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Random walk on a one-dimensional inhomogeneous lattice

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Abstract. The case of a random walk on a one-dimensional inhomogeneous lattice is considered when the rate constants of the particle jumping to adjacent lattice points depend on the particle's position and jumping direction. The macroscopic characteristics of the process are evaluated for the lattice length tending to infinity. The requirements to be met by the sequences of jumping rate constants for the process to be self-averaging are analysed. In this case the macroscopic characteristics are shown to be equivalent to those of the random walk on a homogeneous lattice with an effective jumping rate constant. A method has been found for computing the effective jumping rate constant for a large class of inhomogeneous lattices.

1. Introduction

Random walks on a lattice are widely used in physics for simulating various processes. There is extensive physical and mathematical literature dealing with this classic subject. As a rule, however, the random walk on a homogeneous lattice is considered. The case of an inhomogenous lattice has been studied far less (Temkin 1969, Chernov 1970, Kesten *et al* 1975, Solomon 1975). The probability of the particle jumping on an inhomogeneous lattice depends on the particle's position and jumping direction. This is the case considered in the present paper.

Real systems involving random walks on a one-dimensional inhomogeneous lattice can be found in various fields (strictly speaking, nearly all real systems are inhomogeneous). We shall cite two instances connected with the DNA molecule. The DNA double helix contains two kinds of base pairs (AT and GC) which differ in thermodynamic stability, hence in this respect it is a typical one-dimensional inhomogeneous lattice.

The first instance of a random walk on DNA is RNA polymerase's search for the promoter site. When binding itself to DNA, RNA polymerase creates a locally unwound region in the double helix which it naturally displaces while moving along the DNA chain (Riggs *et al* 1970, Kosaganov *et al* 1980). The shift of RNA polymerase to the next base pair must be preceded (or attended) by a fluctuational opening of that pair, its frequency depending on the kind of pair in question. It should be noted that here the probability of the enzyme's jump does not depend on the jumping direction but only on the kind of pair to which it jumps.

Another instance is the degradation of cruciform structures in DNA molecules (Thompson *et al* 1976). Consider two double-stranded DNA molecules with the same nucleotide sequence in solution. The two molecules may in principle form a metastable

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long-lived cruciform structure (see figure 1). The probability of a spontaneous formation of such structures in solution is negligible but they can be obtained by some special methods (Thompson *et al* 1976). The crossing point in these structures will perform a random walk until it reaches one of the ends and the cross falls into two double-stranded molecules.

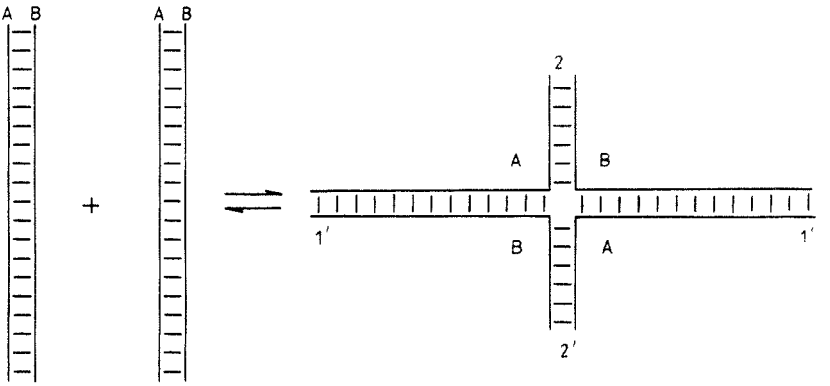

Figure 1. Diagram of the formation of cruciform structures out of two double-stranded DNA molecules.

A shift of the crossing point involves the transfer of two identical base pairs from the 1–1′ helices to 2–2′ and backwards, which must be preceded by a simultaneous opening of two symmetrical base pairs. The reverse jump requires the opening of the same kind of pairs, hence it will be characterised by the same rate constant.

In both cases we deal with the random walk on a one-dimensional inhomogeneous lattice. In the first instance, however, there is the additional condition of equal probabilities of jumping to a given lattice point, while in the second instance each edge of the lattice corresponds to a certain probability of jumping which is the same for motion from left to right and from right to left. The objective of the present study is to analyse the relationship between the distribution of the microscopic probabilities of jumping on a one-dimensional inhomogeneous lattice and the effective macroscopic time characteristics of the random walk process. To be more specific, we shall hereinafter consider the random walk on a stretch with absorbing boundaries and will regard the probability of the particle surviving until time t as the macroscopic characteristic of the process. We hope that for long enough stretches the kinetic curve of particle disappearance at the stretch's ends will be determined only by the average characteristics of the sequence of jumping probabilities. In contrast with references (Temkin 1969, Chernov 1970, Kesten *et al* 1975, Solomon 1975), we treat the case when the random walk may be considered macroscopically as a diffusion problem. We shall attempt to find asymptotic relations between the micro- and macroscopic characteristics of the random walk and assess the extent of their applicability to finite stretches.

Like many other problems involving random inhomogeneities of the medium, the problem in hand may be reduced to finding the asymptotic spectral characteristics of the random matrix. As we shall proceed to show, the resulting matrix is entirely analogous

to the one emerging in the problem of one-dimensional inhomogeneous lattice vibrations (Dyson 1966). Yet, when analysing the random walk, we are interested in the asymptotic behaviour of minimum eigenvalues, whereas in the problem of lattice fluctuations we are after the density of the spectrum of eigenvalues.

2. Formulation of the problem

Consider a one-dimensional lattice containing $N+1$ points. Let a particle perform a random walk over the lattice points and disappear at the terminal points (0 and N). The particle may jump only to adjacent lattice points. The probability of the particle jumping in the small time interval Δt from point k to point $(k+1)$ is $a_k \Delta t$, from point k to point $(k-1)$, $b_k \Delta t$. In the case of a homogeneous lattice $a_k = b_k = a$. Assume that the rate constant sequences for the $\{a_k\}$ and $\{b_k\}$ jumps are macroscopically homogeneous, i.e. the average characteristics of these sequences computed for long enough segments of the sequences do not depend on the segments' position. This requirement is met, for instance, by the typical realisations of ergodic stationary processes.

We seek to answer the following questions:

(1) Are the macroscopic characteristics of the random walk self-averaged, i.e. are the macroscopic time characteristics of the process determined only by the average characteristics of the sequences of microscopic rate constants for the $\{a_k\}$ and $\{b_k\}$ jumps?

(2) If self-averaging does occur, is there a similarity of the macroscopic characteristics, i.e. do the macroscopic characteristics of the random walk on an inhomogeneous lattice coincide for a large enough N with the corresponding characteristics of the random walk on a homogeneous lattice with an effective jumping rate constant a^{eff}?

(3) If the effective jumping rate constant a^{eff} exists, in what way is it expressed through the average characteristics of the sequences $\{a_k\}$ and $\{b_k\}$?

Thus we have to compare the macroscopic characteristics of the random walk on an inhomogeneous lattice with the corresponding characteristics of the random walk on a homogeneous lattice.

We shall regard the probability of the particle surviving until time t as the macroscopic characteristic of the process, provided that at the moment $t = 0$ the particle was at the point αN where $0 < \alpha < 1$, i.e. we shall consider the function

$$P_N(t) = \sum_{k=1}^{N-1} x_k(t). \tag{1}$$

The functions $x_k(t)$ are the probabilities of the particle being at the lattice point k at time t. The change of these probabilities in time is described by the following system of differential equations:

$$\dot{x} = -Ax \tag{2}$$

where

$$x(t) = \begin{pmatrix} x_1(t) \\ \vdots \\ x_{N-1}(t) \end{pmatrix}$$

is an $(N-1)$-dimensional vector and A is a tridiagonal matrix of order $N-1$:

$$A = \begin{pmatrix} a_1+b_1 & -b_2 & 0 & 0 & 0 & \dots & 0 \\ -a_1 & a_2+b_2 & -b_3 & 0 & 0 & \dots & 0 \\ 0 & -a_2 & a_3+b_3 & -b_4 & 0 & \dots & 0 \\ 0 & 0 & -a_3 & a_4+b_4 & -b_5 & \dots & 0 \\ & & & \vdots & & & \\ 0 & 0 & 0 & \dots & -a_{N-3} & a_{N-2}+b_{N-2} & -b_{N-1} \\ 0 & 0 & 0 & \dots & 0 & -a_{N-2} & a_{N-1}+b_{N-1} \end{pmatrix}$$

The solution of system (1) may be represented as follows:

$$x(t) = \sum_{n=1}^{N-1} c_n \exp(-\lambda_n t)\xi^{(n)} \tag{3}$$

where λ_n are the eigenvalues of the matrix A indexed in the order of increasing, $\xi^{(n)}$ are the corresponding eigenvectors and c_n are coefficients dependent on the initial conditions.

If all the a_k and b_k are equal to a, i.e. if the random walk occurs on a homogeneous lattice, then

$$\lambda_n(a) = 4a \sin^2 \frac{\pi n}{2N}, \qquad \xi_k^{(n)}(a) = \left(\frac{2}{N}\right)^{1/2} \sin \frac{\pi k n}{N}. \tag{4}$$

If there exists an effective jumping rate constant a^{eff}, the characteristic time for reaching the boundary will be of the order N^2/a^{eff}. Therefore we are interested in the asymptotic behaviour of the function $P(N^2 t)$ for N large enough. It follows from equations (1)–(3) that

$$P_N(tN^2) = \sum_{k=1}^{N-1} \sum_{n=1}^{N-1} c_n \xi_k^{(n)} \exp(-\lambda_n N^2 t). \tag{5}$$

Since $\lambda_n N^2 \sim a^{\text{eff}} \pi^2 n^2$, the first few terms account for an overwhelming part of the sum over n.

First of all we tried to answer the above questions by a series of computer experiments. The above observations made it possible to analyse only the first eigenvalues and corresponding eigenfunctions in the computer experiments. The results of the experiments were then analytically generalised.

3. Results of computer experiments

Computations were performed for sequences $\{a_k\}$ and $\{b_k\}$ built with the use of the following algorithm:

$$a_k = \begin{cases} 1, & r_k \leqslant \frac{1}{2}, \\ \gamma, & r_k > \frac{1}{2}, \end{cases} \qquad b_{k+1} = a_k, \tag{6}$$

where r_k are pseudorandom numbers rectangularly distributed over the interval $[0, 1]$ and γ is a variable parameter. The case of $\gamma = 1$ corresponds to the random walk on a homogeneous lattice with jumping rate constants $a_k = b_k = 1$.

The eigenvalues λ_n of the matrix A were computed by the method of Givens (Wilkinson 1965) and the eigenvectors $\xi^{(n)}$ by one of the methods presented by Godunov and Riabenkii (1973). The vectors $\xi^{(n)}$ were scaled to unity. Let $\lambda_n(a)$ and $\xi^{(n)}(a)$ denote the eigenvalues and eigenvectors of the matrix for a homogeneous lattice with $a_k = b_k = a$.

Analysis of the dependence of the root-mean-square relative deviation of the first few eigenvalues on N has shown (figure 2) that for N large enough the eigenvalues do not depend on the specific realisation of sequences $\{a_k\}$ and $\{b_k\}$ constructed according to algorithm (6).

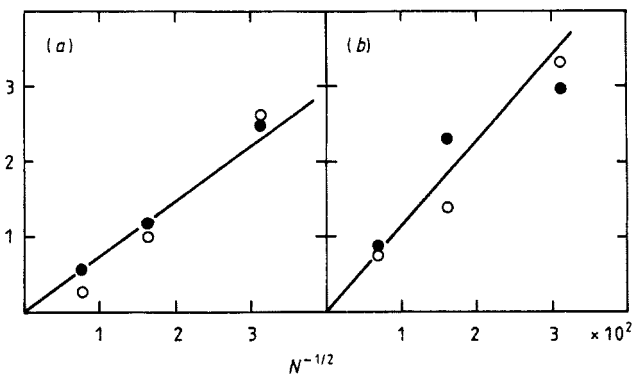

Figure 2. Dependence on the lattice length N of relative root-mean-square deviation of eigenvalues λ_1(○) and λ_5(●) for random matrices A with parameters $\gamma = 4(a)$ and $\gamma = 16$ (b). The root-mean-square deviation was calculated from 16 different realisations of the random matrices for each value of N and γ.

It follows from equation (4) that $\lambda_n(a)/\lambda_1(a) \sim n^2$ for large values of N. Table 1 shows that the same relation holds for $\gamma \neq 1$ if N is large enough ($N = 20\,000$). Besides (see table 2) $\lambda_1/\lambda_1(1)$ does not depend on N if N is large enough. Therefore

$$\frac{\lambda_1}{\lambda_1(1)} = \frac{\lambda_2}{\lambda_2(1)} = \frac{\lambda_3}{\lambda_3(1)} \cdots, \tag{7}$$

and these relations are independent of N if N is large enough.

The results of analysis of the eigenvectors $\xi^{(n)}$ are shown in figure 3. For the first few eigenvectors

$$|\xi^{(n)} - \xi^{(n)}(1)| \sim 1/\sqrt{N} \tag{8}$$

Table 1. Ratios of first eigenvalues for the random matrices A with $\gamma = 4$; case $a_k = b_{k+1}$; $\bar{\lambda}_n$ is obtained by averaging λ_n over 16 realisations of random 20 000-dimensional matrices.

n	$\bar{\lambda}_n/\bar{\lambda}_1$	n^2
1	1	1
2	4.004	4
3	9.008	9
4	16.003	16
5	24.994	25

Table 2. Ratio of first eigenvalue λ_1 of the matrix A with $\gamma = 4$ to first eigenvalue $\lambda_1(1)$ of the matrix for a homogeneous lattice depending upon lattice length N; case $a_k = b_{k+1}$; $\bar{\lambda}_1$ is obtained by averaging over 16 realisations of random N-dimensional matrices.

N	$\bar{\lambda}_1/\lambda_1(1)$
1 000	1.615
4 000	1.603
20 000	1.600

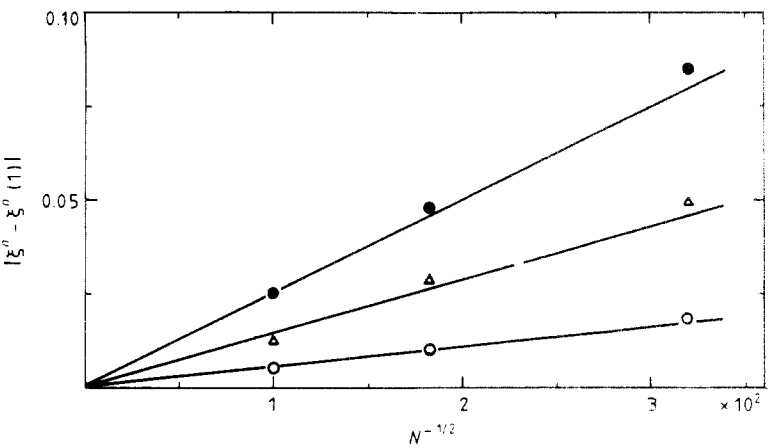

Figure 3. The lattice length dependence of the norm of the difference between eigenvectors of the matrices corresponding to random walks on a homogeneous lattice and an inhomogeneous lattice with the parameter $\gamma = 4$. The dependence is shown for the first (○), third (△) and fifth (●) eigenvectors. For the second and fourth eigenvectors intermediate results were obtained. For each N the averaging was performed over 16 different realisations of the 10 000-dimensional random matrices.

for $N \to \infty$, i.e. for N large enough, $\xi^{(n)}$ do not depend upon the specific realisation of sequences $\{a_k\}$ and $\{b_k\}$ constructed according to algorithm (6), or upon γ.

It follows from expressions (3), (7) and (8) that for sequences $\{a_k\}$ and $\{b_k\}$ based on algorithm (6) the macroscopic characteristics of the random walk on an inhomogeneous lattice asymptotically coincide for $N \to \infty$ with the corresponding characteristics of the random walk on a homogeneous lattice with the jumping rate constant

$$a^{\text{eff}} = \lambda_1/\lambda_1(1). \tag{9}$$

We have succeeded in guessing the equation relating the macroscopic quantity a^{eff} to the microscopic jumping rate constants $\{a_k\}$ for the case when $a_k = b_{k+1}$:

$$a^{\text{eff}} = N \Big/ \sum_{k=1}^{N} a_k^{-1}. \tag{10}$$

For sequences constructed according to algorithm (6) equation (10) is transformed in the following way:

$$a^{\text{eff}} = 2\gamma/(1+\gamma). \tag{11}$$

The results of a comparison of a^{eff} values computed according to equations (9) and (11) are presented in table 3.

Table 3. Values of the effective jumping rate constant a^{eff} computed and obtained from equation (10) for various γ; case $a_k = b_{k+1}$; $\bar{\lambda}_1$ is obtained by averaging over 16 realisations of random 20 000-dimensional matrices.

γ	$a^{\text{eff}} = \bar{\lambda}_1/4 \sin(\pi/2N)$	$a^{\text{eff}} = 2\gamma/(1+\gamma)$
2	1.333	1.333
4	1.600	1.600
8	1.778	1.778
16	1.883	1.882
32	1.942	1.939
64	1.978	1.969

Exactly the same results, including equation (10), were obtained for another class of sequences based on the algorithm $a_k = 1 + \gamma r_k$, $b_{k+1} = a_k$.

One can therefore presume that equation (10) holds for any macroscopically homogeneous sequences $\{a_k\}$ and $\{b_k\}$ which meet the condition $a_k = b_{k+1}$.

We have also investigated an essentially different class of sequences $\{a_k\}$ and $\{b_k\}$ independently constructed according to the algorithm

$$a_k = \begin{cases} 1, & r_{2k-1} \leqslant \frac{1}{2}, \\ \gamma, & r_{2k-1} > \frac{1}{2}, \end{cases} \qquad b_k = \begin{cases} 1, & r_{2k} \leqslant \frac{1}{2}, \\ \gamma, & r_{2k} > \frac{1}{2}. \end{cases} \tag{12}$$

In this case the eigenvalues computed for different realisations of sequences (12) do not show any tendency to approach each other with increasing N. It can therefore be supposed that there is no self-averaging of the macroscopic characteristics of the random walk in this case.

A random walk model similar to the one described by (12) was recently discussed in Sinai (1981). The only difference is that in Sinai (1981) jumps occur at discrete moments of time. The paper demonstrates the lack of self-averaging in a model of this kind; the same ensues from our numerical experiment. The reason for this is that the fixation of a specific pair of random sequences $\{a_k\}$ and $\{b_k\}$, obtained by means of algorithm (12), creates 'holes', i.e. points on the left of which mostly $a_k > b_k$ to a length m and on the right mostly $a_k < b_k$, m being unlimited in contrast to the models discussed above. Self-averaging does not take place because the position of a 'hole' depends on the specific sequence and not only on its average characteristics.

4. Analytical treatment

In this section we shall specify the sufficient requirements to be met by the sequences of jumping rate constants $\{a_k\}$ and $\{b_k\}$ to ensure the self-averaging of the macroscopic characteristics of the random walk on an inhomogeneous lattice. These macroscopic characteristics asymptotically coincide, for N large enough, with the corresponding characteristics of the random walk on a homogeneous lattice with an effective jumping rate constant a^{eff}. We have obtained equations expressing the macroscopic quantity a^{eff}

through the microscopic quantities $\{a_k\}$ and $\{b_k\}$. We shall now apply the approach described in Anshelevich and Vologodskii (1981).

The first step is to compute the characteristic polynomial of the matrix A.

Let $\Delta_{k+1}(\lambda)$ be a kth-order determinant of the matrix $A-\lambda E$. A double expansion of this polynomial results in a situation wherein the sequence of polynomials $\Delta_2(\lambda)$, $\Delta_3(\lambda)$, ... satisfies the recursion relation

$$\Delta_{k+1}(\lambda)=(a_k+b_k-\lambda)\Delta_k(\lambda)-a_{k-1}b_k\Delta_{k-1}(\lambda) \tag{13}$$

with the initial condition

$$\Delta_0(\lambda)=0, \qquad \Delta_1(\lambda)=1.$$

Let

$$\Delta_k(\lambda)=\sum_{n=0}^{\infty}(-1)^n\Delta_k^{(n)}\lambda^n,$$

where for each k only a finite number of coefficients $\Delta_k^{(n)}$ differ from zero.

From the recursion relation (13) for polynomials we obtain a recursion relation for their coefficients:

$$\Delta_{k+1}^{(n)}=(a_k+b_k)\Delta_k^{(n)}-a_{k-1}b_k\Delta_{k-1}^{(n)}+(1-\delta_n)\Delta_k^{(n-1)}$$

with the initial condition

$$\Delta_0^{(n)}=0. \qquad \Delta_1^{(n)}=\delta_n,$$

where

$$\delta_n=\begin{cases}1, & n=0,\\ 0, & n>0.\end{cases}$$

By successively finding from this equation $\Delta_2^{(n)}$, $\Delta_3^{(n)}$, $\Delta_4^{(n)}$, ... and considering $\Delta_k^{(n-1)}$ to have been found already, we obtain

$$\Delta_k^{(n)}=\delta_n\sum_{m=0}^{k-1}\left(\prod_{j=1}^{m}b_j\right)\left(\prod_{j=m+1}^{k-1}a_j\right)+(1-\delta_n)\sum_{l=1}^{k-1}\sum_{m=l}^{k-1}\left(\prod_{j=l+1}^{m}b_j\right)\left(\prod_{j=m+1}^{k-1}a_j\right)\Delta_l^{(n-1)}. \tag{14}$$

Consider the scaling characteristic polynomials

$$y_k=\Delta_k(\lambda/k^2)/\Delta_k(0)$$

and let

$$y_k=\sum_{n=0}^{\infty}(-1)^n y_k^{(n)}\lambda^n. \tag{15}$$

Then

$$y_k^{(n)}=(1/k^{2n})\Delta_k^{(n)}/\Delta_k^{(0)}$$

and from equation (14) we obtain

$$y_k^{(n)}=\delta_n+(1-\delta_n)\frac{1}{k^{2n}}\times\sum_{l=1}^{k-1}\frac{\sum_{m=0}^{l-1}(\prod_{j=1}^{m}b_j)(\prod_{j=m+1}^{l-1}a_j)\sum_{m=l}^{k-1}(\prod_{j=l+1}^{m}b_j)(\prod_{j=m+1}^{k-1}a_j)}{\sum_{m=0}^{k-1}(\prod_{j=1}^{m}b_j)(\prod_{j=m+1}^{k-1}a_j)}l^{2(n-1)}y_l^{(n-1)}. \tag{16}$$

We divide the numerator and the denominator of the above fraction by $a_1 a_2 \dots a_{k-1}$, introduce the notations

$$\omega_m = \prod_{j=1}^{m} \frac{b_j}{a_j}, \qquad d_m = a_m \omega_m,$$

and use the identity

$$\sum_{m=l}^{k-1} \prod_{j=l+1}^{m} \frac{b_j}{a_j} = \omega_l^{-1} \left(\sum_{m=0}^{k-1} \omega_m - \sum_{m=0}^{l-1} \omega_m \right).$$

Then equation (16) becomes

$$y_k^{(n)} = \delta_n + (1-\delta_n) \frac{1}{k^{2n}} \sum_{l=1}^{k-1} \frac{\sum_{m=0}^{l-1} \omega_m \left(\sum_{m=0}^{k-1} \omega_m - \sum_{m=0}^{l-1} \omega_m \right)}{\sum_{m=0}^{k-1} \omega_m} d_l^{-1} l^{2(n-1)} y_l^{(n-1)}. \tag{17}$$

Let the following condition be met: there are limits

$$\omega = \lim_{k \to \infty} \frac{1}{k} \sum_{m=1}^{k-1} \omega_m, \qquad d = \lim_{k \to \infty} \left(\frac{1}{k} \sum_{m=1}^{k-1} d_m^{-1} \right)^{-1}. \tag{18}$$

Then

$$\sum_{m=1}^{l} \omega_m = l(\omega + \delta(l)), \qquad \text{where } \delta(l) \to 0 \text{ if } l \to \infty.$$

We shall now prove, using the method of mathematical induction, that there exists a limit

$$y^{(n)} = \lim_{k \to \infty} y_k^{(n)}$$

and compute it.

$y_k^{(0)} = 1$ by definition, hence $y^{(0)} = 1$.

Assume that

$$y_k^{(n-1)} = y^{(n-1)} + \varepsilon(k),$$

where $\varepsilon(k) \to 0$ for $k \to \infty$. Then, according to formula (17),

$$y_k^{(n)} = \frac{1}{k^{2n}} \sum_{l=1}^{k-1} \frac{l(\omega + \delta(l))[k(\omega + \delta(k)) - l(\omega + \delta(l))]}{k(\omega + \delta(k))} d_l^{-1} l^{2(n-1)} (y^{(n-1)} + \varepsilon(l))$$

$$= \left[\frac{1}{k^{2n+1}} \sum_{l=1}^{k-1} (k-l) l^{2n-1} d_l^{-1} \right] \omega y^{(n-1)} + \theta(k),$$

where $\theta(k) \to 0$ for $k \to \infty$.

Since

$$\lim_{k \to \infty} \frac{1}{k^{2n+1}} \sum_{l=1}^{k-1} (k-l) l^{2n-1} d_l^{-1} = \frac{d^{-1}}{(2n)(2n+1)}$$

it follows that

$$y^{(n)} = \lim_{k \to \infty} y_k^{(n)} = \frac{\omega d^{-1}}{(2n)(2n+1)} y^{(n-1)}.$$

Since $y^{(0)} = 1$ it follows from this recursion relation that

$$y^{(n)} = (\omega d^{-1})^n/(2n+1)!.$$

Recalling (15), we see that

$$\lim_{k\to\infty} y_k(\lambda) = \sum_{n=0}^{\infty} (-1)^n \frac{(\omega d^{-1})^n}{(2n+1)!} \lambda^n = \frac{\sin(\omega\lambda/d)^{1/2}}{(\omega\lambda/d)^{1/2}}. \tag{19}$$

Since the roots of the polynomial $y_N(\lambda)$ are $\lambda_m N^2$ where λ_m denotes the eigenvalues of the matrix A of order $N-1$ indexed in increasing order, it follows from (19) that

$$\lambda_m N^2 \to (d/\omega)\pi^2 m^2$$

for $N \to \infty$.

Hence, if condition (18) is met, the eigenvalues λ_m of the inhomogeneous lattice matrix asymptotically coincide with the eigenvalues $\lambda_m(d/\omega)$ of the matrix for a homogeneous lattice in which $a_k = b_k = d/\omega$.

$$|\lambda_m - \lambda_m(d/\omega)|N^2 \to 0 \tag{20}$$

for $N \to \infty$.

We now go on to the computation of the eigenfunctions of the matrix A.

The system of equations for the eigenvectors and eigenvalues of the matrix A of order $N-1$ is

$$\begin{aligned} &a_{k-1}x_{k-1} - (a_k + b_k)x_k + b_{k+1}x_{k+1} = \lambda x_k, \\ &x_0 = 0, \qquad x_N = 0. \end{aligned} \tag{21}$$

We substitute the variables $u_k = (\Pi_{j=1}^{k} b_j)x_k$. Then this system of equations becomes

$$\begin{aligned} &u_{k+1} = (a_k + b_k - \lambda)u_k - a_{k-1}b_k u_{k-1}, \\ &u_0 = 0, \qquad u_N = 0. \end{aligned} \tag{22}$$

A comparison of this system with the system of equations (13) shows that the solutions of system (13) meeting the additional condition $u_N = 0$ are solutions of system (22). Therefore the vector $(\Delta_1(\lambda_m), \Delta_2(\lambda_m), \ldots, \Delta_{N-1}(\lambda_m))$ is a solution of system (22) for $\lambda = \lambda_m$ where λ_m is an eigenvalue of the matrix A of order $N-1$, and the vector

$$\left(\frac{\Delta_1^{(0)}}{b_1} y_1(\lambda_m 1^2), \frac{\Delta_2^{(0)}}{b_1 b_2} y_2(\lambda_m 2^2), \ldots, \frac{\Delta_{N-1}^{(0)}}{b_1 b_2 \ldots b_{N-1}} y_{N-1}[\lambda_m (N-1)^2]\right)$$

is a solution of system (21) for $\lambda = \lambda_m$ and consequently the eigenvector of the matrix A of order $N-1$ with the eigenvalue λ_m.

By substituting $\Delta_k^{(0)}$ from (14) and using equation (19) and (20) we obtain, for N large enough,

$$\xi_k^{(m)} \sim (2/N)^{1/2}(d^{1/2}/d_k) \sin(\pi m k/N).$$

These eigenvectors are orthonormal relative to the scalar product

$$(x, y) = \sum_{k=1}^{N-1} x_k y_k d_k. \tag{23}$$

Thus, if condition (18) is met, the eigenvectors $\xi^{(m)}$ of the inhomogeneous lattice matrix and the eigenvectors $\xi^{(m)}(d/\omega)$ of the homogeneous lattice matrix with $a_k = b_k =$

d/ω satisfy the relation

$$\max_k |\xi_k^{(m)} - (d^{1/2}/d_k)\xi_k^{(m)}(d/\omega)|\sqrt{N} \to 0 \tag{24}$$

for $N \to \infty$.

Now note that the matrix A is self-adjoint relative to the scalar product in equation (23). Therefore the eigenvectors $\xi^{(m)}$ are orthogonal relative to this scalar product. Hence, if at time $t = 0$ the particle was at point αN where $0 < \alpha < 1$, the coefficients c_m in equation (5) asymptotically satisfy, for N large enough, the relation

$$c_m = \xi_{\alpha N}^{(m)} d_{\alpha N} \sim \sqrt{d}\xi_{\alpha N}^{(m)}(d/\omega) = \sqrt{d}c_m(d/\omega). \tag{25}$$

Besides, it follows from (24) that

$$\sum_{k=1}^{N-1} \xi_k^{(m)} \sim \sqrt{d} \sum_{k=1}^{N-1} d_k^{-1} \xi_k^{(m)}\left(\frac{d}{\omega}\right) \sim \frac{1}{\sqrt{d}} \sum_{k=1}^{N-1} \xi_k^{(m)}\left(\frac{d}{\omega}\right). \tag{26}$$

It follows from equations (5), (20), (25) and (26) that if condition (18) is met, the macroscopic characteristic $P_N(tN^2)$ of the random walk on an inhomogeneous lattice asymptotically coincides, for N large enough, with the corresponding characteristic of the random walk on a homogeneous lattice with $a_k = b_k = d/\omega$.

Note that the sequences $\{a_k\}$ and $\{b_k\}$ enter conditions (18) in a non-symmetrical way. This non-symmetry is due to the non-symmetry of the passage to the limit, which adds new points on the right. However, as can be seen from (18), the physically meaningful value d/ω depends on the sequences $\{a_k\}$ and $\{b_k\}$ in a symmetrical fashion.

We shall now consider a few examples where condition (18) is met.

(1) Let $a_k = b_{k+1}$. Then condition (18) becomes the condition of the existence of a limit

$$\omega = b_1 \lim_{k\to\infty} \frac{1}{k} \sum_{m=1}^{k-1} a_m^{-1}.$$

In this case

$$a^{\text{eff}} = \lim_{k\to\infty} \left(\frac{1}{k} \sum_{m=1}^{k-1} a_m^{-1}\right)^{-1}.$$

(2) Let $a_k = b_{k+2}$. Then condition (18) becomes the condition of the existence of the limits

$$\omega = b_1 b_2 \lim_{k\to\infty} \sum_{m=1}^{k-1} (a_{m-1}a_m)^{-1}, \qquad d = b_1 b_2 \lim_{k\to\infty} \left(\frac{1}{k} \sum_{m=1}^{k-1} a_{m-1}\right)^{-1}.$$

In this case

$$a^{\text{eff}} = \left(\lim_{k\to\infty} \frac{1}{k} \sum_{m=1}^{k-1} (a_{m-1}a_m)^{-1}\right)^{-1} \left(\lim_{k\to\infty} \frac{1}{k} \sum_{m=1}^{k-1} a_{m-1}\right)^{-1}.$$

(3) Let each lattice point k correspond to a positive number u_k and each edge connecting lattice points k and $k+1$ to a positive number v_k. Assume that $a_k = u_k v_k$, $b_k = u_k v_{k-1}$. Then condition (18) becomes the condition of the existence of the limits

$$\omega = v_0 \lim_{k\to\infty} \frac{1}{k} \sum_{m=1}^{k-1} v_m^{-1}, \qquad d = v_0 \lim_{k\to\infty} \frac{1}{k} \sum_{m=1}^{k-1} u_m.$$

In this case

$$a^{\text{eff}} = \left(\lim_{k\to\infty} \frac{1}{k} \sum_{m=1}^{k-1} v_m^{-1} \right)^{-1} \left(\lim_{k\to\infty} \frac{1}{k} \sum_{m=1}^{k-1} u_m \right).$$

Note that any sequences $\{a_k\}$ and $\{b_k\}$ may be represented in this way.

The conditions in examples (1)–(3) are met for a large class of sequences $\{a_k\}$, $\{u_k\}$ and $\{v_k\}$. These include periodical sequences as well as typical realisations of periodical stationary random sequences. The sequences $\{u_k\}$ and $\{v_k\}$ may or may not be intercorrelated.

In the first example the jumping rate constants along each edge from left to right and from right to left are the same. In the second example the jumping rate constant depends only on the lattice point to which the particle jumps. In the third example the jumping rate constant depends on the lattice point from which the particle jumps and the edge it jumps along

5. Discussion

Our results show that the random walk on an inhomogeneous lattice may in a number of cases be approximated by the random walk on a homogeneous lattice with an effective jumping rate constant. It should be emphasised that rigorous analysis was carried out only for $N \to \infty$. The applicability of these results to finite lattices may be assessed on the basis of the numerical experiments.

Analysis of the first two examples treated at the end of § 4 shows that the local strict correlation between sequences $\{a_k\}$ and $\{b_k\}$ ensures the self-averaging of the macroscopic characteristics and the existence of an effective jumping rate constant. The third example shows this to be equally true in the case of a weaker correlation between sequences $\{a_k\}$ and $\{b_k\}$.

The approach elaborated above makes it possible to compute the value of a^{eff} for each specific case.

Note that there is no self-averaging if there is no correlation between sequences $\{a_k\}$ and $\{b_k\}$, as has been shown by the computer experiment.

We shall now analyse the dependence of a^{eff} on sequences $\{a_k\}$ and $\{b_k\}$ in the first two examples treated at the end of § 4. To be more definite, let a_k be independent for various k and

$$a_k = \begin{cases} 1, & \text{with probability } \frac{1}{2}, \\ \gamma, & \text{with probability } \frac{1}{2}. \end{cases} \tag{27}$$

It will be easily seen that these two specific examples correspond to the two real systems considered in the Introduction. Recall that the first instance has been thoroughly computer-analysed.

For sequences based on equation (27) a^{eff} is expressed in the following way: in the first case, when $a_k = b_{k+1}$

$$a^{\text{eff}} = 2\gamma/(1+\gamma),$$

in the second case, when $a_k = b_{k+2}$

$$a^{\text{eff}} = 8\gamma^2/(1+\gamma)^3.$$

These equations show that in the first case a^{eff} as a function of γ monotonically increases and tends to 2 as $\gamma \to \infty$, while in the second case a^{eff} reaches a maximum at $\gamma = 2$ and tends to 0 as $\gamma \to \infty$. Thus even in these two closely related examples the dependence of a^{eff} on the sequences $\{a_k\}$ and $\{b_k\}$ is essentially different.

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