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Velocity and Diffusion Constant of a Periodic One-Dimensional Hopping Model

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The velocity and the diffusion constant are obtained for a periodic one-dimensional hopping model of arbitrary period N. These two quantities are expressed as explicit functions of all the hopping rates. The velocity and the diffusion constant of random systems are calculated by taking the limit $N \to \infty$. One finds by varying the distribution of hopping rates that the diffusion constant and the velocity are singular at different points. Lastly, several possible applications are proposed.

KEY WORDS: Diffusion; random hopping model; disordered lattice.

1. INTRODUCTION

A lot of attention[1] has been given recently to the problem of diffusion on a one-dimensional lattice with random hopping rates. This model gives a satisfactory understanding of conductivity experiments on some anisotropic organic conductors.[2] From a theoretical point of view, it seems to be one of the simplest models of disordered systems. Up to now, physicists have mainly studied the diffusion on a random chain when the transition rates are symmetric. They have developed several methods like the effective medium approximation[3-6] or renormalization group calculations[7] to calculate the diffusion coefficient or the low-frequency dependence of the conductivity and now the problem is well understood.[8]

The case of asymmetric hopping rates has motivated a lot of work in probability theory.[9,10] In particular it was shown that for some distributions, the mean displacement may grow indefinitely, but slower than

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linearly in time. The model usually studied is a discrete time model. If a particle is on site n at time t, it will be at time $t+1$ either on site $n+1$ with probability p_n or on site $n-1$ with probability $q_n = 1 - p_n$. Recently, Sinai[11] has shown that, for random hopping rates p_n which satisfy

$$\langle \log p_n \rangle = \langle \log q_n \rangle \tag{1}$$

the particle is after time t at a distance of order $\log^2 t$ from its starting point. (The averages $\langle\ \rangle$ are performed according to a given distribution of p_n.) When the hopping rates do not satisfy the condition (1), one finds[9,10,12,13] that the mean position $\overline{x(t)}$ of the particle increases linearly in time, i.e., with a finite velocity only if

$$\langle q_n/p_n \rangle < 1 \quad \text{or} \quad \langle p_n/q_n \rangle < 1 \tag{2}$$

One finds

$$\overline{x(t)} \simeq \left\langle \frac{1}{p_n} \right\rangle^{-1} \left(1 - \left\langle \frac{q_n}{p_n} \right\rangle\right) t \qquad \text{if} \quad \left\langle \frac{q_n}{p_n} \right\rangle < 1 \tag{3}$$

whereas

$$\overline{x(t)} \simeq -\left\langle \frac{1}{q_n} \right\rangle^{-1} \left(1 - \left\langle \frac{p_n}{q_n} \right\rangle\right) t \qquad \text{if} \quad \left\langle \frac{p_n}{q_n} \right\rangle < 1 \tag{4}$$

On the contrary, if the condition (2) is not satisfied, the mean position $\overline{x(t)}$ increases like a power law t^β with $\beta < 1$. Then[9,10,12,13], if α is the nonzero solution of

$$\left\langle \left(\frac{1 - p_n}{p_n} \right)^{\alpha} \right\rangle = 1 \tag{5}$$

One finds

$$\begin{aligned} \overline{x(t)} &\sim t^{\alpha} && \text{if} \quad \alpha > 0 \\ &\sim -t^{-\alpha} && \text{if} \quad \alpha < 0 \end{aligned} \tag{6}$$

Bernasconi and Schneider[13] found that these power laws (6) are modulated by a periodic function of $\log t$ for some particular distributions of p_n.

The purpose of this paper is to give an exact expression for the velocity and the diffusion constant of a periodic one-dimensional hopping problem with an arbitrary period N. The method followed is an extension of the approach used in previous work done with Y. Pomeau.[12] It consists in calculating exactly the properties of the steady state. From the exact expressions of the velocity and of the diffusion constant of a periodic chain, one can obtain these quantities for random systems by taking the limit of an infinite period. One finds the conditions under which the velocity and the diffusion constant are both finite. By varying the distribution of hopping rates, one observes that the diffusion constant diverges at a point which differs from the point where the velocity vanishes. The fact that two different quantities are singular at different points is a common feature to several disordered systems.[14] Lastly some possible applications of the results presented here will be proposed.

2. THE STEADY STATE

We shall consider here the continuous time problem. The results will be generalized in Section 5 to the discrete time case. We start with the Master equation which gives the time evolution of $P_n(t)$, the probability for the particle to be on site n at time t:

$$\frac{dP_n}{dt} = W_{n,n+1}P_{n+1} + W_{n,n-1}P_{n-1} - (W_{n+1,n} + W_{n-1,n})P_n \qquad (7)$$

$W_{i,j}$ denotes the probability of jumping from site j to site i per unit time. We do not assume any symmetry of the $W_{i,j}$ (i.e., $W_{i,j}$ has no reason to be equal to $W_{j,i}$).

We consider here a periodic model of period N

$$W_{i,j} = W_{i+N,j+N} \qquad (8)$$

Let us introduce two quantities $\tilde{R}_n(t)$ and $\tilde{S}_n(t)$ which have simple behaviors in the long time limit:

$$\tilde{R}_n(t) = \sum_{k=-\infty}^{\infty} P_{n+Nk}(t) \qquad (9)$$

$$\tilde{S}_n(t) = \sum_{k=-\infty}^{\infty} (n + Nk)P_{n+Nk} \qquad (10)$$

In this section, we are going to calculate the long time behaviors of the $\tilde{R}_n(t)$ and the $\tilde{S}_n(t)$. $\tilde{R}_n(t)$ represents the probability that the particle is on one of the sites $n + Nk$ ($k \in \mathbb{Z}$) at time t. The ratio $\tilde{S}_n(t)/\tilde{R}_n(t)$ represents the average position of the particle when the average is restricted to the sites $n + Nk$ ($k \in \mathbb{Z}$). From the definitions (9) and (10) one sees immediately that

$$\tilde{R}_n(t) = \tilde{R}_{n+N}(t) \qquad (11)$$

$$\tilde{S}_n(t) = \tilde{S}_{n+N}(t) \qquad (12)$$

From Eqs. (7)–(10), one can obtain the time evolution of $\tilde{R}_n(t)$ and

$\tilde{S}_n(t)$:

$$\frac{d\tilde{R}_n}{dt} = W_{n,n+1}\tilde{R}_{n+1} + W_{n,n-1}\tilde{R}_{n-1} - (W_{n+1,n} + W_{n-1,n})\tilde{R}_n \tag{13}$$

$$\frac{d\tilde{S}_n}{dt} = W_{n,n+1}\tilde{S}_{n+1} + W_{n,n-1}\tilde{S}_{n-1} - (W_{n+1,n} + W_{n-1,n})\tilde{S}_n - W_{n,n+1}\tilde{R}_{n+1} + W_{n,n-1}\tilde{R}_{n-1} \tag{14}$$

In the long time limit, one expects to reach a steady state and that the $\tilde{R}_n(t)$ and $\tilde{S}_n(t)$ have a simple behavior:

$$\text{for} \quad t \to \infty \quad \begin{cases} \tilde{R}_n(t) \to R_n & (15) \\ \tilde{S}_n(t) \to a_n t + T_n & (16) \end{cases}$$

where the R_n, a_n, and T_n do not depend on time.

I did not find a simple proof that the long time behaviors of $\tilde{R}_n(t)$ and $\tilde{S}_n(t)$ are actually given by (15) and (16). However, these behaviors seem reasonable if we exclude the case where some W_{ij} vanish. One can at least justify (15) and (16) by considering the hopping problem on a circle of N sites. For this hopping problem on a circle, there exists a dynamical steady state with the particle turning with a constant velocity. R_n is the probability that the particle is on site n in the steady state, whereas $\tilde{S}_n(t)$ is related to the average number of turns done by a particle located on site n at time t.

By replacing in (13) and (14) the $\tilde{R}_n(t)$ and the $\tilde{S}_n(t)$ by their long time behaviors (15) and (16), one finds that the R_n, a_n, and T_n must satisfy the following three equations:

$$0 = W_{n,n+1}R_{n+1} + W_{n,n-1}R_{n-1} - (W_{n+1,n} + W_{n-1,n})R_n \tag{17}$$

$$0 = W_{n,n+1}a_{n+1} + W_{n,n-1}a_{n-1} - (W_{n+1,n} + W_{n-1,n})a_n \tag{18}$$

$$a_n = W_{n,n+1}T_{n+1} + W_{n,n-1}T_{n-1} - (W_{n+1,n} + W_{n-1,n})T_n - W_{n,n+1}R_{n+1} + W_{n,n-1}R_{n-1} \tag{19}$$

whereas the conditions (11) and (12) become

$$R_n = R_{n+N} \tag{20}$$

$$a_n = a_{n+N} \tag{21}$$

$$T_n = T_{n+N} \tag{22}$$

The solution of recurrence (17) contains *a priori* two arbitrary constants. However, the constraint (20) fixes one of these constants and one finds the general solution of (17) and (20) is

$$R_n = C_1 r_n \tag{23}$$

where C_1 is the remaining arbitrary constant and the r_n are given by

$$r_n = \frac{1}{W_{n+1,n}}\left[1 + \sum_{i=1}^{N-1} \prod_{j=1}^{i} \left(\frac{W_{n+j-1,n+j}}{W_{n+j+1,n+j}} \right)\right] \tag{24}$$

The constant C_1 is fixed by the normalization condition

$$\sum_{n=1}^{N} R_n = 1 \tag{25}$$

The expressions of the a_n can be obtained easily because they satisfy the same equations as the R_n. Therefore the a_n are proportional to the R_n:

$$a_n = AR_n \tag{26}$$

where A is *a priori* an unknown constant. This constant A can be fixed by summing Eq. (19) over n:

$$\sum_{n=1}^{N} a_n = \sum_{n=1}^{N} (W_{n+1,n} - W_{n-1,n})R_n \tag{27}$$

Therefore the constant A is given by

$$A = \sum_{n=1}^{N} (W_{n+1,n} - W_{n-1,n})R_n \tag{28}$$

which becomes

$$A = \frac{N}{\sum_{n=1}^{N} r_n}\left[1 - \prod_{n=1}^{N} \left(\frac{W_{n,n+1}}{W_{n+1,n}} \right)\right] \tag{29}$$

when one replaces R_n by $C_1 r_n$.

Let us now find the T_n. To do so it is simpler to introduce the ψ_n defined by

$$\psi_n = W_{n,n+1}T_{n+1} - W_{n+1,n}T_n \tag{30}$$

The equation (19) becomes an equation for the ψ_n:

$$\psi_{n+1} - \psi_n = a_n + W_{n,n+1}R_{n+1} - W_{n+1,n}R_n \tag{31}$$

This equation can be solved easily and one finds that the solution is

$$\psi_n = W_{n+1,n}R_n + \frac{A}{N} \sum_{i=1}^{N} iR_{n+i} + C_2 \tag{32}$$

where C_2 is an arbitrary constant. This constant C_2 will remain everywhere in the calculations but fortunately will disappear in the final expression of the diffusion constant. A useful relation to check that (32) solves (31) is that

$$W_{n+1,n}R_n - W_{n,n+1}R_{n+1} = \frac{A}{N} \sum_{i=1}^{N} R_i \tag{33}$$

This relation is easily verified when one replaces the R_n and A by their expressions (23), (24), and (29).

Now from the knowledge of the ψ_n, we can find the T_n by solving (30):

$$T_n = \frac{-1}{W_{n+1,n}} \frac{1}{1 - \prod_{i=1}^{N}(W_{i,i+1}/W_{i+1,i})} \times \left[\psi_n + \sum_{i=1}^{N-1} \psi_{n+i} \prod_{j=1}^{i} \left(\frac{W_{n+j-1,n+j}}{W_{n+j+1,n+j}} \right) \right] \tag{34}$$

At the end of this section, we have found explicit expressions of the R_n, a_n, and T_n as functions of all the hopping rates. We are now going to use these expressions to calculate the velocity and the diffusion constant.

3. VELOCITY AND DIFFUSION CONSTANT

To calculate the velocity V and the diffusion constant D, we shall use the following definitions:

$$V = \lim_{t\to\infty} \frac{d\overline{x(t)}}{dt} \tag{35}$$

$$D = \frac{1}{2} \lim_{t\to\infty} \frac{d}{dt} \left[\overline{x^2(t)} - \left(\overline{x(t)}\right)^2 \right] \tag{36}$$

where $x(t)$ is the position of the particle at time t and the bar denotes an average over the random walk. Notice that in this section we calculate V and D as functions of all the hopping rates $W_{i,j}$. Therefore there is no average to take with respect to the $W_{i,j}$. By definition one has

$$\overline{x(t)} = \sum_{n=-\infty}^{+\infty} nP_n(t) \tag{37}$$

Therefore

$$\begin{aligned} \frac{d\overline{x(t)}}{dt} &= \sum_{n=-\infty}^{+\infty} n \frac{dP_n}{dt} \\ &= \sum_{n=-\infty}^{-\infty} n\left[W_{n,n+1}P_{n+1} + W_{n,n-1}P_{n-1} - (W_{n+1,n} + W_{n-1,n})P_n \right] \\ &= \sum_{n=-\infty}^{+\infty} (W_{n+1,n} - W_{n-1,n})P_n = \sum_{n=1}^{N} (W_{n+1,n} - W_{n-1,n})\tilde{R}_n(t) \end{aligned}$$

Therefore in the long time limit (15), one finds

$$V = \sum_{n=1}^{N} (W_{n+1,n} - W_{n-1,n})R_n = A \tag{38}$$

One recovers the constant A [see Eq. (28)].

Let us now find the expression of the diffusion constant D. We start from

$$\overline{x^2(t)} = \sum_{n=-\infty}^{+\infty} n^2 P_n(t) \tag{39}$$

After a short calculation, one finds

$$\frac{d\overline{x^2(t)}}{dt} = 2\sum_{n=1}^{N} (W_{n+1,n} - W_{n-1,n})\tilde{S}_n(t) + \sum_{n=1}^{N} (W_{n+1,n} + W_{n-1,n})\tilde{R}_n(t) \tag{40}$$

$$\overline{x(t)} = \sum_{n=1}^{N} \tilde{S}_n(t) \tag{41}$$

$$\frac{d\overline{x(t)}}{dt} = \sum_{n=1}^{N} (W_{n+1,n} - W_{n-1,n})\tilde{R}_n(t) \tag{42}$$

If we replace $\tilde{S}_n(t)$ and $\tilde{R}_n(t)$ by their long time behaviors (15) and (16), one finds

$$\begin{aligned} D &= \frac{1}{2}\lim_{t\to\infty}\left[\frac{d\overline{x^2(t)}}{dt} - \frac{d\left(\overline{x(t)}\right)^2}{dt}\right] \\ &= \sum_{n=1}^{N} (W_{n+1,n} - W_{n-1,n})(a_n t + T_n) + \frac{1}{2}\sum_{n=1}^{N} (W_{n+1,n} + W_{n-1,n})R_n \\ &\quad - \sum_{n=1}^{N} (a_n t + T_n) \sum_{m=1}^{N} (W_{m+1,m} - W_{m-1,m})R_m \end{aligned} \tag{43}$$

Using Eqs. (26)–(28), one finds that the term linear in time disappears and it remains

$$D = \sum_{n=1}^{N} (W_{n+1,n} - W_{n-1,n})T_n + \frac{1}{2}\sum_{n=1}^{N} (W_{n+1,n} + W_{n-1,n})R_n - A\sum_{n=1}^{N} T_n \tag{44}$$

Now we can replace the T_n by their expressions (30) and (34):

$$\begin{aligned} D = &- \sum_{n=1}^{N} \psi_n + \frac{1}{2}\sum_{n=1}^{N} (W_{n+1,n} + W_{n-1,n})R_n \\ &+ A\frac{1}{1 - \prod_{i=1}^{N}(W_{i,i+1}/W_{i+1,i})} \sum_{n=1}^{N} u_n\psi_n \end{aligned} \tag{45}$$

where the u_n are defined by

$$u_n = \frac{1}{W_{n+1,n}}\left[1 + \sum_{i=1}^{N-1}\prod_{j=1}^{i}\left(\frac{W_{n-j,n+1-j}}{W_{n+1-j,n-j}}\right)\right] \tag{46}$$

Replacing again the ψ_n by their expressions (32) and using the relations (23), (24), (25), and (29), one obtains our final expression of the diffusion constant:

$$D = \frac{1}{\left(\sum_{n=1}^{N} r_n\right)^2} \left(A \sum_{n=1}^{N} u_n \sum_{i=1}^{N} i r_{n+i} + N \sum_{n=1}^{N} W_{n+1,n} u_n r_n \right) - A \frac{N+2}{2} \tag{47}$$

The arbitrary constant C_2 disappears in (47) because of the following relation:

$$\sum_{n=1}^{N} u_n = \sum_{n=1}^{N} r_n \tag{48}$$

At the end of this section we have found explicit expressions of the velocity V and the diffusion constant D as functions of all the $W_{i,j}$. For the velocity V we found

$$V = A = \frac{N}{\sum_{n=1}^{N} r_n} \left[1 - \prod_{n=1}^{N} \left(\frac{W_{n,n+1}}{W_{n+1,n}} \right) \right] \tag{49}$$

where the r_n are given by

$$r_n = \frac{1}{W_{n+1,n}} \left[1 + \sum_{i=1}^{N-1} \prod_{j=1}^{i} \left(\frac{W_{n+j-1,n+j}}{W_{n+j+1,n+j}} \right) \right] \tag{50}$$

For the diffusion constant the result is given in Eq. (47) and the u_n and r_n are given in Eqs. (46) and (50). So Eqs. (46)–(50) summarize all the results obtained up to now.

4. APPLICATION TO PURE AND RANDOM CASES

We are now going to calculate the velocity and the diffusion constant in three different situations: a pure asymmetric case, a random symmetric case, and a random asymmetric case. In the first two cases we shall find well-known results. The third case is the most interesting situation.

4.1. The Pure Asymmetric Case

We consider the situation where all the $W_{n+1,n}$ are equal and all the $W_{n-1,n}$ are equal:

$$\begin{aligned} W_{n+1,n} &= W_{\rightarrow} \\ W_{n-1,n} &= W_{\leftarrow} \end{aligned} \tag{51}$$

Then the r_n and the u_n are easy to calculate:

$$u_n = r_n + \frac{1}{W_\rightarrow}\left[1 - \left(\frac{W_\leftarrow}{W_\rightarrow}\right)^N\right] \Big/ \left[1 - \frac{W_\leftarrow}{W_\rightarrow}\right] \tag{52}$$

Therefore the velocity and the diffusion constant are

$$V = W_\rightarrow - W_\leftarrow \tag{53}$$

$$D = \tfrac{1}{2}(W_\rightarrow + W_\leftarrow) \tag{54}$$

These expressions are of course well known and this case is just a verification.

4.2. The Random Symmetric Case

We consider now a situation where the $W_{i,j}$ are different but with the property

$$W_{i,j} = W_{j,i} \tag{55}$$

In this case we have

$$r_n = \sum_{i=1}^{N} \frac{1}{W_{i+1,i}} \tag{56}$$

$$u_n = \frac{N}{W_{n+1,n}} \tag{57}$$

One finds that the velocity V [Eq. (49)] vanishes as it should:

$$V = A = 0 \tag{58}$$

and the diffusion constant becomes here

$$D = N \Big/ \left(\sum_{n=1}^{N} \frac{1}{W_{n+1,n}}\right) \tag{59}$$

If the $W_{n+1,n}$ are distributed according to a distribution $\rho(W)$, one sees that (59) gives in the thermodynamic limit $N \rightarrow \infty$:

$$D = \left\langle \frac{1}{W} \right\rangle^{-1} = \left[\int \rho(W) \frac{dW}{W}\right]^{-1} \tag{60}$$

This result is also well known.[1,8]

4.3. The Random Asymmetric Case

This is a situation for which less is known but which can also be described with the results of Section 3. We consider here the case where the

$W_{i,j}$ are random independent variables except that $W_{i,j}$ and $W_{j,i}$ may be correlated. This means that the two W of the same bond can be correlated but are independent of the W on another bond. When one tries to study this problem, one has to face two difficulties.

Firstly, it is not obvious at all that the velocity and the diffusion constant of the infinite random system are the same as what one finds by taking in expressions (47) and (49) the limit $N \to \infty$. In other words, it could be possible that the limits $N \to \infty$ and $t \to \infty$ do not commute. I believe that these limits actually commute although I do not know how to prove it.

The second difficulty is that the expressions (47) and (49) are complicated enough to make impossible the analytic calculation of the average of V or D for an arbitrary period N. This difficulty is not a serious one because as we shall see it, the problem of calculating V and D becomes simpler in the limit $N \to \infty$. All the limits that we shall calculate will exist with probability 1.

We shall restrict ourselves to the case

$$\left\langle \log\left(\frac{W_{n,n+1}}{W_{n+1,n}} \right) \right\rangle < 0 \tag{61}$$

All the results are easy to transpose to the other case. Let us first calculate the velocity. Because of (61), one has in the limit $N \to \infty$:

$$\lim_{N \to \infty} 1 - \prod_{n=1}^{N} \frac{W_{n,n+1}}{W_{n+1,n}} = 1 \tag{62}$$

This simplifies the expression (49) of the velocity:

$$V = \lim_{N \to \infty} N \Big/ \left(\sum_{n=1}^{N} r_n \right) \tag{63}$$

Now the denominator of (63) can be simplified by replacing the sum by the average of r_n:

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} r_n = \langle r_n \rangle \tag{64}$$

The average of r_n is finite in the limit $N \to \infty$ only if

$$\left\langle \frac{W_{n,n+1}}{W_{n+1,n}} \right\rangle < 1 \tag{65}$$

and one finds that

$$\langle r \rangle = \left\langle \frac{1}{W_{n+1,n}} \right\rangle \left(1 - \left\langle \frac{W_{n,n+1}}{W_{n+1,n}} \right\rangle \right)^{-1} \tag{66}$$

Therefore, if condition (65) is satisfied, one finds that the velocity V is given by

$$V = \left\langle \frac{1}{W_{n+1,n}} \right\rangle^{-1} \left(1 - \left\langle \frac{W_{n,n+1}}{W_{n+1,n}} \right\rangle\right) \tag{67}$$

On the contrary if the condition (65) is not satisfied

$$\left\langle \frac{W_{n,n+1}}{W_{n+1,n}} \right\rangle > 1 \quad \text{and} \quad \left\langle \log \frac{W_{n,n+1}}{W_{n+1,n}} \right\rangle < 0 \tag{68}$$

then $\langle r \rangle = \infty$ and the velocity vanishes:

$$V = 0 \tag{69}$$

One should notice that the calculation of the velocity became simpler in the limit $N \to \infty$, whereas averaging V for finite N seems an impossible task. The reason of this simplification is that, in the limit $N \to \infty$, quantities like (64) do not fluctuate anymore.

Let us now calculate the diffusion constant. To do so we can rewrite (47) using relation (48):

$$D = -\frac{A}{2} + N \frac{\sum_{n=1}^{N} W_{n+1,n} u_n r_n}{\left(\sum_{n=1}^{N} r_n\right)^2} + \frac{A}{\left(\sum_{n=1}^{N} r_n\right)^2} \sum_{i=1}^{N} \left(i - \frac{N+1}{2}\right) \sum_{n=1}^{N} u_n r_{n+i} \tag{70}$$

In the thermodynamic limit $N \to \infty$, each of the sums which appear in (70) has a simple limit. First the constant A is given by (67) [see Eq. (38)]. The sums of r_n have also been calculated [see Eqs. (64) and (66)]:

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} r_n = \left\langle \frac{1}{W_{n+1,n}} \right\rangle \left[1 - \left\langle \frac{W_{n,n+1}}{W_{n+1,n}} \right\rangle\right]^{-1} \tag{71}$$

So we have only two sums to calculate in (70). First by looking at the expressions the u_n and the r_n (46), (50), one shows easily that

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} W_{n,n+1} u_n r_n = \left\langle \frac{1}{W_{n+1,n}} \right\rangle \left(1 - \left\langle \frac{W_{n,n+1}}{W_{n+1,n}} \right\rangle\right)^{-2} \tag{72}$$

The calculation of the remaining sum is a little more complicated. From the expressions of the u_n and the r_n, one can calculate their correlations in the limit $N \to \infty$. One finds in this limit that u_n is not correlated to the r_m with $m > n$ but is correlated to the r_m with $m \leqslant n$. This means that in the thermodynamic limit, one has

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} u_n r_{n-j} = \langle u\rangle\langle r\rangle + f(j) = \langle r\rangle^2 + f(j) \tag{73}$$

where the function $f(j)$ has the following properties:

$$\begin{array}{lll} f(j) \neq 0 & \text{if} & j \geqslant 0 \\ f(j) \to 0 & \text{when} & j \to \infty \\ f(j) = 0 & \text{if} & j < 0 \end{array} \tag{74}$$

Using (73), one can write

$$\begin{aligned} \lim_{N\to\infty} \frac{1}{N^2} \sum_{i=1}^{N} \left(i - \frac{N+1}{2}\right) \sum_{n=1}^{N} u_n r_{n+i} &= \lim_{N\to\infty} \frac{1}{N} \sum_{j=0}^{N} \left(\frac{N-1}{2} - j\right) f(j) \\ &= \frac{1}{2} \sum_{j=0}^{\infty} f(j) \end{aligned} \tag{75}$$

The calculation of this last sum is long but does not present any difficulty since the u_n and the r_n are given and $f(j)$ is defined by (73). One finds that this sum is finite with probability 1 only if

$$\left\langle \left(\frac{W_{n,n+1}}{W_{n+1,n}} \right)^2 \right\rangle < 1 \tag{76}$$

and the result is

$$\sum_{j=0}^{\infty} f(j) = e \frac{1+a}{1-a} \frac{1}{1-b} + 2cd \frac{1+a}{(1-a)^2(1-b)} - c^2 \frac{1+a}{(1-a)^3} \tag{77}$$

where a, b, c, d, and e are defined by

$$a = \left\langle \frac{W_{n,n+1}}{W_{n+1,n}} \right\rangle = \left\langle \frac{W_{\leftarrow}}{W_{\rightarrow}} \right\rangle \tag{78}$$

$$b = \left\langle \left(\frac{W_{n,n+1}}{W_{n+1,n}} \right)^2 \right\rangle = \left\langle \left(\frac{W_{\leftarrow}}{W_{\rightarrow}} \right)^2 \right\rangle \tag{79}$$

$$c = \left\langle \frac{1}{W_{n+1,n}} \right\rangle = \left\langle \frac{1}{W_{\rightarrow}} \right\rangle \tag{80}$$

$$d = \left\langle \frac{W_{n,n+1}}{(W_{n+1,n})^2} \right\rangle = \left\langle \frac{W_{\leftarrow}}{(W_{\rightarrow})^2} \right\rangle \tag{81}$$

$$e = \left\langle \frac{1}{(W_{n+1,n})^2} \right\rangle = \left\langle \frac{1}{(W_{\rightarrow})^2} \right\rangle \tag{82}$$

The notation adopted here is obvious: $W_{\rightarrow}$ replaces $W_{n+1,n}$ and $W_{\leftarrow}$ replaces $W_{n,n+1}$.

Combining all these results, one finds that if

$$\left\langle \left(\frac{W_{\leftarrow}}{W_{\rightarrow}} \right)^2 \right\rangle < 1 \tag{83}$$

The diffusion constant D is given by

$$D = \frac{1 - \langle W_{\leftarrow}/W_{\rightarrow} \rangle^2}{1 - \langle (W_{\leftarrow}/W_{\rightarrow})^2 \rangle} \left\langle \frac{1}{W_{\rightarrow}} \right\rangle^{-3} \times \left[\left\langle \frac{1}{W_{\rightarrow}} \right\rangle \left\langle \frac{W_{\leftarrow}}{(W_{\rightarrow})^2} \right\rangle + \frac{1}{2} \left\langle \frac{1}{(W_{\rightarrow})^2} \right\rangle \left(1 - \left\langle \frac{W_{\leftarrow}}{W_{\rightarrow}} \right\rangle \right) \right] \tag{84}$$

If condition (83) is not satisfied but one has

$$\left\langle \left(\frac{W_{\leftarrow}}{W_{\rightarrow}} \right)^2 \right\rangle > 1 \quad \text{and} \quad \left\langle \frac{W_{\leftarrow}}{W_{\rightarrow}} \right\rangle < 1 \tag{85}$$

Then all the sums which appear in (70) are finite except the last one, which diverges [see condition (76)]. Therefore

$$D = \infty \tag{86}$$

The last region

$$\left\langle \frac{W_{\leftarrow}}{W_{\rightarrow}} \right\rangle > 1 \quad \text{and} \quad \left\langle \log \frac{W_{\leftarrow}}{W_{\rightarrow}} \right\rangle < 0 \tag{87}$$

is more complicated because, in the expression (70), numerators and denominators are both infinite. It is, however, reasonable to expect that the diffusion constant is zero[11] in a whole region which contains the point $\langle \log(W_{\leftarrow}/W_{\rightarrow}) \rangle = 0$.

It is easy to transpose all the expressions given in this section to the case $\langle \log(W_{\leftarrow}/W_{\rightarrow}) \rangle > 0$.

4.4. An Example

In order to illustrate the results of Section 4.3, we are going to study a simple example: the pairs $(W_{n,n+1}, W_{n+1,n})$ can take two values:

$$\begin{aligned} &\text{with probability } \alpha && \begin{cases} W_{n,n+1} = 1 \\ W_{n+1,n} = W \end{cases} \\ &\text{and with probability } 1-\alpha && \begin{cases} W_{n,n+1} = W \\ W_{n+1,n} = 1 \end{cases} \end{aligned} \tag{88}$$

where the constant $W > 1$. The velocity and the diffusion constant are drawn on Figs. 1 and 2.

The critical points α_1 and α_2 are given by

$$\alpha_1 = \frac{W}{W+1} \tag{89}$$

$$\alpha_2 = \frac{W^2}{W^2+1} \tag{90}$$

The model has an obvious symmetry $\alpha \to 1 - \alpha$. One sees that the velocity and the diffusion constant are not singular at the same point. Although this would require more complicated calculations, it is more than likely that higher cumulants of the position $x(t)$ are singular at different points α_n. More precisely the nth cumulant of $x(t)$ is singular at a point α_n given by

$$\left\langle \left(\frac{W_{\leftarrow}}{W_{\rightarrow}} \right)^n \right\rangle = 1 \tag{91}$$

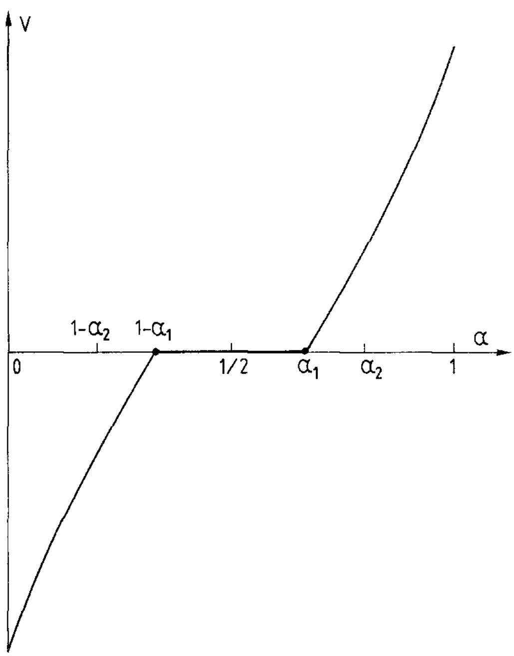

Fig. 1. The velocity of the random asymmetric model defined by (88). The velocity vanishes in a whole region $1 - \alpha_1 < \alpha < \alpha_1$.

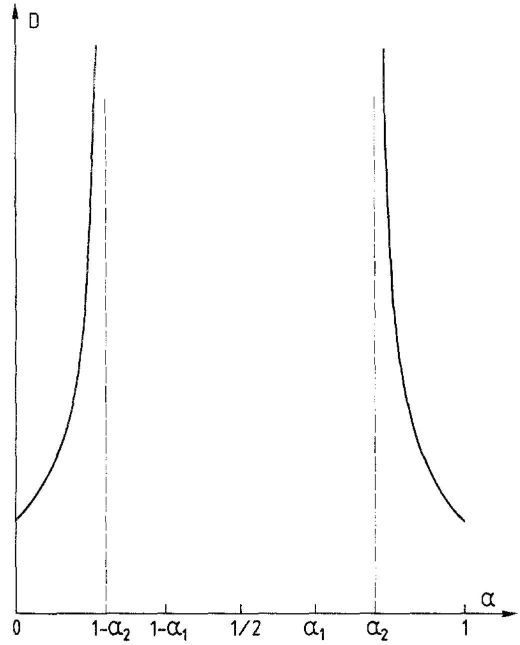

Fig. 2. The diffusion constant of the same model. It diverges at the points α_2 and $1-\alpha_2$ which differ from the points α_1 and $1-\alpha_1$ where the velocity is singular.

5. THE DISCRETE TIME HOPPING MODEL

The hopping model is often considered in a discrete time version. Therefore it is useful to write the results obtained above in that case.

On each site n of the chain, there is a number p_n $(0 < p_n < 1)$. If the particle is at time t on site n, then, at time $t+1$, it will be either on site $n+1$ with probability p_n or on site $n-1$ with probability $q_n = 1 - p_n$. The Master equation becomes here

$$P_n(t+1) = q_{n+1}P_{n+1}(t) + p_{n-1}P_{n-1}(t) \tag{92}$$

where $P_n(t)$ is the probability that the particle is on site n at time t. Here if the lattice has a period N, one has

$$p_n = 1 - q_n = p_{n+N} = 1 - q_{n+N} \tag{93}$$

The calculations given in Sections 2 and 3 can be reproduced here without any difficulty. Therefore it is sufficient to give directly the results. They are again expressed as functions of the r_n and the u_n:

$$r_n = \frac{1}{p_n}\left[1 + \sum_{i=1}^{N-1} \prod_{j=1}^{i} \left(\frac{q_{n+j}}{p_{n+j}}\right)\right] \tag{94}$$

$$u_n = \frac{1}{p_n}\left[1 + \sum_{i=1}^{N-1} \prod_{j=1}^{i} \left(\frac{q_{n+1-j}}{p_{n-j}}\right)\right] \tag{95}$$

The velocity V is given by[12]

$$V = N\left[1 - \prod_{i=1}^{N}\left(\frac{q_i}{p_i}\right)\right] \Big/ \left[\sum_{n=1}^{N} r_n\right] \tag{96}$$

whereas the diffusion constant D is

$$D = -\frac{V^2}{2} - \frac{N+2}{2} V + \frac{N}{\left(\sum_{n=1}^{N} r_n\right)^2} \sum_{n=1}^{N} p_n u_n r_n + \frac{V}{\left(\sum_{n=1}^{N} r_n\right)^2} \sum_{n=1}^{N} \left(u_n \sum_{i=1}^{N} i r_{n+i}\right) \tag{97}$$

One should compare the expressions of the velocity (96) and (49) and the expressions of the diffusion constant (97) and (47). They are almost identical except the term $-V^2/2$ in (97).

If the p_n are randomly distributed according to a distribution $\rho(p_n)$, one finds, using the method described in Section 4, that in the thermodynamic limit ($N \to \infty$), the diffusion constant is finite only if

$$\left\langle \frac{q^2}{p^2} \right\rangle < 1 \tag{98}$$

and the expression of D is

$$D = -\frac{1}{2}\frac{(1 - \langle q/p \rangle)^2}{\langle 1/p \rangle^2} + \frac{(1 - \langle q/p \rangle^2)}{(1 - \langle q^2/p^2 \rangle)} \left\langle \frac{1}{p} \right\rangle^{-3} \times \left[\left\langle \frac{1}{p} \right\rangle \left\langle \frac{q}{p^2} \right\rangle + \frac{1}{2}\left\langle \frac{1}{p^2} \right\rangle \left(1 - \left\langle \frac{q}{p} \right\rangle\right)\right] \tag{99}$$

Similarly, one finds that the velocity is finite if

$$\left\langle \frac{q}{p} \right\rangle < 1 \tag{100}$$

and its expression is

$$V = \left(1 - \left\langle \frac{q}{p} \right\rangle\right) \Big/ \left\langle \frac{1}{p} \right\rangle \tag{101}$$

Expressions (99) and (101) can easily be transposed to cases where $\langle p/q \rangle < 1$ or $\langle p^2/q^2 \rangle < 1$.

6. CONCLUSION

In this paper we have obtained explicit expressions of the velocity (49), (96) and of the diffusion constant (47), (97) of periodic hopping problems with an arbitrary period N. We have seen how from these expressions one can calculate the velocity (67), (101) or the diffusion constant (84), (99) in the random case for an infinite system, at least when the results are finite. I think that from these exact expressions one can obtain, at least numerically, several interesting informations: for finite N and random hopping rates, it would be interesting to know the distributions of V and D and to see how these distributions evolve when N increases. Another possible application is to study the effect of correlations between the $W_{n,n+1}$ of different bonds. In particular, it would be interesting to see what happens when the $W_{n,n+1}$ are quasiperiodic functions of n.

The reason that we could calculate explicitly here V and D is that the steady state can be found exactly. This is not the case in higher-dimensional models or even in one dimension with hopping rates between next nearest neighbors. However, these steady state ideas can be used in all these difficult problems if one tries to make weak disorder expansions of the velocity, the diffusion constant or the frequency-dependent conductivity. The details for lattices in any dimension will be given, I hope, in a forthcoming paper although the method has been described for a one-dimensional model in a recent work done with R. Orbach.[15]

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