IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Diffusion in a one-dimensional lattice with random asymmetric transition rates

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1982 J. Phys. A: Math. Gen. 15 L729

(http://iopscience.iop.org/0305-4470/15/12/013)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 129.252.86.83
The article was downloaded on 30/05/2010 at 15:05

Please note that terms and conditions apply.

J. Phys. A: Math. Gen. **15** (1983) L729–L734. Printed in Great Britain

LETTER TO THE EDITOR

Diffusion on a one-dimensional lattice with random asymmetric transition rates

J Bernasconi and W R Schneider
Brown Boveri Research Center, CH-5405 Baden, Switzerland

Received 31 August 1982

Abstract. We study one-dimensional continuous-time random walks for which the pairs $\{W_n^+, W_{n+1}^-\}$ of nearest-neighbour transition rates are assumed to be independent, equally distributed random variables. The long-time asymptotic behaviour of the mean displacement, $\langle x(t)\rangle$, is determined exactly for a specific model system in which 'diodes' $\{u, 0\}$ and 'two-way bonds' $\{\lambda v, v\}$ occur with probabilities p and $1-p$, respectively. For $\lambda < 1-p$, we find that $\langle x(t)\rangle \sim t^\nu F(\beta^{-1} \ln t)$, where $\nu = \ln(1-p)/\ln \lambda$ and $\beta = -\ln \lambda$, and where F is a periodic function with period 1. The mean displacement thus not only increases slower than linearly in time, but exhibits superimposed, non-decaying oscillations.

Diffusion on a one-dimensional disordered lattice can be modelled by a random walk in a random environment, and corresponding problems have recently attracted considerable attention (see e.g. Alexander *et al* 1981, Derrida and Pomeau 1982, and references therein).

Consider a particle whose motion on the one-dimensional lattice $\mathbb{Z}$, starting at site $n=0$ at time $t=0$, is described by a continuous-time random walk with only nearest-neighbour transition rates $W_n^\pm$. The probabilities $P_n(t)$ of finding the particle at site n at time $t \geq 0$ then obey the master equation

$$dP_n/dt = W_{n-1}^+ P_{n-1} + W_{n+1}^- P_{n+1} - (W_n^+ + W_n^-)P_n, \tag{1}$$

with

$$P_n(0) = \delta_{n0}. \tag{2}$$

The two transition rates associated with the same bond, W_n^+ and W_{n+1}^-, are allowed to be correlated, but the pairs $\{W_n^+, W_{n+1}^-\}$ are assumed to be independent random variables, equally distributed according to a probability density $\rho(w^+, w^-)$. A number of interesting results have been derived (Bernasconi *et al* 1980, Alexander *et al* 1981, Bernasconi and Schneider 1981) for the case of random symmetric transition rates $(W_n^+ = W_{n+1}^-)$, and it is the purpose of this letter to investigate some aspects of the non-symmetric case.

Similar models have been analysed for discrete-time random walks (Solomon 1975, Kesten *et al* 1975, Sinai 1982, Derrida and Pomeau 1982). In these models, a particle at site n will after one time step be either at site $n+1$ or at site $n-1$, with probabilities α_n and $1-\alpha_n$, respectively. For the case that the α_n are independent, identically distributed random variables, a number of remarkable results have been obtained. In particular, it is possible that the mean displacement grows indefinitely, but slower

0305-4470/82/120729+06\$02.00 © 1982 The Institute of Physics

than linearly in time. As one might expect, it will turn out that our continuous-time models lead to essentially the same results as their discrete-time counterparts. We shall, however, find some surprising additional effects which are not immediately apparent from the existing treatments of discrete-time systems.

We now return to our continuous-time random walk described by equations (1) and (2), and our aim is to determine the long-time asymptotic behaviour of the average mean displacement,

$$\langle x(t)\rangle = \sum_{n=-\infty}^{\infty} n\langle P_n(t)\rangle, \tag{3}$$

where $\langle\ldots\rangle$ denotes an ensemble average, i.e. an average with respect to the probability distribution of the random transition rates $W_n^{\pm}$. As already specified after equation (2), we shall restrict our discussion to systems for which the pairs $\{W_n^+, W_{n+1}^-\}$ are independent random variables, equally distributed according to a probability density $\rho(w^+, w^-)$. The two transition rates W_n^+ and W_{n+1}^-, which are associated with the same bond $(n, n+1)$, however, can be correlated.

If the transition rates have fixed values, W^+ and W^- respectively, independent of n, one immediately derives the well known result

$$\langle x(t)\rangle = vt = (W^+ - W^-)t, \tag{4}$$

i.e. the mean displacement varies linearly with time, and $v = W^+ - W^-$ can be identified as a drift velocity.

In the case of random transition rates, our master equation can formally be solved by means of Laplace transformation. Taking equation (2) into account, the Laplace transform of equation (1) becomes

$$(z + W_n^+ - W_n^-)\tilde{P}_n - W_{n-1}^+\tilde{P}_{n-1} - W_{n+1}^-\tilde{P}_{n+1} = \delta_{n0}, \tag{5}$$

where

$$\tilde{P}_n(z) = \int_0^{\infty} dt\, e^{-zt} P_n(t). \tag{6}$$

The solution of equation (5) can be written in the form

$$\tilde{P}_0(z) = (z + X_0 + Y_0)^{-1}, \tag{7}$$

$$\tilde{P}_n(z) = \tilde{P}_0(z) \prod_{m=1}^{n} \frac{X_{m-1}}{z + X_m}, \qquad n = 1, 2, \ldots, \tag{8}$$

$$\tilde{P}_{-n}(z) = \tilde{P}_0(z) \prod_{m=1}^{n} \frac{Y_{m-1}}{z + Y_m}, \qquad n = 1, 2, \ldots, \tag{9}$$

where X_n and Y_n are infinite continued fractions recursively defined by

$$X_n = \cfrac{W_n^+}{1 + \cfrac{W_{n+1}^-}{z + X_{n+1}}}, \qquad n = 0, 1, 2, \ldots, \tag{10}$$

$$Y_n = \cfrac{W_{-n}^-}{1 + \cfrac{W_{-n-1}^+}{z + Y_{n+1}}}, \qquad n = 0, 1, 2, \ldots. \tag{11}$$

The Laplace transform of the average mean displacement $\langle x(t)\rangle$, finally, can be expressed as

$$\langle \tilde{x}(z)\rangle = z^{-1}\sum_{n=0}^{\infty}\langle X_n\tilde{P}_n - Y_n\tilde{P}_{-n}\rangle. \tag{12}$$

If the transition rates $W_n^{\pm}$ are random variables, the problem thus becomes very complicated, and we cannot solve it in its full generality. In the following, we first discuss the results of a self-consistent effective-medium approximation (EMA), and then introduce an interesting special case for which we can determine the long-time asymptotic behaviour of $\langle x(t)\rangle$ exactly. Details of the corresponding calculations will be reported in a more extended publication (Bernasconi and Schneider 1982).

Systems described by a master equation of the type of equation (5), with symmetric transition rates $(W_n^+ = W_{n+1}^-)$, have frequently been analysed in terms of a self-consistent EMA (Alexander *et al* 1981, Odagaki and Lax 1981, Webman 1981). This approach is easily generalised to the case of asymmetric transition rates (Stephen 1981, Bernasconi and Schneider 1982), with an effective medium characterised by two z-dependent transition rates, $W_{\text{eff}}^+(z)$ and $W_{\text{eff}}^-(z)$, which are determined by two coupled self-consistency equations. Within the EMA, one thus has

$$\langle \tilde{x}(z)\rangle = z^{-2}[W_{\text{eff}}^+(z) - W_{\text{eff}}^-(z)] = z^{-2}v_{\text{eff}}(z), \tag{13}$$

and it turns out that

$$v_{\text{eff}}(0) = \begin{cases} (1-\langle w^-/w^+\rangle)/\langle 1/w^+\rangle & \text{if } \langle w^-/w^+\rangle < 1, \\ -(1-\langle w^+/w^-\rangle)/\langle 1/w^-\rangle & \text{if } \langle w^+/w^-\rangle < 1, \end{cases} \tag{14}$$

where here $\langle\ldots\rangle$ denotes the average over the joint probability density $\rho(w^+, w^-)$ for W_n^+ and W_{n+1}^-. Asymptotically, $\langle x(t)\rangle$ is thus predicted to vary linearly with time,

$$\langle x(t)\rangle \approx v_{\text{eff}}(0)t, \qquad t\to\infty, \tag{15}$$

if either $\langle w^-/w^+\rangle$ or $\langle w^+/w^-\rangle$ is smaller than one, and $v_{\text{eff}}(0)$ vanishes if one of these averages approaches 1. If, however, $\rho(w^+, w^-)$ is such that

$$\langle w^-/w^+\rangle \geqslant 1 \qquad \text{and} \qquad \langle w^+/w^-\rangle \geqslant 1, \tag{16}$$

the EMA is not applicable, i.e. it does not lead to physically reasonable results for the long-time behaviour of $\langle x(t)\rangle$. We now introduce a model for which the situation described by equation (16) can be studied in some detail. Consider a probability density $\rho(w^+, w^-)$ of the form

$$\rho(w^+, w^-) = p\,\delta(w^+ - u)\,\delta(w^-) + (1-p)\,\delta(w^+ - \lambda v)\,\delta(w^- - v), \tag{17}$$

with λ, u and v positive and $0<p<1$. This describes a one-dimensional model system in which 'diodes', $\{W_n^+, W_{n+1}^-\} = \{u, 0\}$, and 'two-way bonds', $\{W_n^+, W_{n+1}^-\} = \{\lambda v, v\}$, occur with probabilities p and $1-p$, respectively. It follows that

$$\langle w^-/w^+\rangle = (1-p)/\lambda \qquad \text{and} \qquad \langle w^+/w^-\rangle = \infty, \tag{18}$$

and the interesting region, which cannot be described by the EMA, is thus given by $\lambda \leqslant 1-p$.

For this model, the $z\to 0$ asymptotic behaviour of $\langle \tilde{x}(z)\rangle$ can be determined exactly (Bernasconi and Schneider 1982). One first shows that in the limit as $z\to 0$ it is sufficient to consider configurations for which the bond $(-1, 0)$ is a 'diode'. This implies that all Y_n, equation (11), are zero, so that equation (12) can be written as

$$\langle \tilde{x}(z)\rangle = z^{-1}\left\langle \sum_{n=0}^{\infty}\left(\prod_{m=0}^{n}\frac{X_m}{z+X_m}\right)\right\rangle. \tag{19}$$

We further observe that the value of X_n only depends on $N_+ - n$, where $(N_+, N_+ + 1)$ is the closest 'diode' to the right of site n. For all sites n between two 'diodes', $(N_-, N_- + 1)$ and $(N_+, N_+ + 1)$, we can therefore introduce the notation

$$C_{N_+-n} = X_n/(z+X_n), \qquad N_- + 1 \leq n \leq N_+, \tag{20}$$

and, using equation (10), it follows that

$$C_0 = u/(z+u), \tag{21}$$

$$C_k = \lambda v/[z + v(1+\lambda - C_{k-1})], \qquad k = 1, 2, \ldots, N_+ - N_- - 1. \tag{22}$$

The factors $X_m/(z+X_m)$ in equation (19) can therefore be calculated separately, and with the same recursion, for each segment between two 'diodes'. This makes it possible to perform the average over all configurations explicitly, and one finally obtains

$$\langle \tilde{x}(z)\rangle = z^{-1}\langle S\rangle/(1-\langle R\rangle), \tag{23}$$

where

$$\langle R\rangle = p\sum_{n=0}^{\infty}(1-p)^n R_n, \qquad \langle S\rangle = p\sum_{n=0}^{\infty}(1-p)^n S_n, \tag{24}$$

and

$$R_n = C_0 C_1 \ldots C_n, \tag{25}$$

$$S_n = C_n + C_n C_{n-1} + \ldots + C_n C_{n-1} \ldots C_0. \tag{26}$$

The recursion defined by equations (21) and (22) can be solved, so that the $z \to 0$ behaviour of $\langle \tilde{x}(z)\rangle$ can be determined analytically. The long-time asymptotic behaviour of $\langle x(t)\rangle$ then follows from general theorems about inverse Laplace transforms (Doetsch 1971).

The corresponding calculations are rather lengthy (Bernasconi and Schneider 1982), and we restrict ourselves to a summary and discussion of the long-time behaviour of the average mean displacement. We obtain that

$$\langle x(t)\rangle \approx \begin{cases} v_\infty t, & \lambda > 1-p, \\ \alpha p^{-2} ct/\ln(ct), & \lambda = 1-p, \\ p^{-2}(ct)^\nu F[\beta^{-1}\ln(ct)], & \lambda < 1-p, \end{cases} \tag{27}$$

where

$$v_\infty = \frac{uv(\lambda - 1 + p)}{(1-p)u + p\lambda v}, \qquad c = \frac{uv(1-\lambda)^2}{u + v(1-\lambda)}, \tag{28}$$

$$\alpha = -\ln(1-p), \qquad \beta = -\ln\lambda, \qquad \nu = \alpha/\beta. \tag{29}$$

The function F is periodic with period 1, and explicitly given by

$$F(\tau) = \sum_{n=-\infty}^{\infty}\frac{f_n}{\Gamma(\nu + 1 + 2\pi i n/\beta)}\,e^{2\pi i n\tau}, \tag{30}$$

where the f_n are determined by

$$\sum_{n=-\infty}^{\infty} f_n\, e^{2\pi i n\tau} = \left(\sum_{k=-\infty}^{\infty} \frac{e^{-\alpha(k-\tau)}}{1+e^{-\beta(k-\tau)}}\right)^{-1}\left(\sum_{k=-\infty}^{\infty} g_k\, e^{2\pi i k\tau}\right)^{-1}, \tag{31}$$

with

$$g_k = \frac{\pi}{\beta}\left(\sin \pi\nu \cosh \frac{2\pi^2 k}{\beta} - \mathrm{i} \cos \pi\nu \sinh \frac{2\pi^2 k}{\beta}\right)^{-1}. \tag{32}$$

For $\lambda > 1-p$ we can compare our exact result with that obtained from the self-consistent EMA. Evaluating $v_{\text{eff}}(0)$, equation (14), for the $\rho(w^+, w^-)$ defined in equation (17), we find that $v_{\text{eff}}(0) = v_\infty$. If the parameters p and λ are such that an asymptotic drift velocity exists, it is thus correctly reproduced by the EMA.

For $\lambda < 1-p$, the asymptotic behaviour of $\langle x(t)\rangle$ is very remarkable. The average mean displacement not only increases slower than linearly in time, $\langle x(t)\rangle \sim t^\nu$, but exhibits superimposed, non-decaying oscillations as a function of $\ln t$. The period of these oscillations, $\beta = -\ln \lambda$, as well as their amplitude, increases with decreasing λ, and we note that λ characterises the asymmetry of the 'two-way bonds'. As $\langle x(t)\rangle$ represents an average over all possible configurations of 'diodes' and 'two-way bonds', the persistence of these oscillations is rather surprising. It is possible, however, to give a simple intuitive interpretation of their origin (see below).

To perform numerical simulations, it is convenient to use the following discrete-time analogue of our 'diode model'. If $x_t = n$ denotes the position of the particle at time t, one has $x_{t+1} = n+1$ with probability α_n, and $x_{t+1} = n-1$ with probability $1-\alpha_n$, and

$$\frac{1-\alpha_n}{\alpha_n} = \begin{cases} 0, & \text{with probability } p, \\ \lambda^{-1}, & \text{with probability } 1-p. \end{cases} \tag{33}$$

This model has been analysed by Solomon (1975), and his results imply that the asymptotic behaviour of $\langle x_t\rangle$ is qualitatively the same as in our continuous-time model, equation (27). In particular, it turns out that the expressions for the exponent ν and for the oscillation period β coincide with those given in equation (29), although the oscillatory behaviour of $\langle x_t\rangle$ is only obtained implicitly.

In our simulations we have chosen $p = 0.7$ and $\lambda = 0.09$ (implying $\nu = \frac{1}{2}$), and corresponding results are displayed in figure 1. They represent an average over 10 000 Monte Carlo samples and exhibit the oscillatory behaviour of $\ln(t^{-\nu}\langle x_t\rangle)$ against $\ln t$ very clearly. Even–odd effects are important for small (integer) t values, but the asymptotic oscillations with period $\beta = -\ln \lambda$ develop very rapidly, and at least qualitatively they compare very well with our continuous-time predictions, equations (27)–(32), which we have evaluated with $u = 1$ and $v = (1+\lambda)^{-1}$.

It can be demonstrated that the oscillatory behaviour of the average mean displacement is connected with the discrete nature of the slowing-down process in our models. Consider the average time t_k it takes a particle to go beyond the first k-tuple of consecutive 'two-way sites' (or 'two-way bonds') it encounters on its path. This can be estimated as follows (Bernasconi and Schneider 1982):

$$t_k \approx (1-p)^{-k} + \sum_{m=1}^{k} (1-p)^{m-k}\tau_m, \tag{34}$$

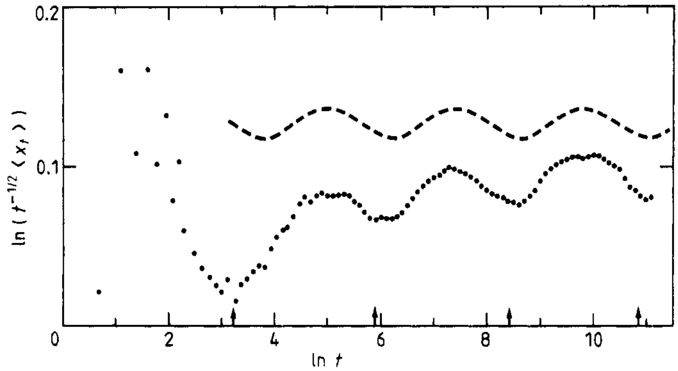

Figure 1. Average mean displacement $\langle x_t \rangle$ for the model described by equation (33), with $p=0.7$ and $\lambda=0.09$. The numerical results represent an average over 10 000 Monte Carlo samples, and the broken curve is the continuous-time result for the asymptotic behaviour of $\langle x(t) \rangle$ (equations (27)–(32), evaluated for $p=0.7$, $\lambda=0.09$, $u=1$, and $v=(1+\lambda)^{-1}$). The arrows indicate simple estimates for the locations t_k of the first minima (equation (34); $k=1,\ldots,4$).

where

$$\tau_m = 2\lambda^{-m} \sum_{j=1}^{m} j\lambda^{j-1} \tag{35}$$

is the average waiting time at an m-tuple of consecutive 'two-way sites', and where the average separation of two m-tuples has been approximated by $(1-p)^{-m}$. For $\lambda < 1-p$, t_k becomes dominated by τ_k, so that we may expect $\ln(t^{-\nu}\langle x_t \rangle)$ to exhibit minima at $t \approx t_k$. This intuitive argument is rather accurately confirmed by the numerical simulations in figure 1, and we note that $(\ln t_{k+1} - \ln t_k) \to \ln \lambda^{-1}$ for $k \to \infty$, in agreement with the analytic predictions for the asymptotic oscillation period.

The above arguments, finally, indicate that the oscillations are not an exclusive consequence of our 'diode models'. Similar effects should also be observed in systems with a more general transition rate distribution, provided that this is (a) *discrete* and (b) such that $\langle x(t) \rangle$ increases slower than linearly in time. In this connection we note that the saddlepoint-type approach of Derrida and Pomeau (1982) would be insensitive to such superimposed oscillations.

References

Alexander S, Bernasconi J, Schneider W R and Orbach R 1981 *Rev. Mod. Phys.* **53** 175
Bernasconi J and Schneider W R 1981 *Phys. Rev. Lett.* **47** 1643
—— 1982 to be published
Bernasconi J, Schneider W R and Wyss W 1980 *Z. Phys.* B **37** 175
Derrida B and Pomeau Y 1982 *Phys. Rev. Lett.* **48** 627
Doetsch G 1971 *Handbuch der Laplace-Transformation I und II* (Basel: Birkhäuser)
Kesten H, Koslov M V and Spitzer F 1975 *Compositio Math.* **30** 145
Odagaki T and Lax M 1981 *Phys. Rev.* B **24** 5284
Sinai Ya G 1982 *Lecture Notes in Physics* (Berlin: Springer) **153** 12
Solomon F 1975 *Ann. Prob.* **3** 1
Stephen M J 1981 *J. Phys. C: Solid State Phys.* **14** L1077
Webman I 1981 *Phys. Rev. Lett.* **47** 1496