Journal of Statistical Physics, Vol. 30, No. 2, 1983

Diffusion in Random One-Dimensional Systems

J. Bernasconi[1] and W. R. Schneider[1]

Diffusion on the one-dimensional lattice $\mathbb{Z}$ is described by a master equation with nearest-neighbor transfer rates (symmetric or asymmetric). The transfer rates associated with bonds are assumed to be independent, equally distributed random variables. Under various conditions on their common distribution the large time behavior of averaged site probabilities and/or related quantities is exhibited.

KEY WORDS: Diffusion; one-dimensional; lattice; master equation; nearest neighbor; transfer rates; random variables.

1. INTRODUCTION

We consider a particle moving randomly on the one-dimensional lattice $\mathbb{Z}$ starting at site j. This motion is conveniently described by the probability $P_n(t)$ of finding the particle at time $t \geqslant 0$ on the site n. Obviously,

$$P_n(0) = \delta_{nj}, \qquad n \in \mathbb{Z} \tag{1.1}$$

as the particle starts with certainty at j. The simplest equation describing the change in time of these probabilities is a first-order linear differential equation, i.e.,

$$\dot{P}_n(t) = \sum_m T_{nm} P_m(t) \tag{1.2}$$

As the particle does not get lost, destroyed, or trapped, the total probability is conserved:

$$\sum_n P_n(t) = 1, \qquad t \geqslant 0 \tag{1.3}$$

Presented at the Symposium on Random Walks, Gaithersburg, MD, June 1982.

[1] Brown Boveri Research Center, CH-5405 Baden, Switzerland.

0022-4715/83/0200-0355$03.00/0

Differentiating (1.3), inserting (1.2), and setting $t = 0$ yields

$$\sum_n T_{nj} = 0 \tag{1.4}$$

As the equation of motion should not depend on the initial condition, we require (1.4) to hold for any j. This allows us to rewrite (1.2) as

$$\dot{P}_n(t) = \sum_{m \neq n} T_{nm} P_m(t) - \Big(\sum_{m \neq n} T_{mn} \Big) P_n(t) \tag{1.5}$$

The first term corresponds to gains by hops ending in n implying for the so-called transfer rates

$$T_{nm} \geqslant 0, \qquad n \neq m \tag{1.6}$$

whereas the second term describes the losses by hops starting in n. We restrict ourselves to the case of nearest-neighbor hopping, i.e.,

$$T_{nm} = 0, \qquad |n - m| > 1. \tag{1.7}$$

It is convenient to set

$$W_{n+1}^- = T_{n,n+1}, \qquad W_n^+ = T_{n+1,n} \tag{1.8}$$

Note that the pair (W_n^+, W_{n+1}^-) is associated with the bond $(n, n+1)$. Inserting (1.7), (1.8), into (1.5) leads to

$$\dot{P}_n = W_{n-1}^+ P_{n-1} + W_{n+1}^- P_{n+1} - (W_n^+ + W_n^-) P_n \tag{1.9}$$

Symmetric diffusion is characterized by a symmetric transfer rate matrix, i.e., $T_{mn} = T_{nm}$ for all m, n. For nearest-neighbor hopping this implies

$$W_n^+ = W_{n+1}^- \equiv W_n \tag{1.10}$$

In ordered systems the transfer rates have fixed nonnegative values independent of n. Fourier transformation of the corresponding version of (1.9) yields

$$\dot{Q}_k = (e^{ik} W^+ + e^{-ik} W^- - W^+ - W^-) Q_k, \qquad Q_k = \sum_n P_n e^{ink} \tag{1.11}$$

with $k \in [0, 2\pi)$. Taking (1.1) with $j = 0$ into account, (1.11) is solved by

$$Q_k(t) = \exp t(e^{ik} W^+ + e^{-ik} W^- - W^+ - W^-) \tag{1.12}$$

Inversion of the Fourier transform yields

$$P_n(t) = e^{-t(W^+ + W^-)} \left(\frac{W^+}{W^-} \right)^{n/2} I_{|n|}\left[2(W^+ W^-)^{1/2} t \right] \tag{1.13}$$

where I_κ denotes the modified Bessel function of order κ. For the mean displacement of the particle we obtain

$$x(t) \equiv \sum_n n P_n(t) = (W^+ - W^-) t \tag{1.14}$$

using the generating function of the modified Bessel functions. Similarly, the mean square displacement is given by

$$x^2(t) \equiv \sum_n n^2 P_n(t) = (W^+ - W^-)^2 t^2 + (W^+ + W^-)t \qquad (1.15)$$

By setting $W^+ = W^- = W$ we obtain the corresponding results for symmetric diffusion.

2. ASYMMETRIC RANDOM DIFFUSION

In ordered systems only the motion of the particle is stochastic, whereas the lattice in which the motion takes place does not contain any randomness. This is an idealization. Real lattices are always to a certain degree disordered (defects, impurities, etc.). A possibility to introduce disorder into our description of diffusion by (1.9) is to assume that the transfer rates $W_n^{\pm}$ are random variables. In view of (1.9) also the site probabilities $P_n(t)$ and quantities derived thereof become random variables. The connection to observable quantities is established by averaging over all random transfer rates, denoted by $\langle\ \rangle$.

To be specific, we assume that the pairs (W_n^+, W_{n+1}^-) are independent, equally distributed $\mathbb{R}_+^2$-valued random variables. Their distribution is described by the probability measure ν with support in $\mathbb{R}_+^2$. The particular choice

$$\nu = p\delta_{(u,0)} + (1-p)\delta_{(\lambda v, v)} \qquad (2.1)$$

with $\lambda, u, v > 0$ and $0 < p < 1$ describes a model in which

$$(W_n^+, W_{n+1}^-) = (u, 0) \qquad (2.2)$$

with probability p and

$$(W_n^+, W_{n+1}^-) = (\lambda v, v) \qquad (2.3)$$

with probability $1-p$. For this model the following large time behavior of the average mean displacement has been obtained[1]:

$$\langle x(t)\rangle \sim \begin{cases} wt, & \lambda > 1-p \\ \alpha p^{-2} ct/\ln(ct), & \lambda = 1-p \\ p^{-2}(ct)^{\gamma}\phi(\beta^{-1}\ln(ct)), & \lambda < 1-p \end{cases} \qquad (2.4)$$

where

$$w = \frac{uv(\lambda - 1 + p)}{p\lambda v + (1-p)u}, \qquad c = \frac{uv(1-\lambda)^2}{u + v(1-\lambda)} \qquad (2.5)$$

and

$$\alpha = -\ln(1-p), \qquad \beta = -\ln\lambda, \qquad \gamma = \alpha/\beta \tag{2.6}$$

The function ϕ is periodic with period 1; explicitly,

$$\phi(\tau) = \sum_{n=-\infty}^{\infty} \frac{c_n}{\Gamma(\gamma + 1 + 2\pi i n/\beta)} e^{2\pi i n\tau} \tag{2.7}$$

with

$$\sum_{n=-\infty}^{\infty} c_n e^{2\pi i n\tau} = \left[\sum_{k=-\infty}^{\infty} \frac{e^{-\alpha(k-\tau)}}{1 + e^{-\beta(k-\tau)}} \right]^{-1} \tag{2.8}$$

3. SYMMETRIC RANDOM DIFFUSION

Symmetric (nearest neighbor) random diffusion is described by (1.9) and (1.10), i.e.,

$$\dot{P}_n = W_{n-1}(P_{n-1} - P_n) + W_n(P_{n+1} - P_n) \tag{3.1}$$

where the random transfer rates W_n, $n \in \mathbb{Z}$, are assumed to be independent, equally distributed random variables. Their distribution is given by a probability measure ν whose support has to be in $\mathbb{R}_+$, as negative transfer rates do not occur. A Laplace transform in time,

$$\tilde{P}_n(s) = \int_0^\infty dt\, e^{-st} P_n(t) \tag{3.2}$$

leads to

$$s\tilde{P}_n - \delta_{n0} = W_{n-1}(\tilde{P}_{n-1} - \tilde{P}_n) + W_n(\tilde{P}_{n+1} - \tilde{P}_n) \tag{3.3}$$

having set $j = 0$ in the initial condition (1.1).

We introduce auxiliary random variables X_n and Y_n, $n = 0, 1, 2, \ldots$, by setting

$$X_n = \cfrac{1}{\cfrac{1}{W_n} + \cfrac{1}{s + \cfrac{1}{\cfrac{1}{W_{n+1}} + \cdots}}},$$

$$Y_n = \cfrac{1}{\cfrac{1}{W_{-n-1}} + \cfrac{1}{s + \cfrac{1}{\cfrac{1}{W_{-n-2}} + \cdots}}} \tag{3.4}$$

In terms of these variables the solution of (3.3) is given by

$$\tilde{P}_{-n} = \tilde{P}_0 \prod_{m=1}^{n} Y_{m-1}(Y_m + s)^{-1}, \qquad n = 1,2,\ldots$$
$$\tilde{P}_0 = (s + X_0 + Y_0)^{-1} \tag{3.5}$$
$$\tilde{P}_n = \tilde{P}_0 \prod_{m=1}^{n} X_{m-1}(X_m + s)^{-1}, \qquad n = 1,2,\ldots$$

Together with the transfer rates W_n also X_n and Y_n are all equally distributed. However, the independence of the former only implies that all X_n are independent of all Y_n. From (3.4) we read off

$$X_n = \left[W_n^{-1} + (s + X_{n+1})^{-1} \right]^{-1} \tag{3.6}$$

(and a similar formula for Y_n) showing clearly that X_n and X_{n+1} are dependent. However, W_n and X_{n+1} are independent as the latter depends only on W_m, $m > n + 1$. Hence, we obtain from (3.6) the integral equation

$$\mu_s(B_x) = \iint_{A_{s,x}} d\nu(y)\, d\mu_s(z) \tag{3.7}$$

for the probability measure μ_s describing the distribution of all X_n, Y_n. Here, we have set

$$\sigma(B_x) = \int_{B_x} d\sigma(x'), \qquad B_x = [0, x) \tag{3.8}$$

for an arbitrary probability measure σ on $\mathbb{R}_+$ [note that σ is uniquely defined if $\sigma(B_x)$ is given for all $x \geqslant 0$]. The domain $A_{s,x}$ of integration is given by

$$A_{s,x} = \left\{ (y,z) \in \mathbb{R}_+^2 \mid \left\{ y^{-1} + (s + z)^{-1} \right\}^{-1} < x \right\} \tag{3.9}$$

It has been shown[2] that (3.7) has a unique solution which may be obtained as follows: Define the sequence of probability measures $\mu_s^{(n)}$, $n = 0,1,2,\ldots$ with $\mu_s^{(0)} = \nu$ by

$$\mu_s^{(n+1)}(B_x) = \iint_{A_{s,x}} d\nu(y)\, d\mu_s^{(n)}(z), \qquad n = 0,1,2,\ldots \tag{3.10}$$

Then

$$\mu_s(B_x) = \lim_{n\to\infty} \mu_s^{(n)}(B_x) \tag{3.11}$$

The extremal cases $s = 0$ and $s = \infty$ are explicitly solvable for arbitrary ν:

$$\mu_0 = \delta_0, \qquad \mu_\infty = \nu \tag{3.12}$$

(δ_a is the Dirac measure situated at a). For $\nu = \delta_w$, $w \geqslant 0$ (corresponding to the ordered system with all $W_n = w$) the solution for arbitrary s is

$$\mu_s = \delta_{a(s)}, \qquad a(s) = \tfrac{1}{2}\left[\left(4ws + s^2\right)^{1/2} - s \right] \tag{3.13}$$

The behavior of μ_s as s approaches zero has been investigated in Refs. 3 and 4 for ν belonging to one of three classes of probability measures characterized by their behavior near zero. Apart from more technical assumptions these classes are characterized by the following:

(C1) The probability measures ν belonging to C1 satisfy

$$a = \int_0^\infty x^{-1}\, d\nu(x) < \infty \tag{3.14}$$

(C2) The probability measure ν belongs to C2 if there are positive constants a and c such that

$$\int_0^c |\nu(B_x) - ax| x^{-2}\, dx < \infty \tag{3.15}$$

(C3) The probability measure ν belongs to C3 if there are positive constants a and α, $\alpha < 1$, such that

$$\lim_{x \downarrow 0} \nu(B_x) x^{\alpha - 1} = a^{1-\alpha} \tag{3.16}$$

Simple but typical examples are the following probability measures ν with density $\rho = d\nu/dx$:

$$\begin{aligned} &\rho(x) = 1, && 1 \leqslant x \leqslant 2\text{: C1} \\ &\rho(x) = 2x, && 0 \leqslant x \leqslant 1\text{: C1} \\ &\rho(x) = 1, && 0 \leqslant x \leqslant 1\text{: C2} \\ &\rho(x) = (1-\alpha)x^{-\alpha}, && 0 \leqslant x \leqslant 1\text{: C3} \end{aligned} \tag{3.17}$$

The behavior of μ_s near $s = 0$ is described as follows[3,4]: set

$$\epsilon(s) = a^{-1} h(as) \tag{3.18}$$

where a is the constant in (3.14), (3.15), (3.16), respectively, and where h is given by

$$h(x) = x^{1/2}, \qquad (-2x/\ln x)^{1/2}, \qquad x^{1/(2-\alpha)} \tag{3.19}$$

for ν in C1, C2, C3, respectively. Then

$$\lim_{s \downarrow 0} \mu_s(B_{\epsilon(s)x}) = \pi(B_x) \tag{3.20}$$

with the probability measure π given by

$$\pi = \delta_1 \tag{3.21}$$

for $\nu \in C1, C2$. For $\nu \in C3$ the density of π is given by

$$\frac{d\pi}{dx} = \frac{\beta\gamma}{\Gamma(\beta)} H_{12}^{20}\left(\gamma x \middle| \begin{matrix} (-1, 1) \\ (-\beta, \beta)(0, \beta) \end{matrix} \right), \qquad \beta = (2-\alpha)^{-1}, \quad \gamma = \left[\beta^2 \Gamma(\alpha) \right]^{\beta} \tag{3.22}$$

where H_{pq}^{mn} denotes a Fox function[5] (one of the generalizations of hypergeometric functions).

With the help of the probability measure μ_s we may express the average $\langle \tilde{P}_0(s) \rangle$ (which involves integration over all random variables W_n) as follows:

$$\langle \tilde{P}_0(s) \rangle = \int\int d\mu_s(x)\, d\mu_s(y)\, (s + x + y)^{-1} \tag{3.23}$$

This follows immediately from (3.5) in view of the fact that X_0 and Y_0 are independent and both distributed according to μ_s. From (3.20)–(3.23) the following behavior of $\langle \tilde{P}_0(s) \rangle$ as s tends to zero is obtained:

$$\lim_{s \downarrow 0} \langle \tilde{P}_0(s) \rangle / \left[a f(as) \right] = 1 \tag{3.24}$$

For ν in C1, C2, C3 the function f is given by

$$f(x) = \tfrac{1}{2} x^{-1/2}, \qquad 2^{-3/2}(-\ln x / x)^{1/2}, \qquad C_\alpha x^{-\beta} \tag{3.25}$$

respectively, with

$$C_\alpha = \int\int d\pi(x)\, d\pi(y)\, (x + y)^{-1} \tag{3.26}$$

This integral may be evaluated using (3.22) with the result[6]

$$C_\alpha = \frac{\pi}{\sin \pi\beta} \frac{1-\alpha}{\Gamma(\beta)^2} \gamma \qquad [\beta, \gamma \text{ as in } (3.22)] \tag{3.27}$$

By different methods (3.24)–(3.27) have been obtained in Ref. 7. The behavior of $\langle \tilde{P}_n(s) \rangle$, $n \neq 0$, as s tends to zero was obtained in Ref. 4 from the behavior of $\langle \tilde{P}_0(s) \rangle$ using a scaling hypothesis. Recently, a theorem was announced[8] confirming this assumption. Thus, it is possible to determine the behavior of the diffusion function

$$D(s) = \tfrac{1}{2} s^2 \sum_n n^2 \langle \tilde{P}_n(s) \rangle \tag{3.28}$$

for $s \downarrow 0$:

$$\lim_{s \downarrow 0} D(s) / \left[a^{-1} g(as) \right] = 1 \tag{3.29}$$

with

$$g(x) = 1, \qquad 2/(-\ln x), \qquad D_\alpha x^{\alpha/(2-\alpha)} \tag{3.30}$$

for C1, C2, C3, respectively. A direct approach to the behavior of $D(s)$ has been presented in Ref. 7 where also an expression for the constant D_α is derived. By means of general Abelian and Tauberian theorems the large time behavior of $\langle \tilde{P}_n(t) \rangle$ and of the mean square displacement may be obtained. We refrain from reproducing these results. They may be found in Ref. 9 where also a comprehensive review of applications to a large variety of physical problems has been given.

REFERENCES

1. J. Bernasconi and W. R. Schneider, *J. Phys. A: Math. Gen.* **15**:L729 (1982).
2. W. R. Schneider, *Commun. Math. Phys.* **87**:303 (1982).
3. W. R. Schneider and J. Bernasconi, *Mathematical Problems in Theoretical Physics*, R. Schrader, R. Seiler, and D. A. Uhlenbrock, eds., Springer Lecture Notes in Physics, Vol. 153 (Springer, Berlin, 1982), p. 389.
4. J. Bernasconi, W. R. Schneider, and W. Wyss, *Z. Phys.* **B37**:175 (1980).
5. B. L. J. Braaksma, *Compos. Math.* **15**:239 (1963).
6. W. R. Schneider, unpublished.
7. M. J. Stephen and R. Kariotis, *Phys. Rev. B* **26**:2917 (1982).
8. A. Golosov, private communication.
9. S. Alexander, J. Bernasconi, W. R. Schneider, and R. Orbach, *Rev. Mod. Phys.* **53**:175 (1981).