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LETTER TO THE EDITOR

Diffusion laws for random walks on various heterogeneous lattices

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Abstract. Diffusion laws and diffusion coefficients are given for random walks on lattices whose scattering probabilities differ from site to site.

Random walks are models for transport phenomena such as diffusion. For heterogeneous media one studies heterogeneous lattices, that is lattices where the transition probabilities differ from site to site. Some models of this type were studied by Seshadri *et al* (1979), Westcott (1982), Heyde (1982), Heyde *et al* (1982) and Anshelevich and Vologodskii (1981).

We consider here models with a more realistic scattering process in which the direction of the particle (walker) after scattering depends on its direction before scattering.

One dimension

A particle starts at 0 with velocity to the east and moves with unit speed on the integer lattice $\mathbb{Z}$. Its direction (velocity) $V_t = \pm 1$ at time t conditional on its direction V_{t-1} at time $t-1$ when scattered at site $i \in \mathbb{Z}$ has probability

$$p_i \text{ if } V_t = -V_{t-1} \qquad 1-p_i \text{ if } V_t = V_{t-1} \tag{1}$$

i.e. the particle is reflected (back scattered) at site i with probability $p_i \neq 1$.

The diffusion behaviour of the particle depends on how the p_i vary over sites $i \in \mathbb{Z}$. Many materials are heterogeneous on a microscopic scale but are essentially homogeneous on a macroscopic or laboratory scale. In the first approximation, such materials can be modelled by p_i which are periodic in i with period M, say, which can be as large as desired. For the displacement

$$X_t = V_0 + V_1 + V_2 + \ldots + V_{t-1}$$

of such walks we can derive the diffusion law (central limit theorem)

$$X_t/(Dt)^{1/2} \text{ tends in distribution to a standard normal variable as } t \to \infty, \tag{2}$$

where

$$D = \left(\frac{1}{M}\sum_{i=1}^{M} \frac{p_i}{1-p_i}\right)^{-1} \tag{3}$$

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is the diffusion coefficient. One can further show that the mean square displacement $\langle X_t^2 \rangle$ satisfies

$$\langle X_t^2 \rangle \sim Dt \qquad \text{as } t \to \infty. \tag{4}$$

We note that D depends only on the sum of the $p_i/(1-p_i)$ and not on their order within the period. This exemplifies, for more general models, the point made by Shuler and Mohanty (1982); other instances date back to Rayleigh and Maxwell. For further comments see Heyde *et al* (1982).

An important special case of the model contains a proportion ρ of sites with symmetric scatterers ($p_i = \frac{1}{2}$), the remaining sites being empty ($p_i = 0$): then $D = 1/\rho$. We call this the *dilute simple random walk* (DSRW). It is a lattice version of the famous *wind-tree* model of Ehrenfest.

The value of D for models with two or more scatterer types in any proportions is readily obtained from (3).

More realistically, we can replace strict periodicity by a condition of *macroscopic homogeneity*,

$$\frac{1}{M} \sum_{i=j}^{j+M-1} \frac{p_i}{1-p_i} \to \frac{1}{D} \text{ uniformly in } j \text{ as } M \to \infty \tag{5}$$

for some $D > 0$. Again (2) and (4) can be derived. The uniformity condition may be merely a limitation of our method: it is not a severe condition for physical materials. Heyde *et al* (1982) proved similar results for a simpler model under an assumption like (5) but without the uniformity. They used a general theory due to Stone (1963). This theory and its extensions (e.g. theorem 2.1 of Helland 1982) seem not to be useful in our model for technical reasons involving random time changes.

In the periodic case, the results (2) and (4) are obtained by application of two theorems of Smith (1955) for cumulative processes. Theorem 8 implies that

$$\langle X_t^2 \rangle \sim t \langle Y^2 \rangle / \langle \tau \rangle \tag{6}$$

where $Y = \text{integer} \times M$ is the displacement at first recurrence of the walk (where the walker reaches a point a whole number of periods from the initial point and has the initial direction of motion), and τ is the time (step number) of first recurrence. Now in the manner of Westcott (1982) one writes recurrence relations for the mean numbers m_j^{E} (m_j^{W}) of steps to reach this recurrence point from site j with velocity to the east (west), and solves these to obtain the surprisingly simple result

$$\langle \tau \rangle = 2M. \tag{7}$$

To obtain $\langle Y^2 \rangle$ we note that $Y/M = 1, 0, -1, -2, \ldots$ only. Then one finds that

$$\Pr(Y = -kM) = (1-a)^2 a^k \qquad \text{for } k = 0, 1, 2, \ldots$$

where

$$a = \Pr(Y = M) \tag{8}$$

so that

$$\langle Y \rangle = 0 \qquad \text{and} \qquad \langle Y^2 \rangle = 2aM^2/(1-a). \tag{9}$$

To evaluate a, one adds all contributions from walks starting at 0 which reach M before -1 (they may hit 0 any number of times). This yields, with $p_0 = p_M$,

$$a = (1-p_0) \sum_{j=0}^{\infty} [p_0(1-f_1^E)]^j f_1^E = \frac{(1-p_0) f_1^E}{1-p_0(1-f_1^E)} \tag{10}$$

where f_j^E is the probability of reaching 0 before M, starting at $j \in [1, M]$ with velocity to the east. Writing recurrence relations for the f_j^E in the manner of Westcott (1982) and solving them gives

$$f_1^E = \left(1 + \sum_{i=1}^{M-1} \frac{p_i}{1-p_i}\right)^{-1}. \tag{11}$$

Combining (6)–(11) gives the desired result (4). Then (2) is deduced from theorem 9 of Smith (1955).

Our method for the non-periodic case (5) is very involved. It is based on the extension of Smith's theorem 9 by Westcott (1982) for a simpler type of random walk, where one dissects the lattice $\mathbb{Z}$ into blocks of length M. Here, however, we make M increase with t: fast enough to ensure that (5) converges as $t \to \infty$, but slowly enough with t to ensure that the model remains close enough to the periodic case. This can be achieved with

$$(t\delta\sqrt{t})^{1/2} \ll M \ll \sqrt{t} \qquad \text{as } t \to \infty \tag{12}$$

where $\delta_M > 0$ bounds the magnitude of the difference between the two sides of (5) (it is independent of j and converges to zero as $M \to \infty$).

Two dimensions

A particle starts at $\mathbf{0}$ and moves with unit speed on the bonds (i.e. four directions) of the two-dimensional integer lattice $\mathbb{Z}^2$. Its direction $\boldsymbol{V}_t$ at time t conditional on its direction $\boldsymbol{V}_{t-1}$ at time $t-1$ when scattered at site $(i, j) \in \mathbb{Z}^2$ has probability

$$p_{ij} \text{ for back scatter } (\boldsymbol{V}_t = -\boldsymbol{V}_{t-1}) \qquad q_{ij} \text{ for forward scatter } (\boldsymbol{V}_t = \boldsymbol{V}_{t-1})$$
$$\tfrac{1}{2}(1 - p_{ij} - q_{ij}) \text{ for left turn and for right turn.} \tag{13}$$

Our results are confined to certain periodic cases. For definiteness, assume the initial velocity is to the east, and that $p_{ij} + q_{ij} < 1$ for all (i, j).

For a layered material one can take an $M \times 1$ periodic cell on $\mathbb{Z}^2$. Now the p and q have no j dependence. The displacement

$$X_t = |\boldsymbol{V}_0 + \boldsymbol{V}_1 + \ldots + \boldsymbol{V}_{t-1}|$$

then satisfies (4) with

$$D = \frac{1}{2}\left(\frac{1}{M}\sum_{i=1}^{M} \lambda_i\right)^{-1} + \frac{1}{2}\frac{1}{M}\sum_{i=1}^{M} \lambda_i^{-1} \tag{14}$$

$$\lambda_i = (1 - q_i + p_i)/(1 + q_i - p_i). \tag{15}$$

We note again the lack of dependence on order among the λ_i.

The first term in (14) corresponds to horizontal displacements and is similar to (3). It can be derived by the method outlined in the preceding paragraph. To obtain the second term corresponding to the vertical displacement, we write the vertical displacement Z at first recurrence of the walk (hitting any point (iM, j) with velocity to the east) in terms of the horizontal displacement $Y = kM$ ($k = 1, 0, -1, -2\ldots$) at first recurrence:

$$Z = \begin{cases} Z^{\mathrm{E}}_{0,M} & \text{if } k=1 \\ Z^{\mathrm{E}}_{0,-1} + \sum_{j=0}^{|k|-1} Z^{\mathrm{W}}_{-jM-1,-(j+1)M-1} + Z^{\mathrm{W}}_{kM-1,kM} & \text{if } k = 0, -1, -2, \ldots \end{cases} \tag{16}$$

where $Z^{\mathrm{E}}_{m,n}$ ($Z^{\mathrm{W}}_{m,n}$) is the vertical displacement during a horizontal displacement from column m to column n, starting from m with velocity to the east (west). This expresses Z as a sum of independent variables for each k.

By Smith's theorem 8 the vertical component of the mean square displacement is then

$$\sim t\langle Z^2\rangle/\langle\tau\rangle \tag{17}$$

where here $\langle\tau\rangle = 4M$ by a calculation similar to the previous one. Now one derives recurrence relations for the variances and covariances of terms in (16) in the manner of Westcott (1982). For example, the first term in (16) contributes ω^{E}_0, where

$$\omega^{\mathrm{E}}_j = \langle Z^{\mathrm{E}}_{j,-1}{}^2\rangle, \tag{18}$$

and if ω^{W}_j is defined likewise we find for $j = 0, 1, \ldots, M-1$

$$\begin{aligned} \omega^{\mathrm{E}}_j &= \pi_j\omega^{\mathrm{E}}_{j+1} + (1-\pi_j)\omega^{\mathrm{E}}_{j-1} + \eta_j \\ \omega^{\mathrm{W}}_j &= (1-\pi_j)\omega^{\mathrm{E}}_{j+1} + \pi_j\omega^{\mathrm{W}}_{j-1} + \eta_j \\ \omega^{\mathrm{E}}_M &= \omega^{\mathrm{W}}_{-1} = 0 \end{aligned} \tag{19}$$

where

$$\begin{aligned} \pi_j &= \tfrac{1}{2}(1 + q_j - p_j) \\ \eta_j &= (f^{\mathrm{E}}_{j+1} + f^{\mathrm{W}}_{j-1})/(2\lambda_j) \end{aligned} \tag{20}$$

and the f are defined previously and satisfy recurrence relations for the horizontal motion. Solving these for ω^{0}_{E}, and solving similar equations for the other terms in (16), gives eventually, on substitution in (17), the second term in (14).

A 2×2 periodic cell gives full two-dimensional heterogeneity. In this case the particle has only 16 inequivalent states (four positions and four velocities), so that the walk can be described by a 16×16 transition matrix. Then by diagonalising this matrix one obtains, after a rather elaborate calculation, the result (4) with

$$D = \tfrac{1}{4}[2(\lambda_{11}+\lambda_{12})^{-1} + 2(\lambda_{12}+\lambda_{22})^{-1} + 2(\lambda_{22}+\lambda_{21})^{-1} + 2(\lambda_{21}+\lambda_{11})^{-1}] \tag{21}$$

where

$$\lambda_{ij} = (1 - q_{ij} + p_{ij})/(1 + q_{ij} - p_{ij}). \tag{22}$$

One can readily check that (14) and (21) agree for the 2×1 periodic cell.

The formula

$$D = \frac{1}{2}\left[\frac{1}{M}\sum_{i=1}^{M}\left(\frac{1}{N}\sum_{j=1}^{N}\lambda_{ij}\right)^{-1} + \frac{1}{N}\sum_{j=1}^{M}\left(\frac{1}{M}\sum_{i=1}^{M}\lambda_{ij}\right)^{-1}\right] \tag{23}$$

reduces to (14) when $N = 1$, to (16) when $M = N = 2$ and to $1/\rho$ for the DSRW ($p_{ij} = q_{ij} = \frac{1}{4}$ or $q_{ij} = 1$). It is therefore a plausible conjecture for the diffusion coefficient in the general $M\times N$ periodic cell case.

To date we have not verified this formula beyond these special cases. Our method for the $M \times 1$ cell does not readily extend even to the $M \times 2$ cell. The transition matrix method for the 3×2 cell gives a 24×24 matrix which we have not been able to diagonalise.

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