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COMMENT

Dispersion in first passage time for biased diffusion

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Abstract. This comment presents Monte Carlo simulations of first passage times for biased diffusion on randomly dilute lattices, as a model for hydrodynamic dispersion. The calculated distributions show non-monotonic curves and non-monotonic derivatives. Possibly there is a simple exponential decay for large times. Fourier transformations demonstrate *no* $1/f$ frequency dependence.

This comment tries to model the flow through inhomogeneous media. The starting point of the following simulations is the so-called 'ant in the labyrinth' problem, which is well known in percolation theory (Stauffer 1985b). A cubic or triangular lattice is occupied with probability p. Above the percolation threshold p_c we obtain a path of occupied positions through the lattice ($p_{c,\text{cubic}} = 0.3117$; $p_{c,\text{triangular}} = 0.5$). In this comment we will discuss lattices with $p = 0.8 > p_c$ and lattice sizes of $L_{\text{cubic}} = 176^3$ and $L_{\text{triangular}} = 2560^2$. At the beginning of the simulation we select n occupied positions as starting points for ants. To achieve a flux through the lattice it is necessary to install a constant bias force BF to the random walkers. Physically BF may be a field, pushing the ants in one direction. In the simulations we set BF between 0.6 and 0.8 to obtain a rapid flux. This means with probability $(1+5\text{BF})/6$ the ant selects the field direction (x direction) and with probability $(1-\text{BF})/6$ any other direction for its next attempt to move. Biased diffusion has been studied in various ways (Pandey 1984, Seifert and Suessenbach 1984, Stauffer 1985a, Barma and Dhar 1983, Böttger and Bryskin 1982). If we observe the ants during their walk, we realise that the average time the ants need to reach distance r differs. In this way we can calculate so-called first passage time distributions (figures 1 and 2). Another possible way to analyse the distributions is to calculate Fourier transformations from the following autocorrelation function in the stationary case:

$$\langle n(0)n(t)\rangle_{\text{eq}} \tag{1}$$

where $n(t)$ is the number of ants having reached a distance $\geqslant r$ after t steps (figures 3 and 4).

The Cyber 205 vector computer at Bochum University was used to calculate the first passage times. In figures 1 and 2 about 5 million ants walk up to 5000 time steps to reach a given distance in x direction. In these cases cubic lattices and $\text{BF} = 0.8$ were used. Figure 1 shows the logarithm $n(t)$ of ants for distance 10 against time steps; figure 2 shows the distribution for distance $r = 90$ (r = lattice position difference in the x direction). Both figures give very asymmetric shapes. Many ants need long times to reach the given distance. For large times there is a tendency for an exponential decay, but better statistics for $t > 3000$ may show a more complex behaviour. If we

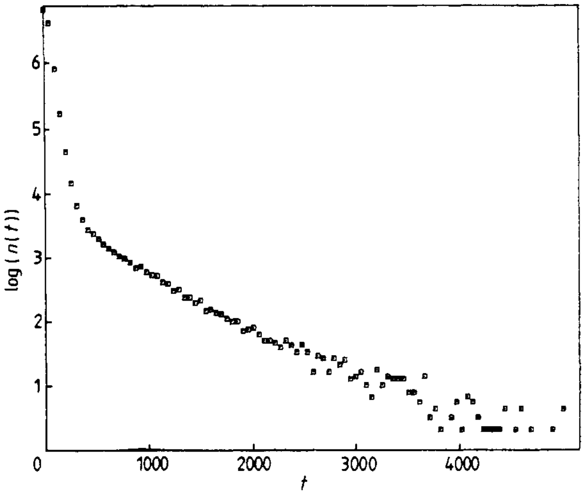

Figure 1. log($n(t)$) against t. $n(t)$: number of ants having reached a distance $r \geqslant 10$ after t time steps.

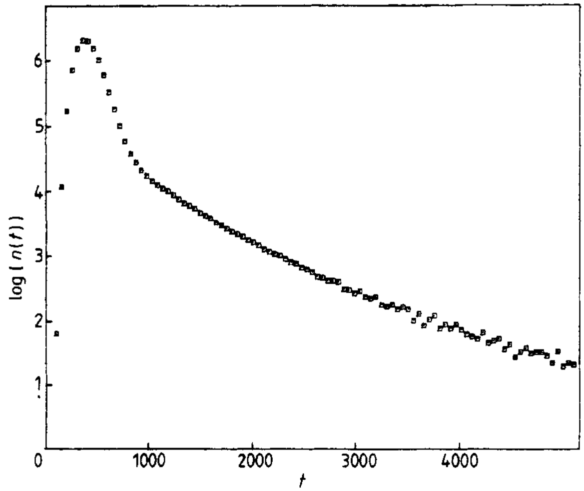

Figure 2. log($n(t)$) against t. $n(t)$: number of ants having reached a distance $r \geqslant 90$ after t time steps.

assume an exponential law $n(t) \propto e^{-at}$, we find $a \simeq 0.0012$. In the case of BF $= 0.8$ we found an apparent constant slope a between $r = 10$ and $r = 100$. Also in a triangular lattice there may be an exponential decay; here we find $a \simeq 0.0067$. In calculations with BF $= 0.6$ the exponential decay is less clear; further examinations seem to be necessary. In no case did we find a behaviour in the form $n(t) \propto t^{-a}$.

Figures 3 and 4 show the discrete Fourier transformations FT of the data presented in figures 1 and 2. In each diagram we find three curves: the real part (Re), the imaginary part (Im) of FT and the FT belonging to autocorrelation function (1) (A). The curves show a very complex behaviour and not a simple $1/f$ frequency dependence. If the distance r increases, the A curves reach zero earlier. This means that for greater distances, only lower frequencies play a significant part.

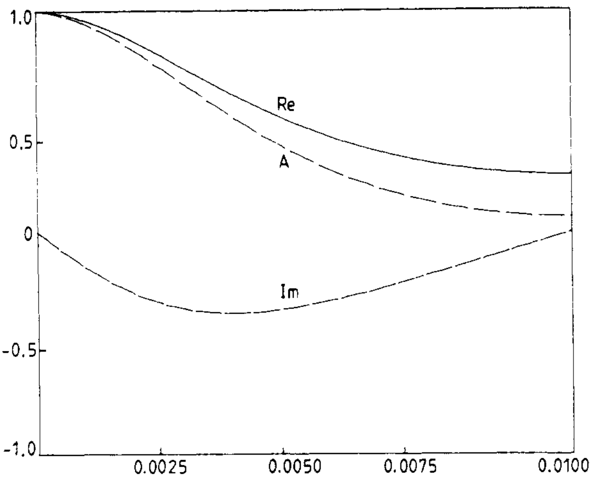

Figure 3. Real part (Re), imaginary part (Im) and Re^2+Im^2 (A) of discrete Fourier transformation against frequency for distance $r=10$.

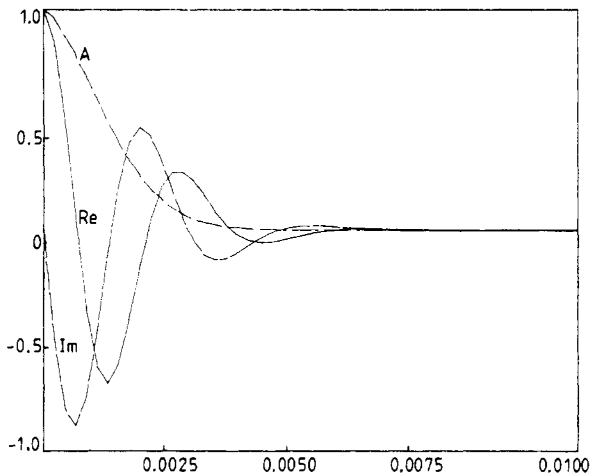

Figure 4. Real part (Re), imaginary part (Im) and Re^2+Im^2 (A) of discrete Fourier transformation against frequency for distance $r=90$.

In summary we have seen that the distribution of first passage times is quite complex for biased diffusion in random media.

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Note added in proof. Different simulations have been done by L de Arcangelis, J Koplick, S Redner and D Wilkinson (*Preprint*) and by S Roux, C Mitescu, E Charlaix and C Baudet (*Preprint*).

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