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LETTER TO THE EDITOR

Resistance and related scaling properties of self-avoiding random walks

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Abstract. Three scaling exponents for random and self-avoiding chains are studied by direct renormalisation. These describe the end-to-end resistance of a conducting chain; the arc length of the shortest path traceable between the chain ends; and the arc length of chain in no loop. The scaling behaviours of these quantities are identical to first order in $\varepsilon = 4 - d$. (d is the space dimension.) For a long self-avoiding chain, we predict that each one is proportional to the chain length.

Recently, interest has been generated in the scaling properties of the end-to-end resistance, R, of random walks in d dimensions. Banavar *et al* (1983) considered unrestricted lattice chains. They found, by several methods including a Hamiltonian renormalisation group (RG) analysis, the following scaling law for the mean resistance of a random walk of length S: $\langle R(S) \rangle \sim S^{x(d)}$, where $x(d) \simeq \frac{1}{4}d$ for $2 < d < 4$.

In this letter we study the effect of 'excluded volume' or a self-avoiding tendency (see de Gennes 1979) on the resistance of a continuous random chain or walk. We also consider F, the fraction of chain arc in no loop, and L, the arc length of the shortest path between the chain ends; we discuss these in relation to R.

Our results are of general interest to the discussion of transport on fractal structures (Alexander and Orbach 1982, Leyvraz and Stanley 1983). When self-intersections are carefully treated, the unconstrained and self-avoiding chains provide two examples of inhomogeneous connected random fractals. By inhomogeneous, we mean that they contain bottlenecks which hinder the diffusion of a random walker on the fractal (Leyvraz and Stanley 1983, Rammal and Toulouse 1983).

It might be argued that the resistance of a *self-avoiding* chain or walk (SAW) is, trivially, proportional to its length, since it never intersects itself (by definition). This reasoning is insufficient. For example, consider a lattice SAW, constrained as usual not to occupy the same site twice. One can now make a (non-trivial) circuit by placing unit conductors not just along the chain backbone, but between any two *adjacent* sites occupied by the chain. The circuit which results contains many loops: in fact in our (off-lattice) calculation the number of such loops is infinite. Nonetheless, we predict that $\langle R(S) \rangle \sim S$, because $\langle F(S) \rangle$ remains finite as $S \to \infty$. The resistance is dominated by the fact that there are some places in the circuit where all the current must flow down a single strand; and the fraction $\langle F \rangle$ of chain in such strands is non-vanishing. In other words, the SAW is so extremely inhomogeneous that typically the end-to-end circuit may be broken with a single cut.

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Our calculation is to first order in ε, but the structure of the resulting flow diagram strongly suggests that this conclusion will not be altered by higher terms. Below we give an outline account of the calculation method and our results; a physical discussion follows.

We consider a Brownian chain, $X(s)$, $0<s<S$. The scale of s is chosen so that $\langle (X(S)-X(0))^2\rangle_0 = Sd$. Here '$\langle\ \rangle_0$' denotes average over the Wiener probability, P:

$$P[X(s)] = \exp\left(-\tfrac{1}{2}\int_0^S (\partial X/\partial s)^2\,\mathrm{d}s\right).$$

We refer to S as the arc length of the chain (des Cloizeaux 1980). The unit of resistance is chosen so that in the absence of any loops, $R = S$. The ensemble of Brownian chains is decomposed according to n, the number of conducting contacts, by using the identity

$$1 = \mathrm{e}^{-w_0\Delta}\sum_n (w_0\Delta)^n/n!$$

where $\Delta = \frac{1}{2}\iint \delta(X(s)-X(s'))\,\mathrm{d}s\,\mathrm{d}s'$, and w_0 is an arbitrary (positive) weight. We obtain, for the unconstrained (i.e. gaussian) case,

$$\langle R(S)\rangle_0 = \left\langle \mathrm{e}^{-w_0\Delta}\boldsymbol{R}\sum_n (w_0\Delta)^n/n!\right\rangle_0. \tag{1}$$

Here $\boldsymbol{R}$ acts to the right on a product of δ-functions, $\Pi_i\,\delta(X(s_i)-X(s_i'))$, by taking the resistance of the chain with contacts present between each pair of points (s_i, s_i') in the product. Note that if (1) is now expanded in powers of w_0 there are also δ-functions present to the left of $\boldsymbol{R}$; these must *not* be counted as conducting contacts.

We also define operators $\boldsymbol{L}$ and $\boldsymbol{F}$; $\boldsymbol{L}$ takes the arc length of the shortest path between the chain ends (allowing short-cuts at each s_i, s_i' pair) and $\boldsymbol{F}$ takes the fraction of arc points, s, for which there is no pair (s_i, s_i') in the product such that $s_i < s < s_i'$.

To include the effects of self-avoidance, we modify (1) by the weight $\mathrm{e}^{-w_s\Delta}$; w_s is the excluded volume parameter. Hence, for the general case,

$$\langle R(S)\rangle = \langle \mathrm{e}^{-w_s\Delta}\rangle_0^{-1}\left\langle \mathrm{e}^{-(w_0+w_s)\Delta}\boldsymbol{R}\sum_n (w_0\Delta)^n/n!\right\rangle_0. \tag{2}$$

We have used this expression to obtain an ε-expansion by the direct renormalisation method of des Cloizeaux (1980, 1981).

First (2) is expanded to second order in the dimensionless variables $y = w_0(2\pi)^{-d/2}S^{\varepsilon/2}$ and $z = w_s(2\pi)^{-d/2}S^{\varepsilon/2}$. This gives

$$\langle R(S)\rangle/S = 1 + [-2+\mathrm{O}(\varepsilon)]y\varepsilon^{-1} + [6+\mathrm{O}(\varepsilon)]y^2\varepsilon^{-2} + [12+\mathrm{O}(\varepsilon)]yz\varepsilon^{-2}. \tag{3}$$

Then the following are defined as series in y and z:

$$p(y,z) = \mathrm{d}(\ln\langle R\rangle)/\mathrm{d}(\ln S) - 1; \qquad V(y,z) = \partial p/\partial(\ln S).$$

We also define $g(z)$, the dimensionless second virial coefficient for the SAW, which characterises the chain swelling, and $W(z) = \partial g/\partial(\ln S)$. All these series diverge as $S\to\infty$. However, they may be rearranged to obtain series for V and W in terms of p and g (which remain finite). These are, to leading order,

$$V(p,g) = 2p(\varepsilon/4 - 3g + p) \tag{4}$$

$$W(g) = g(\varepsilon/2 - 4g). \tag{5}$$

These equations give, to first order in ε, a full description of the flow in the (p, g) plane as S is increased. This flow behaviour is shown schematically in figure 1. We have also obtained similar series for the exponents which describe the behaviour of $\langle F\rangle$ and $\langle L\rangle$. To this order $\langle R(S)\rangle$, $S\langle F(S)\rangle$, and $\langle L(S)\rangle$ *all scale exactly alike.*

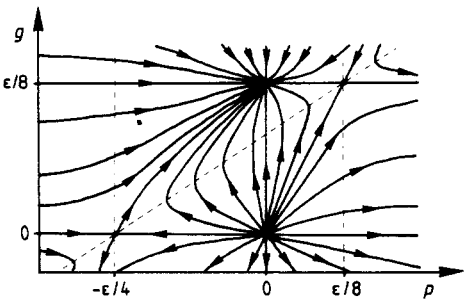

Figure 1. The motion in the parameter space (p, g) as $\ln S$ is increased (schematic). Tangents to the curves are $(V, W) = \partial(p, g)/\partial(\ln S)$. On the line $\varepsilon/4 - 3g + p = 0$, the tangents are vertical (i.e. $V(p, g) = 0$). The region $p > 0$ is physically inaccessible.

The scaling exponents are obtained as follows:

As $S \to \infty$, $\langle R(S)\rangle \sim S^{1+p^*(d)}$, where the fixed-point (FP) value, $p^*(d)$, is obtained by setting $V(p^*, g^*) = W(g^*) = 0$. Then the corresponding resistance exponent $x = 1 + p^*(d)$. There is one such exponent associated with each FP; the FP values, (p^*, g^*), are:

$$(p^*, g^*) = (0, 0), (-\varepsilon/4, 0), (0, \varepsilon/8) \text{ and } (\varepsilon/8, \varepsilon/8).$$

For a gaussian chain (i.e. $g = 0$) the FP at $(-\varepsilon/4, 0)$ is reached, giving $\langle R(S)\rangle_0 \sim S^{d/4}$, in agreement with Banavar *et al* (1983). However, for g non-zero (the case of a SAW) the corresponding solution of $V = 0$ in (4) gives an unstable FP at $(\varepsilon/8, \varepsilon/8)$. This FP can never be reached physically, since it has $p^* > 0$. The only stable FP is at $(0, \varepsilon/8)$. Thus, to first order in ε, for a self-avoiding chain, $\langle R(S)\rangle \sim S$ as $S \to \infty$.

To interpret figure 1 in a direct physical way, the parameter $x(S) = p(S) + 1$ may be thought of as a local 'exponent' or slope on the log/log plot of $R(S)$ against S. The final asymptotic exponent is that obtained as S tends to infinity. Rather than plotting $p(S)$ against S itself, it is more convenient to plot p against the parameter $g(S)$, which remains finite as $S \to \infty$. The asymptotic (FP) value of p is obtained when g reaches its own fixed-point value, g^*.

This use of g may at first seem slightly obscure; but des Cloizeaux (1980) has shown that in fact g (and not S) is the physically relevant parameter for the SAW. (Our results for the behaviour of g *itself* reproduce those given by des Cloizeaux (1981); this is because equation (5) above for $W(g)$ does not depend on p.)

In discussing the relative significance of F, R, and L, we note the following bounds (which are physically obvious)

$$S\langle F(S)\rangle \leqslant \langle R(S)\rangle \leqslant \langle L(S)\rangle \leqslant S. \tag{6}$$

The calculation given above is unable to distinguish between the first three of these quantities. For the case of a gaussian chain, they seem intuitively to be very different (in, e.g., $d = 3$). To check this point, the exponents must be obtained to greater accuracy;

this requires a calculation to order ε^2. We do not attempt this here. However it seems certain that all the exponents will be altered by higher terms, and that they will all become different.

In considering the resistance exponent for the unconstrained walk with conducting self-intersections, it is interesting to calculate the spectral dimension, d_s, of such a fractal. The result, which may be obtained easily by scaling arguments, is $d_s(d) = 2/(1+x(d))$. If one uses the first-order result for $x(d)$, (i.e., $x = \frac{1}{4}d$) the function $d_s(d)$ 'crosses' the celebrated Alexander–Orbach (1982) value of $d_s = \frac{4}{3}$ when $d = 2$. This suggests an intuitively appealing conjecture—that the conducting gaussian walk may become homogeneous, or nearly so, as $d \to 2$ (see Leyvraz and Stanley 1983).

We now consider the effect of higher terms on the asymptotic behaviour of $\langle R(S)\rangle$ for the SAW. Suppose we take the calculation to order ε^2. It is simple to show that there will still be a FP at $p^* = 0$ (with $g^* = \varepsilon/8 + O(\varepsilon^2)$). This is because there is a factor y in the series $p(y, z)$ and, correspondingly, a factor p in equation (4) to all orders. Unless the second-order shift of the unphysical FP at $(\varepsilon/8, \varepsilon/8)$ is so large as to move it into the physical half plane ($p^* < 0$), the resistance exponent for the SAW will be *unaffected.* Furthermore, in view of the flow pattern of figure 1, it seems improbable that *any* higher-order calculation would give a FP with g^* non-zero *and* $p^* < 0$. Unless this occurs, the asymptotic behaviour is always governed by the FP at $(0, \varepsilon/8 + \ldots)$. This argument applies equally to the quantities $\langle L(S)\rangle$ and $S\langle F(S)\rangle$. We therefore speculate that $\langle F(S)\rangle \to$ constant as $S \to \infty$, for all values of the space dimension, d. The resistance and shortest path, being bounded below by $S\langle F(S)\rangle$, are consequently proportional to the chain length.

These results are, at first sight, rather surprising. We offer the following comments.

The SAW ensemble is obtained from the gaussian ensemble by discarding all walks with any self intersections. (This must be contrasted with the 'true' self-avoiding walk of Amit *et al* (1983).) Because of the nature of this definition, it can be somewhat misleading to think of the SAW as though it were taken step by step in time. If one insists on such a picture, and wishes to consider a monodisperse ensemble of chain lengths, it is necessary to allow a very high degree of 'anticipation' on the part of the walker. In effect, the previous path of a random walker must be thought of as an *absorbing* barrier. Since we require the walk to survive for a certain number of steps (i.e., S is large and fixed), the entropic choice of the random walker is severely reduced if it comes even *remotely near* any region of space where it has been before.

It has, of course, been previously remarked (de Gennes 1979, McKenzie 1976) that the probability of an N-step SAW ending on a site very close to where it started is very small. However, it should also be noted that the relative probability of such a closed loop occurring *within* a *longer* SAW is much smaller still—because of the entropic constraints which the loop imposes on the *rest* of the SAW (by forcing its two 'tails' into proximity).

In the light of these remarks, our central conclusion, that $\langle F(S)\rangle$ tends to a constant for a long SAW (in any d), is perhaps easier to understand than it might at first seem.

Finally we record some further consequences of equations (4) and (5). By considering $D = \partial(V, W)/\partial(p, g)$ at the fixed points, we have obtained (to first order) exponents characterising the leading corrections to scaling.

At $(p^*, g^*) = (-\varepsilon/4, 0)$ the eigenvectors of D are along the directions $(2, 3)$ and $(1, 0)$. Hence for the gaussian chain ($g = 0$), the approach to $p^* = -\varepsilon/4$ is given by $(p - p^*) \sim S^{-\lambda}$, where $\lambda = -\partial V/\partial p|_{p^*} = \varepsilon/2 + O(\varepsilon^2)$. At the stable FP, $(0, \varepsilon/8)$, the eigenvectors of D are $(0, 1)$ and $(1, 0)$. Whilst the approach of g to $g^* = \varepsilon/8$ is given by

$(g - g^*) \sim S^{-\epsilon/2}$, we find that $p \sim S^{-\epsilon/4}$. Hence p for the SAW approaches its asymptotic value of zero *very slowly*. The corresponding behaviour of $\langle F \rangle$ is given by

$$\langle F(S) \rangle \sim (A + BS^{-\epsilon/4}),$$

whereas for the gaussian chain, one has

$$\langle F(S) \rangle_0 \sim S^{-\epsilon/4}(1 + CS^{-\epsilon/2}).$$

Here A, B and C are (non-universal) constants.

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