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LETTER TO THE EDITOR

**Biased diffusion on random networks: mean first passage time and DC conductivity**

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**Abstract.** Biased diffusion on a segment with a dangling end is considered, employing a method previously developed by the authors. It is shown that a definition of the drift velocity which is different from that of White and Barma leads to non-singular behaviour as a function of bias. The two approaches to biased diffusion are compared and a critique of their validity is presented.

In a recent publication, White and Barma (1984) studied the problems of diffusion on certain networks, including percolation clusters, under the influence of external bias. One of their results is that the drift velocity corresponding to a one-dimensional lattice with random length branches ('random comb' cf figure 1(a)) varies non-monotonically as a function of bias: it first increases, then decreases to zero. For a certain distribution of the branch lengths they find that the drift velocity vanishes above a critical (finite) value of the bias.

In the present letter we wish to revisit this problem on the basis of an exact method for analysing properties of random walks on networks, which we have recently developed (Goldhirsch and Gefen 1985a, b). Using our approach we present a new method for calculating the DC resistance (and consequently the drift velocity). We show that an identification of the drift velocity which is different from the one defined by White and Barma involves no singularity as a function of the bias. The alternative definition we propose seems to us physically appropriate. This drift velocity, which is proportional to the mean value of the DC current, actually increases with the bias. In the limit of infinite bias the mean first passage time diverges, but this fact describes a transient property of the system and does not imply a vanishing conductivity. Finally we verify that for the specific choice of the distribution of lengths of the side branches which was made by White and Barma, the average mean first passage time  $\langle t \rangle_{\text{MFT}}$  indeed undergoes a phase transition. This does not happen for most choices of such a distribution—and should be regarded as an artefact of this specific choice (which may not be of general applicability for percolation clusters). Moreover, in the calculation of White and Barma the effect of any side branch on the motion of the random walker is decoupled from the effects of the other side branches. This decoupling property does not seem to be of general validity (e.g. it is not valid for mean first passage times).

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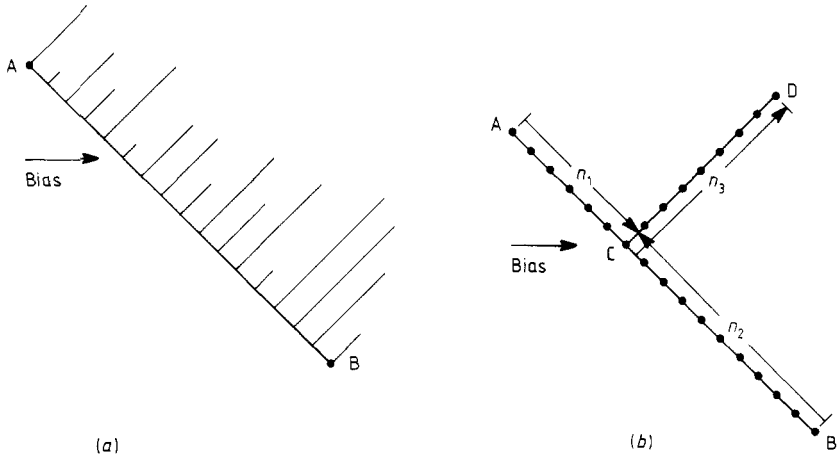


Figure 1. (a) A 'random comb'. (b) A segment with a single dangling end.

Consider for simplicity the network depicted in figure 1(b). There are  $n_1 + 1$  points on the segment AC,  $n_2 + 1$  points on CB and  $n_3 + 1$  points on CD. The field direction is as shown in the figure. A random walker is assumed to have a probability  $p_1 > 0$  (per step) to move parallel to the projection of the field and  $p_2 < p_1$  to move against it. A 'step' is assumed to last for a time  $\Delta t$  and lead the walker to a nearest neighbour only.

It is convenient to define the following quantities:

(a)  $\tilde{X}_i(n)$ —the probability to stay at a vertex for  $n$  steps. Hence:  $\tilde{X}_A(n) = (1 - p_1)^n$ ;  $\tilde{X}_C(n) = (1 - 2p_1 - p_2)^n$ ;  $\tilde{X}_B(n) = (1 - p_2)^n$ .

(b)  $\tilde{T}_{i,j}(n)$ —the probability to leave a vertex  $i$  (e.g. A) on the first step and reach vertex  $j$  for the first time after  $n$  steps, without having ever returned to  $i$ .

(c)  $\tilde{Q}_{i,j}(n)$ —the probability to leave vertex  $i$  on the first step and return to  $i$  for the first time after  $n$  steps, without having reached vertex  $j$  in the process.

(d)  $\tilde{G}_{i,j}(n)$ —the probability to start at  $i$  and reach  $j$  for the first time, after  $n$  steps (it is allowed to revisit  $i$ ).

Let  $P(n)$  be any of the above probability functions. It is convenient to define a corresponding generating function or  $\phi$  probability:

$$P(\phi) = \sum_{n=0}^{\infty} \tilde{P}(n) e^{i\phi n} \quad 0 \leq \phi < 2\pi. \tag{1}$$

It follows that  $G_{ij}(\phi = 0) = 1$  and that  $\langle t \rangle_{\text{MFT}}$  from A to B is:

$$\langle t \rangle_{\text{MFT}} = dG_{AB}/di\phi|_{\phi=0}. \tag{2}$$

(Note the difference between  $\langle t \rangle_{\text{MFT}}$  and the transversal time, as defined by White and Barma (1984).)

It is known that generating functions or  $\phi$  probabilities add and multiply like regular probabilities, except that one does not have to keep track of the number of steps involved. For example if  $\tilde{T}_{AC}(n)$  and  $\tilde{G}_{CB}(n)$  are as defined before then we obtain for  $\tilde{G}_{AB}$ :

$$\tilde{G}_{AB}(n) = \sum_{n_1=0}^n \tilde{T}_{AC}(n - n_1) \tilde{G}_{CB}(n_1). \tag{3}$$

The corresponding  $\phi$  probabilities satisfy

$$G_{AB}(\phi) = \tilde{T}_{AC}(\phi)G_{CB}(\phi) \tag{4}$$

which demonstrates our point.

Let  $(\alpha, \beta)$  be a segment of  $(n + 1)$  points with no branches (e.g. AC). Define  $T_n^+(\phi)$  as  $T_{\alpha\beta}(\phi)$  when the field points from  $\alpha$  to  $\beta$ ,  $T_n^-(\phi)$  as  $T_{\beta\alpha}(\phi)$  and  $Q_n(\phi)$  as  $Q_{\alpha\beta}(\phi)$ . It can be shown that  $Q_{\alpha\beta}(\phi) = Q_{\beta\alpha}(\phi)$  and

$$T_n^+(\phi) = (p_1/p_2)^n T_n^-(\phi), \tag{5}$$

cf Goldhirsch and Gefen (1985b). It follows that:

(a) The  $\phi$  probability  $Q_c(\phi)$  to walk from C to C without reaching A, B or D in the process is (the explicit dependence on  $\phi$  is suppressed for notational simplicity):

$$Q_c(\phi) = X_c / (1 - X_c(Q_{n_1} + Q_{n_2} + Q_{n_3})). \tag{6}$$

(b) The  $\phi$  probability to go from A to A without reaching C is

$$Z_A = X_A / (1 - X_A Q_{n_1}). \tag{7}$$

(c) Similarly for the vertex D

$$Z_D = X_D / (1 - X_D Q_{n_3}). \tag{8}$$

(d) The  $\phi$  probability  $S_C$  to leave C and return to C for the first time after having visited A or D is

$$S_C(\phi) = T_{n_1}^+ T_{n_1}^- Z_A + T_{n_3}^+ T_{n_3}^- Z_D. \tag{9}$$

(e) The  $\phi$  probability  $R_c$  to start at C and return to C without reaching B is

$$R_c(\phi) = Q_c / (1 - Q_c S_c). \tag{10}$$

(f) Finally

$$G_{AC}(\phi) = Z_A T_{n_1}^+ \tag{11}$$

$$G_{AB}(\phi) = Z_A T_{n_1}^+ R_c T_{n_2}^+ \tag{12}$$

Equation (12) expresses the generating function for the mean first passage time as an algebraic form in the basic  $\phi$  probabilities:  $T^{\pm}$ 's,  $Q$ 's and  $X$ 's. These quantities can be calculated (cf Goldhirsch and Gefen 1985b). We quote some of the results

$$T_n^+(\phi = 0) = (p_1 - p_2) / (1 - r^n) \quad T_n^-(\phi = 0) = r^n (p_1 - p_2) / (1 - r^n) \tag{13}$$

where  $r = p_2/p_1$ ; and

$$Q_n(\phi = 0) = p_2(1 - r^{n-1}) / (1 - r^n) \tag{14}$$

and

$$\langle t \rangle_{\text{MFT}} = \left. \frac{dG_{AB}(\phi)}{d\phi} \right|_0 \cdot \Delta t = \frac{p_1 r^{-n_3}}{(p_1 - p_2)^2} (1 - r^{n_3}) + \frac{n_1 + n_2}{p_1 - p_2} + O(nr^n) \cdot \Delta t \tag{15}$$

in the limit of large  $n_i$ 's.

For a sufficiently large branch length  $n_3$  the leading term in (15) is proportional to  $r^{-n_3}$  or  $\exp[n_3 \log(p_1/p_2)]$ . If we consider a distribution in the lengths of the side branch as chosen by Whitè and Barma (1984):

$$\text{Pr}(n_3) = C e^{-an_3} \quad 0 \leq n_3 < \infty \tag{16}$$

then  $\langle t \rangle_{\text{MFT}}$  diverges when  $\log p_1/p_2 > a$ . Hence  $p_1/p_2 = e^a$  is a singular point for  $\langle t \rangle_{\text{MFT}}$ . This criticality is not generic; had we chosen  $\text{Pr}(n_3) \propto \exp(-bn_3^k)$  or a power law  $\text{Pr}(n_3) \propto n_3^{-k}$ , no criticality would have resulted. ( $\langle t \rangle_{\text{MFT}}$  never diverges for  $k' > 1$ . It diverges for any non-zero bias for  $k' < 1$  and for any  $k$ . At percolation  $\text{Pr}(n) \sim n^{-k}$  and above it  $\text{Pr}(n) \sim \exp(n^{1-1/d})$ , see e.g. Stauffer (1979). In both cases no criticality exists at finite bias. (For the latter, however, we may have criticality due to atypical clusters.) We also remark that in the case of many branches or the 'random comb' that was originally considered by White and Barma, the contributions of the different branches do not decouple (Goldhirsch and Gefen 1985b) in the calculation of the  $\langle t \rangle_{\text{MFT}}$ .

Returning to the question of conductivity we note that if we assume a time independent density  $\rho$  of non-interacting particles at both end points A and B (e.g. by connecting both end points to large particle reservoirs of the same chemical potential), the current from A to B is given by

$$I_{\text{AB}} = \rho(T_{\text{AB}}^+ - T_{\text{AB}}^-)|_{\phi=0}/\Delta t. \quad (17)$$

Equation (17) follows from the fact that  $T_{\text{AB}}^+(\phi=0)$  is the total probability of a particle leaving A to reach B, without returning to A, and thus contribute to the net forward current. Similarly  $T_{\text{BA}}^-$  is proportional to the net backward current. It is rather easy to see that  $T_{\text{AB}}^\pm(\phi=0)$  does not depend on the existence of a side branch. All the side branch can do is *delay* the arrival of a particle. The *total* probability of arrival is unaffected by its existence. Another way to see this fact is by noting that the total probability of a walker who wandered into the sidebranch CD—to return to C is 1 for every finite length branch. This observation is, of course, verified on the relevant formulae (Goldhirsch and Gefen 1985b). Let thus  $V$  be the potential difference between points A and B. It follows from the above discussion that the resistance between these points is given by

$$R_{\text{AB}} = \frac{V\Delta t}{\rho(T_{n_1+n_2}^+(\phi=0) - T_{n_1+n_2}^-(\phi=0))}. \quad (18)$$

Assuming  $p_1 = K \exp(E/k_B T)$ ,  $p_2 = K \exp(-E/k_B T)$  where  $E$  is the field component along AB and  $k_B T$ , the Boltzmann factor, and denoting  $n = n_1 + n_2$  we obtain

$$R_{\text{AB}} = \frac{V\Delta t}{[\exp(V/nk_B T) - \exp(-V/nk_B T)] \cdot \rho K} \quad (19)$$

where use was made of  $E = V_{\text{AB}}/n$  and (13). In the limit of small bias  $R \propto n$  as expected. Since  $p_1 + p_2 \leq 1$ ,  $K \leq [2 \cosh(V/nk_B T)]^{-1}$ . Assuming for simplicity  $p_1 + p_2 = 1$  (i.e. no staying at a point):

$$R_{\text{AB}} = (V\Delta t/\rho) \coth(V/nk_B T). \quad (20)$$

When  $V \rightarrow \infty$ ,  $R_{\text{AB}} \rightarrow V$  or  $1/R_{\text{AB}} \rightarrow 0$ , namely the conductance vanishes. No singular behaviour at any finite bias is found.

One may relate these results to the drift velocity. The current  $I_{\text{AB}} \equiv \rho v_D$ . This expression can be considered as a definition of a drift velocity  $v_D$ . Since  $I_{\text{AB}} = E/R_{\text{AB}}$  it follows that  $v_D = E/\rho R_{\text{AB}}$  i.e.

$$v_D = (1/n\Delta t) \tanh(V/nk_B T). \quad (21)$$

Consequently  $v_D$  increases monotonically with the voltage and no singularity at finite bias occurs.

White and Barma in their analysis chose to adopt a different definition of the drift velocity, which we denote by  $v_{\text{WB}}$ . According to them, the current through a point A on a one-dimensional ring,  $I_A = (N/n)v_{\text{WB}}$ , where  $n$  is the linear length of the system and  $N$  is the total number of particles in the system. The traversal time  $\tilde{T}_N$  is defined as  $N/I_A$ . Therefore,  $\langle v_{\text{WB}} \rangle = \langle n/\tilde{T}_N \rangle$ , where  $\langle \rangle$  denotes the time average (and configuration average). Since  $\tilde{T}_N \propto N$ , for fixed  $I_A$  (i.e. fixed backbone density)  $\tilde{T}_N$  will diverge when  $N$  does. Approximating  $\langle 1/\tilde{T}_N \rangle$  by  $1/\langle \tilde{T}_N \rangle$ , White and Barma obtain  $\langle v_{\text{WB}} \rangle = \langle n/\tilde{T}_N \rangle$  and thus the vanishing of  $\langle v_{\text{WB}} \rangle$ , when  $N$  diverges. This should be contrasted with  $\langle v_{\text{D}} \rangle$ , which does not diverge even when  $\langle t \rangle_{\text{MFT}}$  does.

It seems to us that since in a realistic system (i.e. *with* many-body interactions) the particles in the dangling bonds do not allow the entrance of new particles from the backbone (where the net flow goes), our definition of drift velocity is more appropriate. The drift velocity of the particles which are trapped in the dangling bond(s) is basically zero and since they form the majority of particles for some probability distributions for the lengths of the side branches (as explained before), the 'average drift' is zero as predicted by White and Barma. Thus the two definitions of drift velocity do not 'contradict' each other but refer to different physical questions.

Finally, we wish to dwell on the question whether the influence of a dangling branch on average quantities is decoupled from the other branches. In the picture of White and Barma, which allows particles which reached an end point to return from it, the effect of the various branches on the mean transversal time is decoupled. They also consider a periodic system (e.g. identical reservoirs connected to both end points). We consider a different set up, i.e. the two reservoirs connected to the end points of the backbone are different (e.g. one boundary can be fully absorbing) and thus  $\langle t \rangle_{\text{MFT}}$ , in our case, seems to be a more appropriate time. In that case we have shown that (even in the case of zero bias) the effect of the branches is not decoupled (see Goldhirsch and Gefen 1985b).

In summary, one has to be extremely cautious when identifying the physically relevant quantities in the problem of biased diffusion. Non-monotonic dependence of the resistance on the bias (which is a result of e.g. the existence of bends in the backbone) will not be affected by the presence of dead ends.

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