## TRANSPORT IN STRONGLY DISORDERED CHAINS

#### J. VAN POLEN and H. VAN BEIJEREN

Institute for Theoretical Physics, Princetonplein 5, P.O. Box 80006, 3508 TA Utrecht, The Netherlands

Received 27 June 1990

A one-dimensional hopping model is studied with a translation invariant hopping rate distribution proportional to  $\nu^{-\alpha}$  ( $0 < \alpha < 1$ ) for hopping rate  $\nu$  approaching zero. The long time behavior of the return probability and the mean square displacement of the hopping particle are calculated with the aid of a transfer matrix method. Previous results of Bernasconi et al. and of Stephen and Kariotis, obtained by different methods, are confirmed; results of Nieuwenhuizen and Ernst are found to be partly in agreement and partly in disagreement with the former.

## 1. Introduction

Approximately ten years ago Bernasconi et al. [1, 2] addressed the problem of hopping transport on disordered chains, in which the hopping rates between neighboring sites are independent random variables. If the average waiting time between subsequent jumps is finite, the hopping process approaches ordinary diffusion for long times [1-4], although the disorder in the chain does give rise to long time tail effects [3]. On the other hand, if the average waiting time is divergent, the hopping process does not approach diffusion for long times: the mean square displacement of a particle does not increase proportionally to time, but rather as a power  $t^{\alpha}$  with  $\alpha < 1$  [1-4], and the probability distribution function for a particle starting out at a given point at t = 0 does not approach a Gaussian for long times. The model addressed here can be used to describe conduction in quasi-one-dimensional superionic conductors [1]. In addition it can be mapped on to several other interesting disordered models in one dimension. Examples [2] are the harmonic chain with random masses or spring constants, excitations at low temperature in a Heisenberg chain and electrical lines with random conductances or capacitances.

In this paper we will treat the hopping process with divergent average waiting time by means of a transfer matrix method, which has been employed before to treat the stochastic one-dimensional Lorentz gas [5, 6]. Different

0378-4371/91/\$03.50 (C) 1991 - Elsevier Science Publishers B.V. (North-Holland)

methods have been used before: integral equation techniques were introduced by Bernasconi et al. [1, 2] and extended by Nieuwenhuizen and Ernst [3]; Stephen and Kariotis employed the replica method [4].

The main results of our calculations are expressions for the long time behavior of the probability for having returned to the origin and for the mean square displacement of a hopping particle. Our expressions fully agree with those of Stephen and Kariotis, so, strictly spoken, we have not obtained any new results. Yet we think the paper is useful, for the following reasons:

i) Bernasconi et al. do not give an exact expression for the long time behaviour of the mean square displacement, and Nieuwenhuizen and Ernst give an expression that is at variance with that of Stephen and Kariotis. Our results, obtained by an entirely different method, provide a useful confirmation of the latter's results.

ii) The physical interpretation of our method is quite straightforward, which, to our feeling, cannot be said of the replica method.

The plan of the paper is as follows: In section 2 we introduce the master equation and the hopping time distributions, describing our system. Next we introduce a dual transformation of the master equation to make it more tractable. In section 3 we express the average Green's function for the hopping process in terms of the stationary eigenvector of a transfer matrix, and in section 4 we calculate the long time behaviour of the probability of being back at the origin and of the mean squared displacement. Finally, in section 5 we discuss our results and make comparisons to previous work.

## 2. Master equation

The probability  $P_n(t)$  to find a particle at site *n* at time *t* evolves in time according to the master equation

$$\frac{\mathrm{d}}{\mathrm{d}t} P_n(t) = \frac{1}{2} \nu_n [P_{n+1}(t) - P_n(t)] + \frac{1}{2} \nu_{n-1} [P_{n-1}(t) - P_n(t)].$$
(1)

The transfer rates  $\nu_n$  are independent random variables distributed according to a position-independent probability density function  $\rho(\nu)$ , given as<sup>#1</sup>

$$\rho(\nu) = \begin{cases} (1-\alpha)2^{\alpha-1}\nu^{-\alpha}, & 0 < \nu \le 2, \\ 0, & \text{elsewhere}. \end{cases}$$
(2)

This distribution has been studied before in refs. [1-4]. A quantity of central

<sup>#1</sup> The quantity  $\nu$  in our notation corresponds to 2W in refs. [1-4].

interest is the Green's function  $\langle G_n(t) \rangle$ , the average probability of finding a particle starting at the origin (n = 0) at t = 0, at site *n* at time *t*. The brackets indicate a combined average over all realizations of the hopping process at given values of the jump rates  $\nu_n$ , and over the jump rate distributions  $\rho(\nu_n)$ .

The latter average does include an average over a stationary initial distribution of the hopping particle, in which the lattice sites are relabeled such that the starting position always is the origin. In principle this leads to an extra weighing factor for each set of jump rates  $\{\nu_n\}$ , proportional to the stationary probability of finding the jumping particle at the origin under the realization  $\{\nu_n\}$ . However, the stationary solution of (1) is of the form  $P_n = \text{constant}$ , independently of  $\{\nu_n\}$ , hence this weighing factor for the present problem is simply unity.

Accordingly  $\langle G_n(t) \rangle$  may be found by solving (1) with the initial condition  $P_n(0) = \delta_{n0}$  and averaging the solution over the probability distribution

$$W\{\nu_n\} = \prod_{n=-\infty}^{\infty} \rho\{\nu_n\}.$$
 (3)

For general *n* no simple closed form expression for  $\langle G_n(t) \rangle$  has been found so far, but for  $\langle G_0(t) \rangle$  and for the second moment  $\langle x^2(t) \rangle = \sum_{n=-\infty}^{\infty} n^2 \langle G_n(t) \rangle$  different closed form expressions have been given in refs. [1-4]. Here we will evaluate these quantities by means of a transfer matrix method, which has been used before [5, 6], and reproduce the expressions given by Stephen and Kariotis [4].

For this transfer matrix method to be applicable one has to apply a dual transformation. Introducing

$$j_n(t) = P_n(t) - P_{n+1}(t)$$
(4)

one may rewrite (1) as<sup>#2</sup>

$$\frac{\mathrm{d}}{\mathrm{d}t} j_n(t) = \frac{1}{2} \left[ \nu_{n-1} j_{n-1}(t) + \nu_{n+1} j_{n+1}(t) - 2\nu_n j_n(t) \right].$$
(5)

To obtain  $\langle G_n(t) \rangle$  from (5) one has to solve it with initial condition  $j_n(0) = \delta_{n0} - \delta_{n+1,0}$  and average  $P_n(t)$ , to be constructed from  $j_n(t)$ , over  $W\{\rho_n\}$ .

<sup>&</sup>lt;sup>\*2</sup> Eq. (5) can also be interpreted as a master equation for occupation probabilities  $j_n(t)$ , with jump rates  $\nu_n$  that depend only on the site from which the jump originates. However, this process has as stationary solution  $j_n = \nu_n^{-1}$  (the stationary solution of (1) corresponds to the trivial stationary solution  $j_n = 0$  of (3)). As a consequence the average over the jump rate distributions is ill-defined, because the probability of starting at the origin now has to be weighted by  $\nu_0^{-1}$  and with the distribution (2) the integral over  $\nu_0^{-1}\rho(\nu_0)$  is divergent.

Instead we may consider the solution  $\overline{j}_n(t)$  of (5), with initial condition  $\overline{j}_n(0) = \delta_{n0}$ , and average this over the same probability distribution. To understand this, first note that

$$\langle \overline{j_n}(t) \rangle - \langle \overline{j_{n+1}}(t) \rangle = \langle j_n(t) \rangle$$
 (6)

because of translation invariance for averaged quantities. From the definition of  $\langle j_n(t) \rangle$  it follows that

$$\langle j_n(t) \rangle = \langle P_n(t) \rangle - \langle P_{n+1}(t) \rangle \tag{7}$$

with initial condition  $P_n(0) = \delta_{n0}$ . Hence one may conclude to

$$\langle \overline{j_n}(t) \rangle = \langle P_n(t) \rangle + f(t)$$
 (8)

with f(t) independent of n. From (1) and (5) one readily derives the relations

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{n}P_{n}(t)=0,$$
(9a)

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{n}\overline{j_{n}}(t)=0.$$
(9b)

From the initial conditions one finds  $\sum P_n(t) = \sum \overline{j_n}(t) = 1$ , therefore f(t) = 0, and indeed  $\langle \overline{j_n}(t) \rangle = \langle P_n(t) \rangle$ . Hence, replacing the notation  $\overline{j_n}(t)$  by  $P_n(t)$ , one finds the original problem may be replaced by that of finding  $\langle P_n(t) \rangle$  for  $P_n(t)$ satisfying (5) with initial condition  $P_n(0) = \delta_{n,0}$ .

# 3. Transfer matrix method. Formal expressions for $\langle P_n(z) \rangle$ , G(k, z) and $\langle x^2(z) \rangle$

In this section, we will derive expressions for  $\langle P_n(z) \rangle$ , the Laplace transform of  $\langle P_n(t) \rangle$ , for G(k, z), defined as the Fourier transform of  $\langle P_n(z) \rangle$ :

$$G(k, z) = \sum_{n=-\infty}^{\infty} \langle P_n(z) \rangle e^{-ikn}, \qquad (10)$$

and for  $\langle x^2(z) \rangle$ , which, of course, is the Laplace transform of the averaged second moment  $\langle x^2(t) \rangle$ . We start with some further definitions: Let  $W_n(t)$  be the probability that the particle, arriving at site *n*, will have to wait there for a period of time  $\geq t$  before it jumps again. For the process described by (5) we

have

$$W_n(t) = e^{-\nu_n t}$$
 (11)

Let  $I_n(t)$  denote the probability density (p.d.) for a jump from n to n + 1 at time t, under the condition that the particle arrived at n at time 0 and stayed there between times 0 and t. By symmetry the p.d. for a jump from n to n - 1 under the same conditions is the same.  $W_n(t)$  and  $I_n(t)$  are related through

$$W_n(t) = 1 - 2 \int_0^t I_n(t') \, \mathrm{d}t' \,. \tag{12}$$

(11) and (12) yield

$$I_n(t) = \frac{1}{2}\nu_n \,\mathrm{e}^{-\nu_n t} \,. \tag{13}$$

Finally, let  $\psi_n(k, t)$  be the p.d. for the *n*th return to k at time t, under the conditions:

1) at t = 0, the particle is at site k;

2) from k, it can only jump to the right, with jumping time distribution  $I_k(t)$ ; (This means that all jumps from k to the left are disregarded.)

3) the averages with respect to the  $\rho(\nu_i)$  (i > k) have been taken.

We want to derive a connection between the return probability to k and that to k + 1. Suppose the particle starts at site k at t = 0, makes n returns to k from the right, the last one at time t, and within this time interval also makes m returns to k + 1 from the right. (See fig. 1.) There are  $\binom{m+n-1}{m}$  ways of



Fig. 1. Illustration of the path of the particle between scatterers k-k+2.

ordering the sequence of returns to k + 1 in time, where we use the convention  $\binom{m-1}{m} = \delta_{m0}$ . In consequence, the Laplace transform of  $\psi_n(k, t)$  satisfies the equation

$$\psi_{n}(k, z) = \sum_{m=0}^{\infty} \int_{0}^{\infty} d\nu_{k+1} \rho(\nu_{k+1}) [I_{k}(z)]^{n} [I_{k+1}(z)]^{n} \\ \times \left(\frac{m+n-1}{m}\right) \psi_{m}(k+1, z) , \qquad (14)$$

where  $I_k(z)$  is the Laplace transform of  $I_k(t)$  (known already) and  $\psi_0(k+1, z)$ = 1. From (13), we see

$$I_k(z) = \frac{\frac{1}{2}\nu_k}{z + \nu_k} \,. \tag{15}$$

To stress the dependence on  $\nu_k$ , we will write  $I(\nu_k)$  and  $\psi_n(\nu_k)$  instead of  $I_k(z)$ and  $\psi_n(k, z)$ . When we define

$$\psi_n^T = \frac{\psi_n(\nu_k)}{\left[I(\nu_k)\right]^n} \tag{16}$$

(14) can be written as

$$\boldsymbol{\psi}^{T} = T\boldsymbol{\psi}^{T} \,, \tag{17}$$

where the operator T has matrix elements

$$T_{nm} = \left(\frac{m+n-1}{m}\right) \int_{0}^{\infty} \mathrm{d}\nu \,\rho(\nu) \left(\frac{\frac{1}{2}\nu}{z+\nu}\right)^{n+m}.$$
 (18)

Here we used (15); note that  $\psi_n^T$  is independent of  $\nu_k$ ! From the probabilistic interpretation of  $\psi_n(k, t)$  and eq. (14) we obtain

$$\boldsymbol{\psi}_0^T = \boldsymbol{1} \,. \tag{19}$$

In addition, from (15)-(18) and (2) one may derive

$$\lim_{n \to \infty} \psi_n^T = 0 . \tag{20}$$

The small-z behaviour of  $\psi_n^T$  will be calculated in section 4. Next, we want to express  $\langle P_n(z) \rangle$  in terms of  $\psi^T$  and some operators acting

on it. For this purpose, we define still another probability density. Let  $\mathcal{P}_n(t)$  be the p.d. for the arrival of the particle at site *n* exactly at time *t*, under the condition that it resided at site 0 at t = 0. Its Laplace transform,  $\mathcal{P}_n(z)$ , satisfies the relation

$$P_n(z) = W_n(z) \mathcal{P}_n(z) = \frac{1}{z + \nu_n} \mathcal{P}_n(z) , \qquad (21)$$

where  $W_n(z)$  is the Laplace transform of  $W_n(t)$ , defined in (11).  $\mathcal{P}_n(z)$  can be expressed in terms of the Laplace transformed return probability densities in the following way: For n = 0 we have

$$\mathscr{P}_0(z) \equiv \mathscr{P}(\nu_0) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} {\binom{m+n}{m}} \psi_n(\nu_0) \psi_m(\nu_0) .$$
(22)

The explanation is as follows: suppose the particle returns to the origin m times from the right and n times from the left. The total time spent on the right of the origin is t' and on the left it is t - t'. The total number of different sequences of returns from right and left is  $\binom{n+m}{m}$ . Hence the probability density for these events to occur is given by

$$\binom{m+n}{m}\int_0^t \mathrm{d}t' \,\psi_m(0,\,t')\,\psi_n(0,\,t-t')\,.$$

Laplace transformation and summation over m and n leads to (22). Note that we tacitly used left/right symmetry at each site.

The same kind of reasoning gives for  $\mathcal{P}_1(z)$ 

$$\mathcal{P}_{1}(z) \equiv \mathcal{P}_{1}(\nu_{0}, \nu_{1})$$

$$= \sum_{m=0}^{\infty} \psi_{m}(\nu_{0}) \sum_{n=0}^{\infty} {\binom{m+n}{n}} \sum_{l=0}^{\infty} {\binom{n+l}{l}} [I(\nu_{0})]^{n+1} [I(\nu_{1})]^{n} \psi_{l}(\nu_{1}) .$$
(23)

This may be written as

$$\mathscr{P}_{1}(\nu_{0}, \nu_{1}) = (\psi(\nu_{0}), RS(\nu_{0}, \nu_{1}) \psi(\nu_{1})), \qquad (24)$$

where (, ) denotes the usual inner product and the operators R and  $S(\nu_0, \nu_1)$  are defined through

$$R_{mn} = \binom{m+n}{n} \tag{25}$$

and

$$S_{mn}(\nu_0, \nu_1) = \left(\frac{m+n}{n}\right) [I(\nu_0)]^{m+1} [I(\nu_1)]^m .$$
<sup>(26)</sup>

Generalizing this analysis one obtains

$$P_n(\nu_0, \ldots, \nu_n) = (\psi(\nu_0), RS(\nu_0, \nu_1) \cdots S(\nu_{n-1}, \nu_n) \psi(\nu_n)), \qquad (27)$$

which holds for  $n \ge 1$ . When we define

$$S_{mn}(\nu_k) = \left(\frac{m+n}{m}\right) \left[I(\nu_k)\right]^{n+m+1}$$
(28)

and use (16), it is a matter of algebra to show that

$$\mathcal{P}_n(\nu_0,\ldots,\nu_n) = \frac{1}{I(\nu_n)} \left( \psi^T, S(\nu_0) S(\nu_1) \cdots S(\nu_n) \psi^T \right).$$
<sup>(29)</sup>

From (15) and (21) we obtain

$$P_n(z) \approx \left(\psi^T, S(\nu_0) \ S(\nu_1) \cdots S(\nu_{n+1}) \ \frac{2S(\nu_n)}{\nu_n} \ \psi^T\right), \tag{30}$$

which holds for  $n \ge 0$ . Now take the average

$$\langle P_n(z) \rangle = \left( \psi^T, \left\langle S(\nu_0) \right\rangle_{\nu_0} \left\langle S(\nu_1) \right\rangle_{\nu_1} \cdots \left\langle S(\nu_{n-1}) \right\rangle_{\nu_{n-1}} \left\langle \frac{2S(\nu_n)}{\nu_n} \right\rangle_{\nu_n} \psi^T \right)$$

$$= \left( \psi^T, \left[ \left\langle S(\nu) \right\rangle_{\nu} \right]^n \left\langle \frac{2S(\nu)}{\nu} \right\rangle_{\nu} \psi^T \right),$$
(31)

where, for instance,  $\langle S(\nu) \rangle_r = \int_0^\infty S(\nu) \rho(\nu) d\nu$ .

As a last step, writing S for  $\langle S(\nu) \rangle_{\nu}$ , we will express  $\langle 2S(\nu)/\nu \rangle_{\nu} \psi^{T}$  in terms of S acting on  $\psi^{T}$ . From (15) and (28), we have

$$S_{mn} = \left(\frac{m+n}{n}\right) 2^{-(m+n+1)} \int_{0}^{\infty} d\nu \,\rho(\nu) \left(\frac{\nu}{z+\nu}\right)^{m+n+1}$$
(32)

and

$$\left(\left\langle \frac{2S(\nu)}{\nu}\right\rangle_{\nu}\right)_{mn} = \left(\frac{m+n}{m}\right) 2^{-(m+n)} \int_{0}^{\nu} d\nu \ \rho(\nu) \ \frac{1}{\nu} \left(\frac{\nu}{z+\nu}\right)^{m+n+1}.$$
 (33)

254

Comparison of (32) and (18) yields

$$S_{mn} = T_{m+1,n} \tag{34}$$

and, likewise, we find

$$\left(\left\langle \frac{2S(\nu)}{\nu} \right\rangle_{\nu}\right)_{mn} = \frac{1}{z} \left( T_{m+1,n-1} + T_{mn} - 2T_{m+1,n} \right).$$
(35)

Using (17) and (34), (35) yields

$$\left\langle \frac{2S(\nu)}{\nu} \right\rangle_{\nu} \psi^{T} = \frac{1}{z} \left( S^{2} \psi^{T} + \psi^{T} - 2S \psi^{T} \right), \qquad (36)$$

which is inserted into (31) to give our formula for  $\langle P_n(z) \rangle$ :

$$\langle P_n(z)\rangle = \frac{1}{z} \left(\psi^T, S^n(1-S)^2\psi^T\right), \qquad n \ge 0.$$
(37)

In case n < 0, we simply have

$$\langle P_n(z) \rangle = \langle P_{-n}(z) \rangle$$
 (38)

owing to the left/right symmetry at each site and the averaging procedure. In particular, for n = 0 we find

$$\langle P_0(z) \rangle = \frac{1}{z} \left( \psi^T, (1-S)^2 \psi^T \right) = \frac{1}{z} \left( (1-S) \psi^T, (1-S) \psi^T \right)$$
  
=  $\frac{1}{z} \sum_{n=0}^{\infty} \left( \psi^T_n - \psi^T_{n+1} \right)^2.$  (39)

Here we used the fact that S is symmetric (from (32) and (17) and (34)) to give  $(S\psi^T)_n = \psi_{n+1}^T$ . This will enable us to calculate  $\langle P_0(z) \rangle$  for  $z \to 0$  once  $\psi^T$  has been found.

It will prove helpful considering the Green's function G(k, z), as defined in (10). Insertion of (37) into (10), and using the formal expression

$$\sum_{n=0}^{\infty} (e^{\pm ik}S)^n = \frac{1}{1 - e^{\pm ik}S} , \qquad (40)$$

leads to

$$G(k, z) = \frac{1}{z} \left( \psi^{T}, \frac{(1 - S^{2})(1 - S)^{2}}{1 + S^{2} - 2S \cos k} \psi^{T} \right).$$
(41)

Expanding (41) in powers of k, we find

$$G(k, z) = \frac{1}{z} \left[ 1 + \left( \psi^{T}, \left( 2 + S - \frac{2}{1 - S} \right) \psi^{T} \right) k^{2} + \left( \psi^{T}, \left( -\frac{7}{6} - \frac{1}{12} S + \frac{25}{6} \frac{1}{1 - S} - \frac{5}{(1 - S)^{2}} + \frac{2}{(1 - S)^{3}} \right) \psi^{T} \right) k^{4} + \mathcal{O}(k^{6}) \right].$$

$$(42)$$

Note that indeed  $G(0, z) = \sum_{n=-\infty}^{\infty} \langle P_n(z) \rangle = 1/z$ . From (41), this can be seen as follows:

$$G(0, z) = \frac{1}{z} \left( \psi^{T}, (1 - S^{2})\psi^{T} \right) = \frac{1}{z} \left[ (\psi^{T}, \psi^{T}) - (S\psi^{T}, S\psi^{T}) \right]$$
$$= \frac{1}{z} \left( \sum_{n=0}^{\infty} (\psi^{T}_{n})^{2} - \sum_{n=0}^{\infty} (\psi^{T}_{n+1})^{2} \right) = \frac{1}{z} (\psi^{T}_{0})^{2} = \frac{1}{z} ,$$

where we used (19), (32) and (34).

It is seen that in using G(k, z) instead of  $\langle P_n(z) \rangle$ , the problem is shifted from studying the action of the operator  $S^n$  on  $\psi^T$  to doing the same for the operator  $1/(1-S)^n$ . Unfortunately, this will not be any simpler. We will use (42) to find the second moment. A general formula for G(k, z) reads [5]

$$G(k, z) = \frac{1}{z} + \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n)!} k^{2n} \langle x^{2n}(z) \rangle , \qquad (43)$$

where  $\langle x^{2n}(z) \rangle$  denotes the Laplace transform of  $\langle x^{2n}(t) \rangle$ . Equating the second terms of (42) and (43) gives the desired expression for  $\langle x^2(z) \rangle$ :

$$\langle x^{2}(z) \rangle = \frac{2}{z} \left[ 2(\psi^{T}, \psi^{S}) - 2(\psi^{T}, \psi^{T}) - (\psi^{T}, S\psi^{T}) \right], \qquad (44)$$

where we have introduced

$$\psi^S = \frac{1}{1-S} \ \psi^T \ . \tag{45}$$

## 4. Explicit calculations

In this section, we briefly outline how to calculate  $\psi^T$  and  $\psi^s$ , which were defined in the previous section and derive from this the small-z behaviour of  $\langle P_0(z) \rangle$  and  $\langle x^2(z) \rangle$ . More details are presented in ref. [9].

# 4.1. Calculation of $\psi^T$

Remember  $\psi^{T}$  satisfies eq. (17), i.e.

$$\sum_{n} T_{mn} \boldsymbol{\psi}_{n}^{T} = \boldsymbol{\psi}_{m}^{T} \,, \tag{46}$$

where  $T_{mn}$  is defined in (18). First, we will put  $T_{mn}$  into a more usable form. Inserting (2) into (18) and then changing the variable of integration to  $\tau = 1/\nu$ , we obtain

$$T_{mn} = {\binom{m+n-1}{n}} 2^{-(m+n)} (1-\alpha) 2^{\alpha-1} \int_{1/2}^{\infty} d\tau \, \tau^{\alpha-2} \, \frac{1}{(1+z\tau)^{m+n}} \,. \tag{47}$$

The integral can be expressed in a hypergeometric function (ref. [7], (3.194.2)). Making extensive use of its properties, we find for  $z \rightarrow 0$ 

$$T_{mn} \approx {\binom{m+n-1}{n}} 2^{-(m+n)} \times \left(1 + 2^{\alpha-1}(1-\alpha)(\alpha-2)! \frac{(n+m-\alpha)!}{(n+m-1)!} z^{1-\alpha}\right).$$
(48)

Here we made some assumptions, concerning the scaling of n and z. They can be justified afterwards by the results we find in this way. Using Stirlings formula in the form

$$N! = N^{N} e^{-N} (2\pi N)^{1/2} [1 + \mathcal{O}(1/N)]$$
(49)

and the approximation  $(1 - \epsilon)^{\mu} = 1 - \mu \epsilon$  ( $\epsilon \rightarrow 0$ ;  $\mu > 0$ ), one may rewrite (48) as

$$T_{mn} \approx {\binom{m+n-1}{n}} 2^{-(m+n)} (1-\epsilon)^{(m+n)^{1-\alpha}},$$
 (50)

where

$$\epsilon = 2^{\alpha - 1} \Gamma(\alpha) \, z^{1 - \alpha} \,. \tag{51}$$

We now return to (46). We assume that the dependence of  $T_{mn}\psi_n^T$  on *n* is sufficiently smooth to write

$$\sum_{n} T_{mn} \psi_n^T = \int_0^\infty T(m, n) \psi_n^T \,\mathrm{d}n \,.$$
<sup>(52)</sup>

Furthermore, we suppose that  $T(m, n) \psi^{T}(n)$  has a maximum for, say,  $n = n_0$ . So

$$\left(\frac{\partial}{\partial n} T(m, n) \psi_n^T\right)_{n=n_0} = 0.$$
(53)

The idea now is to expand the logarithm of  $T(m, n) \psi^{T}(n)$  in a Taylor series about  $n = n_0$ . Doing so, we obtain

$$\sum_{n} T_{mn} \psi_{n}^{T} \approx T_{mn_{0}} \psi_{n_{0}}^{T} \int_{-\infty}^{\infty} \exp[a(x - n_{0}) - b(x - n_{0})^{2} + c(x - n_{0})^{3} + d(x - n_{0})^{4} + \cdots] dx$$
$$\approx T_{mn_{0}} \psi_{n_{0}}^{T} \sqrt{\frac{\pi}{b}} \left(1 + \frac{3}{4} \frac{d}{b^{2}} + \frac{15}{16} \frac{c^{2}}{b^{3}}\right).$$
(54)

Here

$$a = \left(\frac{\partial}{\partial n}\log[T(m, n) \psi_n^T]\right)_{n=n_0} = 0 \quad (\text{from (53)}),$$
$$-b = \frac{1}{2!} \left(\frac{\partial^2}{\partial n^2}\log[T(m, n) \psi_n^T]\right)_{n=n_0}, \quad \text{etc.}$$
(55)

The calculation of  $n_0$ , b, c and d is laborious, but straightforward.  $n_0$  is determined by (55). Inserting (50) into (55), the differentiation can be carried out if we apply Stirling's formula (49) to the factor  $\binom{m+n-1}{n}$ . Then the derivatives of log  $T(m, n_0)$  with respect to  $n_0$  are computed and inserted into (54). Finally, expanding log  $\psi_n^T$  about  $n_0$  as well, we find from (46) that  $\psi_n^T$  has to satisfy

$$\frac{\mathrm{d}^2\psi_n^T}{\mathrm{d}n^2} - \epsilon 2^{1-\alpha}n^{-\alpha}\psi_n^T = 0.$$
(56)

A general solution can be found in ref. [7], (8.494.10); the solution that satisfies (19) and (20) is readily found to be

$$\psi_n^T = A(z)\sqrt{n} K_{1/(2-\alpha)} \left( \frac{2\sqrt{\Gamma(\alpha)}}{2-\alpha} z^{(1-\alpha)/2} n^{(2-\alpha)/2} \right),$$

where

$$A(z) = \frac{2}{\Gamma(1/(2-\alpha))} \left[ \frac{\Gamma(\alpha)}{(2-\alpha)^2} \right]^{1/2(2-\alpha)} z^{(1-\alpha)/2(2-\alpha)} .$$
 (57)

Here  $K_{1/(2-\alpha)}$  denotes a modified Bessel function of order  $1/(2-\alpha)$ .

# 4.2. Calculation of $\psi^{s}$

The vector  $\psi^s$  was defined in (45) as

$$\psi^{S} = \frac{1}{1-S} \ \psi^{T}$$

or

$$\psi^{S} - S\psi^{S} = \psi^{T} . \tag{58}$$

For  $z \rightarrow 0$ , we find from (34) and (50)

$$S_{mn} \approx {\binom{m+n}{n}} 2^{-(m+n+1)} (1-\epsilon)^{(m+n+1)^{1-\alpha}}.$$
 (59)

 $\Sigma_n S_{mn} \psi_n^s$  can be treated much the same way as was  $\Sigma_n T_{mn} \psi_n^T$ ; as a result we find the approximation

$$\sum_{n} S_{mn} \psi_{n}^{S} \approx \exp\left(my^{2} - y - m \frac{\mathrm{d}y}{\mathrm{d}m} - \epsilon 2^{1-\alpha} m^{1-\alpha}\right) \psi_{m}^{S}, \qquad (60)$$

where

$$y(m) = -\frac{\partial}{\partial m} \log \psi_m^S \,. \tag{61}$$

Expanding the exponent in (60), inserting the result into (58) and substituting (61) for y leads to the following differential equation for  $\psi_m^S$  ( $\psi_m^T$  being a known function; see (57)):

$$m \frac{\partial^2 \psi_m^S}{\partial m^2} + \frac{\partial \psi_m^S}{\partial m} - \epsilon 2^{1-\alpha} m^{1-\alpha} \psi_m^S = -\psi_m^T, \qquad (62)$$

which may be written as

$$m^{1/2} \left( \frac{\partial^2}{\partial m^2} + \frac{1}{4m^2} - \epsilon 2^{1-\alpha} m^{-\alpha} \right) \left( m^{1/2} \psi_m^S \right) = -\psi_m^T \,. \tag{63}$$

From (19), (20) and (45) we conclude that  $\psi_m^s$  has to satisfy

259

$$\lim_{m \to \infty} \psi_m^S = 0 \tag{64}$$

and

$$\lim_{m \to 0} \psi_m^S \quad \text{exists} \,. \tag{65}$$

A solution of the homogeneous equation corresponding to (63) can be found in ref. [7], (8.491.2). The method of variation of the constants of integration, combined with the conditions (64) and (65), leads to

$$\psi_{m}^{S} = \left(\frac{1}{1-S} \psi^{T}\right)_{m} = \frac{2}{2-\alpha} \left(K_{0}(Bm^{(2-\alpha)/2}) \int_{0}^{m} I_{0}(Bk^{(2-\alpha)/2}) \psi_{k}^{T} dk + I_{0}(Bm^{(2-\alpha)/2}) \int_{m}^{\infty} K_{0}(Bk^{(2-\alpha)/2}) \psi_{k}^{T} dk\right),$$
(66)

where

$$B = \frac{2\sqrt{\Gamma(\alpha)}}{2-\alpha} \ z^{(1-\alpha)/2}$$

So 1/(1-S) acts on  $\psi^T$  as an integral operator, at least approximately. The Green's function, which is made up of terms like  $(\psi^T, [1/(1-S)^n]\psi^T)$ , can now be expressed in terms of integrals over Bessel functions. Unfortunately, it seems that these integrals cannot be evaluated analytically.

## 4.3. Evaluation of $\langle P_0(z) \rangle$

Now that we have found  $\psi_n^T$ , the calculation of  $\langle P_0(z) \rangle$  is straightforward. Owing to the factor  $z^{(1-\alpha)/2}$  in the argument of  $\psi_n^T$  (see (57)), we can write (39) for  $z \to 0$  as

$$\langle P_0(z) \rangle = \frac{1}{z} \int_0^\infty \left( \frac{\mathrm{d}\psi_n^T}{\mathrm{d}n} \right)^2 \mathrm{d}n \;.$$
 (67)

After insertion of (57) some algebra gives

$$\langle P_0(z) \rangle = \frac{(2-\alpha)A^2(z)}{2z} \int_0^\infty x K_{1+1/(2-\alpha)}^2(x) \, \mathrm{d}x \,.$$
 (68)

Again, the integral can be found in ref. [7], (6.576.4); the result reads

$$\langle P_0(z)\rangle = \frac{C(\alpha)}{z^{1/(2-\alpha)}},$$
(69)

where

$$C(\alpha) = \left(\frac{\Gamma(\alpha)}{(2-\alpha)^2}\right)^{1/(2-\alpha)} \frac{\Gamma(2-1/(2-\alpha))}{\Gamma(1+1/(2-\alpha))} .$$
(70)

This result agrees with previous ones (see section 5).

## 4.4. The second moment $\langle x^2(z) \rangle$

To calculate the second moment, we recall (44); inserting (57) and (66) one finds that the first term is dominant for  $z \rightarrow 0$ :

$$\langle x^2(z) \rangle \approx \frac{4}{z} \left( \psi^T, \psi^S \right) = D(\alpha) I(\alpha) \frac{1}{z^{(4-3\alpha)/(2-\alpha)}},$$
(71)

where

$$D(\alpha) = \frac{256}{2^{6/(2-\alpha)}(2-\alpha)^{(2-3\alpha)/(2-\alpha)}\Gamma^2(1/(2-\alpha))\left[\Gamma(\alpha)\right]^{2/(2-\alpha)}}$$

and

$$I(\alpha) = \int_{0}^{\infty} x^{(1+\alpha)/(2-\alpha)} K_{1/(2-\alpha)}(x) K_{0}(x)$$
$$\times \left( \int_{0}^{x} t^{(1+\alpha)/(2-\alpha)} K_{1/(2-\alpha)}(t) I_{0}(t) dt \right) dx .$$
(72)

## 5. Discussion

The results (69) and (70) for  $\langle P_0(z) \rangle$  have been obtained before in exactly the same form by Stephen and Kariotis [4] and by Nieuwenhuizen and Ernst [3]. Bernasconi et al. find the same z-dependence for  $\langle P_0(z) \rangle$ . They also give an explicit expression for the coefficient  $C(\alpha)$ , but this does not obviously coincide with (70) although numerically it is at least very close (see fig. 2). The results for  $\langle x^2(z) \rangle$  contained in (71) and (72) have been given before by Stephen and Kariotis, who obtained them by an entirely different method [4]. Nieuwenhuizen and Ernst and Bernasconi et al. present the same exponent for

261



Fig. 2. The inverse coefficient  $1/C(\alpha)$  as a function of  $\alpha$ . Curve: eq. (70); dots: expression of Bernasconi et al.

z. Bernasconi et al. do not give the prefactor, while the expression given by Nieuwenhuizen and Ernst leads to values two to four times as large as the ones we computed. Since Stephen and Kariotis and we got the same expression along completely different routes we strongly expect this to be the correct one.

It is interesting to compare the system under consideration to the trivial case where all transfer rates equal the same constant, say,  $\nu_0$ . (This is sometimes called: the ordered case.) For this purpose, we transform back (69) and (71) to find

$$\langle P_0(t) \rangle = \frac{C(\alpha)}{\Gamma(1/(2-\alpha))} \frac{1}{t^{(1-\alpha)/(2-\alpha)}}$$
(73)

and

$$\langle x^{2}(t) \rangle = \frac{D(\alpha) I(\alpha)}{\Gamma((4-3\alpha)/(2-\alpha))} t^{2(1-\alpha)/(2-\alpha)} , \qquad (74)$$

whereas in an ordered system

$$P_0(t) = \frac{1}{\sqrt{2\pi\nu_0 t}}$$
(75)

and

$$\langle x^2(t) \rangle = \nu_0 t . \tag{76}$$

So, as expected, for our problem particle transport is slower. But there is more. In an ordered system, we have

$$P_0^2(t) \langle x^2(t) \rangle = \frac{1}{2\pi} ,$$
 (77)

which is characteristic of the Gaussian profile of  $P_n(t)$  as a function of n. For our system, we find

$$\langle P_0(t) \rangle^2 \langle x^2(t) \rangle \equiv H(\alpha)$$
 (78)

with H depending explicitly on  $\alpha$ .

For some  $\alpha$ -values, we computed  $H(\alpha)$  numerically (see fig. 3). Our results



Fig. 3. The product  $\langle P_0(t) \rangle^2 \langle x^2(t) \rangle$  for long times, plotted as a function of  $\alpha$ .

indicate that  $H(0) = 1/2\pi$  and  $H(\alpha) > 1/2\pi$  ( $0 < \alpha < 1$ ). This means that the profile of  $\langle P_n(t) \rangle$  is not a Gaussian, but, given its height at the origin, it is broader! So the time-development of the system under consideration is not only slowed down in comparison to the corresponding ordered system, it differs from it in a more fundamental way.

In conclusion we want to indicate how in principle our results could be extended. First of all the vectors  $[1/(1-S)^n]\Psi^T$  may in principle be calculated by replacing on the right-hand side of (66)  $\Psi^T$  successively by  $\Psi^S$ ,  $[1/(1-S)]\Psi^S$ , etc. This causes no problems of principle, but control of the accuracy of all successive integrals may readily become a numerical problem. Another strategy would be approximating S by a finite-dimensional matrix, in which case the matrices  $S^n$ ,  $1/(1-S)^n$  as well as  $1/(1+S^2-2S\cos k)$ , appearing in (37), (42) and (41), respectively, could be calculated algebraically.

Finally the calculation of corrections to the leading asymptotic behaviour of the various quantities of interest can in principle be done as well, but for this purpose probably the methods of refs. [3, 4] are more suitable.

### Acknowledgements

Extensive use was made of the Diplomarbeit of Christian Hemsing [8], which treats the case of finite average waiting time. Erik Hummel performed the numerical computation of the coefficient  $C(\alpha)$  as given by Nieuwenhuizen and Ernst.

### References

- [1] J. Bernasconi, W.R. Schneider and W. Wyss, Z. Phys. B 37 (1979) 176.
- [2] S. Alexander, J. Bernasconi J., W.R. Schneider and R. Orbach, Rev. Mod. Phys. 53 (1981) 175.
- [3] Th.M. Nieuwenhuizen and M.H. Ernst, Phys. Rev. B 31 (1985) 3518.
- [4] M.J. Stephen and R. Kariotis, Phys. Rev. B 26 (1982) 2917.
- [5] H. van Beijeren, Rev. Mod. Phys. 54 (1982) 195.
- [6] H. van Beijeren and H. Spohn, J. Stat. Phys. 31 (1983) 231.
- [7] J.S. Gradshteyn and J.M. Ryzhik, Table of Integrals, Series and Products (Academic Press, Orlando, 1980).
- [8] C. Hemsing, Diplomarbeit at RWTH, Aachen, Fed. Rep. Germany, unpublished.
- [9] J. van Polen, doctoraalscriptie, University of Utrecht, unpublished.