time the application of probability distribution scaling methods to an interacting walk model; in particular this enables us to get a direct grasp on configurational properties of polymers that can be represented by this two-state rotational isomeric model. The quantity $G(k)$ which we calculate is related to measurable neutron scattering cross sections and the system of equations (29)–(32) enables us in principle to look at chains of arbitrary length N .

The possible extensions of this work fall therefore into two main categories: modifications of the methods of §§ 2.1–2.3 and 3 should allow us to investigate related problems in kinetics, as well as walks with other types of short-range interactions, which could be based on different polymer models from the one we have chosen. Some of these extensions, including an interacting walk/polymer with a continuously variable bond angle (Mehta and Stinchcombe 1986), are currently being treated.

We now comment on the connection of our work to other work in this field. The crossover behaviour of our model bears a strong formal resemblance to that arising in the de Gennes model of a polymer in a good solvent (de Gennes 1979) though the

basic systems are quite different. The dilute limit of that model (density $\rho \rightarrow 0$) corresponds to the polymer showing strongly self-avoiding behaviour (cf our limit $x \rightarrow 0$). In the concentrated solution limit, interactions between different polymer chains cancel to give effectively non-interacting units (de Gennes 1979), so that the polymer chain can be satisfactorily modelled by a RW in this limit (cf our $x \rightarrow 1$). In the semidilute regime there is a crossover controlled by a characteristic length ξ (the 'blob' size) which is such that for all length scales $r < \xi$, the polymer shows self-avoiding behaviour, whereas for all $r > \xi$, it shows random-walk-type behaviour; this is exactly equivalent to the behaviour of our walk model for $0 \leq x \leq 1$, for $N < N_c$ and $N > N_c$ respectively, with N_c , the characteristic length given by e^{2K} .

Finally we discuss the relationship of our results to those of Bruce (1981) in his analysis, using transfer matrix methods, of universal block probability distributions for large one-dimensional Ising-like systems. The recursive scaling technique used by us is a much more direct way of approaching the scaling behaviour than transfer matrix approaches. Moreover this technique addresses (via (29)–(32)) chains of arbitrary length N and arbitrary characteristic length N_c . However, in the scaling regime of large N and N_c (equations (34)ff), the invariant forms we obtain for $P(R)$ are in agreement with those obtained by Bruce, and we display explicitly the crossover (dependent on the ratio N/N_c) that connects them.

Appendix. Derivation of \mathcal{R}_n^2

If we define

$$\alpha_n(k) \equiv \sqrt{2\pi}^{\frac{1}{2}}(1+t)F_{ns}(k) \quad (\text{A1})$$

$$\beta_n(k) \equiv e^{ika}\sqrt{2\pi}^{\frac{1}{2}}(1-t)F_{nr}(k) \quad (\text{A2})$$

$$\gamma_n(k) \equiv \sqrt{2\pi}^{\frac{1}{2}}(1+t)F_{ns}(-k) \quad (\text{A3})$$

the system of equations (30) and (31) take the form

$$\alpha_{n+1} = \alpha_n^2 + \beta_n^2 \quad (\text{A4})$$

$$\gamma_{n+1} = \gamma_n^2 + \beta_n^2 \quad (\text{A5})$$

$$\beta_{n+1} = \beta_n(\alpha_n + \gamma_n) \quad (\text{A6})$$

where the arguments of the functions α , β , γ are taken to be understood above, and hereafter. With u_n , v_n defined by

$$u_n \equiv \alpha_n - \gamma_n \quad (\text{A7})$$

$$v_n \equiv \alpha_n + \gamma_n \quad (\text{A8})$$

equations (A4)–(A6) take the form

$$u_{n+1} = u_n v_n \quad (\text{A9})$$

$$v_{n+1} = \frac{1}{2}[u_n^2(1+\lambda) + v_n^2] \quad (\text{A10})$$

where λ is a constant under scaling which can be evaluated from initial conditions.

Finally, if we define

$$l_n \equiv \frac{1}{2}[v_n + u_n(1 + \lambda)^{1/2}] \quad (\text{A11})$$

$$m_n \equiv \frac{1}{2}[v_n - u_n(1 + \lambda)^{1/2}] \quad (\text{A12})$$

equations (A9) and (A10) take the form

$$l_{n+1} = l_n^2 \quad (\text{A13})$$

$$m_{n+1} = m_n^2. \quad (\text{A14})$$

Using (32) and (A1)–(A14) we obtain

$$G_n(k) = \frac{1}{\sqrt{2\pi}} [(l_0^{2^n} + m_0^{2^n}) + \cos ka \left(\frac{\lambda}{1 + \lambda} \right)^{1/2} (l_0^{2^n} - m_0^{2^n})]. \quad (\text{A15})$$

If we now realise that our initial conditions for the zeroth-order distribution are

$$P_{0s}(R) = P_{0r}(-R) = \delta(R - a) \quad (\text{A16})$$

$$P_{0r}(R) = P_{0s}(-R) = \delta(R + a) \quad (\text{A17})$$

we can use the above to evaluate $F_{0s}(\pm k)$ and $F_{0r}(\pm k)$, where, for instance,

$$F_{0s}(k) = \frac{1}{\sqrt{2\pi}} \int e^{ikR} dR P_{0s}(R). \quad (\text{A18})$$

Using all the above equations, we can find $l_0(k)$, $m_0(k)$ and λ , and insert in (A15) to give us $G_n(k)$. We evaluate $G_n(k)$ in this manner to order (k^2) , which is sufficient to give us \mathcal{R}_n^2 from equation (33), and the result is equation (34).

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