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Solvable models of temporally correlated random walk on a lattice

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Abstract. We seek the conditional probability function $P(\mathbf{m}, t)$ for the position of a particle executing a random walk on a lattice, governed by the distribution $W(n, t)$ specifying the probability of n jumps or steps occurring in time t. Uncorrelated diffusion occurs when W is a Poisson distribution. The solutions corresponding to two different families of distributions W are found and discussed. The Poissonian is a limiting case in each of these families. This permits a quantitative investigation of the effects, on the diffusion process, of varying degrees of temporal correlation in the step sequences. In the first part, the step sequences are regarded as realizations of an ongoing renewal process with a probability density $\psi(t)$ for the time interval between successive jumps. W is constructed in terms of ψ using the continuous-time random walk approach. The theory is then specialized to the case when ψ belongs to the class of special Erlangian density functions. In the second part, W is taken to belong to the family of negative binomial distributions, ranging from the geometric (most correlated) to the Poissonian (uncorrelated). Various aspects such as the continuum limit, the master equation for P, the asymptotic behaviour of P, etc., are discussed.

Keywords. Jump diffusion; continuous-time random walk; special Erlangian distribution; negative binomial distribution; master equation.

1. Introduction

Consider a particle performing a random walk on an infinite lattice in the following manner: the particle resides at a site for a random duration of time, before jumping instantaneously and at random to a nearest neighbour site. We want to calculate the probability $P(\mathbf{m}, t)$ of finding it at the site $\mathbf{m}$ at time t, given that it was at an arbitrary origin $\mathbf{0}$ at $t = 0$. This quantity can be written as

$$P(\mathbf{m}, t) = \sum_{n=0}^{\infty} W(n, t)\, p_n(\mathbf{m}), \tag{1}$$

where $W(n, t)$ is the probability of n jumps occurring in the interval $(0, t)$ and $p_n(\mathbf{m})$ is the probability of reaching the point $\mathbf{m}$ from $\mathbf{0}$ in n steps. The latter is known in principle for all lattice graphs, being the solution to the standard random walk problem. The former, $W(n, t)$, characterizes the evolution in time of the jump diffusion process. If the successive jumps are completely uncorrelated in time, the stationary, discrete random variable n has a Poisson distribution

$$W(n, t) = (1/n!)\,(\lambda t)^n \exp(-\lambda t), \tag{2}$$

where λ is the mean jump rate. *All* other probability distributions imply a memory or correlation in the jump sequence, and hence in the diffusion process itself. It is this sort of *temporally correlated* random walk that we study in what follows, with the help of certain solvable models—*i.e.*, specific classes of distributions $W(n, t)$ that generalize (2) in a natural manner, and for which analytical solutions to the jump diffusion problem can be found.

The notation used in an earlier paper on a two-state random walk on a lattice (Balakrishnan and Venkataraman 1981, referred to as BV hereafter) will be retained. For simplicity of notation, we restrict ourselves to a cubic lattice in d dimensions, with the lattice constant set equal to unity. Thus $\mathbf{m} = (m_1, m_2, \ldots, m_d)$. Let L denote the generating function of $P(\mathbf{m}, t)$, *i.e.*,

$$L(z_1, \ldots, z_d, t) = \sum_{m_i = -\infty}^{\infty} P(\mathbf{m}, t)\, z_1^{m_1}, z_2^{m_2}, \ldots, z_d^{m_d}, \tag{3}$$

and further let

$$H(z, t) = \sum_{n=0}^{\infty} W(n, t)\, z^n \tag{4}$$

be the generating function for the step number distribution $W(n, t)$. Then L is determined in terms of H according to

$$L(z_1, \ldots, z_d, t) = H(g), (z)t, \tag{5}$$

where $$g(z) = \sum_{i=1}^{d} (r_i z_i + l_i z_i^{-1}) \tag{6}$$

generates a single step on the lattice. The positive numbers (r_i, l_i) satisfying $\Sigma(r_i + l_i) = 1$ are the *a priori* probabilities for jumps in the $+i$ and $-i$ directions respectively. They allow for a biased random walk. In the absence of any bias, each $r_i = l_i = 1/(2d)$. Once H is known, $P(\mathbf{m}, t)$ may be found in principle by inverting (3). The mean square displacement is given by

$$\langle \mathbf{m}^2(t) \rangle = \nu(t) + \nu_2(t) \sum_{i=1}^{d} (r_i - l_i)^2, \tag{7}$$

where $$\nu(t) = [\partial H(z, t)/\partial z]_{z=1} \tag{8}$$

is the first moment of $W(n, t)$ (the mean number of jumps in a time interval t), and

$$\nu_2(t) = [\partial^2 H/\partial z^2]_{z=1} \tag{9}$$

is the second factorial moment of $W(n, t)$. Specifying the jump statistics thus specifies the random walk. We shall concentrate on two distinct families of distributions

$W(n, t)$, in each of which the Poissonian (2) occurs as a limiting case. This will help us understand the effects of temporal correlations in the jump process in a graded, quantitative manner.

Before proceeding to these distributions, we must record the already known solution in the Poissonian case (see BV and references therein). It is trivial to see that

$$H(z, t) = \exp\,[\lambda t\,(z-1)], \tag{10}$$

and that $\nu(t) = \lambda t$ in this case. Further, $P(\mathbf{m}, t)$ is found to be

$$P(\mathbf{m}, t) = \exp\,(-\lambda t) \prod_{i=1}^{d} (r_i/l_i)^{m_i/2}\, I_{m_i}(2\lambda t (r_i l_i)^{1/2}), \tag{11}$$

where I_m is the modified Bessel function of order m. Equation (11) is the basic solution for diffusion *via* uncorrelated, nearest-neighbour jumps on a cubic lattice, in the presence of directional bias. It can be shown (see, *e.g.*, BV) to satisfy the conventional Markovian master equation

$$\frac{\partial}{\partial t} P(\mathbf{m}, t) = \lambda \sum_{i=1}^{d} [r_i \{P(m_1, \ldots, m_i - 1, \ldots, m_d, t) - P(\mathbf{m}, t)\}$$
$$+ l_i \{P(m_1, \ldots, m_i + 1, \ldots, m_d, t) - P(\mathbf{m}, t)\}], \tag{12}$$

for instance by observing that the corresponding step-generating function (10) obeys the differential equation

$$\partial H(z, t)/\partial t + \lambda (1-z) H(z, t) = 0. \tag{13}$$

2. A class of continuous-time random walks

2.1 *Continuous-time random walk (CTRW)*

A rather general approach to the problem is to regard the sequence of jumps as an ongoing *equilibrium renewal process* (see, *e.g.* Cox 1967): the time interval between successive jumps is assumed to be governed by a common normalized probability density $\psi(t)$. The mean residence time at a site is therefore

$$\tau = \int_0^\infty t\psi(t)\, dt\,. \tag{14}$$

The probability density for the *first* jump time from a *randomly* chosen origin of time is given by (Feller 1966, Cox 1967; see BV)

$$\psi_0(t) = (1/\tau) \int_t^\infty \psi(t')\, dt'. \tag{15}$$

The n-jump probability $W(n, t)$ can then be expressed as a multiple integral involving $\psi(t)$, according to the standard procedure of CTRW theory (Montroll and Weiss 1965). One obtains (BV) the following answer for the Laplace transform of the generating function $H(z, t)$:

$$\tilde{H}(z, s) = \frac{1 - \tilde{\psi}_0(s) - z(\tilde{\psi}(s) - \tilde{\psi}_0(s))}{s(1 - z\tilde{\psi}(s))}, \tag{16}$$

where a tilde denotes the Laplace transform.* Replacing z by $g(z)$ in (16) then yields the generating function for the random walk on the lattice. In principle, therefore, this represents a general solution to the problem. Note, incidentally, that

$$\tilde{\nu}(s) = 1/\tau s^2, \text{ or } \nu(t) = t/\tau, \tag{17}$$

in this class of models, regardless of the functional form of $\psi(t)$; the mean square displacement for unbiased random walks remains proportional to t.

2.2 *Special Erlangian distributions* $\psi(t)$

It is easy to verify that the Poisson distribution (2) for $W(n, t)$, with the generating function (10), corresponds to the functional form

$$\psi(t) = \lambda \exp(-\lambda t) \quad (= \psi_0(t) \text{ in this case}), \tag{18}$$

in the CTRW formalism. Now, the ratio of the jump probability density $\psi(t)$ to the corresponding holding time distribution, namely,

$$\phi(t) = \psi(t) \Big/ \Big[1 - \int_0^t \psi(t')\, dt'\Big], \tag{19}$$

measures the probability of an imminent jump at time t, given that the preceding one occurred at $t = 0$. In analogy with the renewal theory, we may call $\phi(t)$ the 'age-specific jump rate'. In these terms, the exponential distribution (18) is singled out by a special feature: a constant ($= \lambda$) age-specific jump rate. For all other distributions, ϕ is time-dependent. For correlated jumps, we expect $\phi(t)$ to have the following sort of general behaviour: it must increase from a vanishing value at $t = 0$ to the uncorrelated limit (λ) for very large values of t. A family of distributions $\psi(t)$ for which $\phi(t)$ has this behaviour is the 'special Erlangian' one,

$$\psi(t) = \lambda \frac{(\lambda t)^{M-1}}{(M-1)!} \exp(-\lambda t), \quad M = 1, 2, \ldots \tag{20}$$

*Instead of $\psi(t)$, one may also work with the holding-time distribution $p(t)$, called the 'survivor function' in renewal theory. This is related to $\psi(t)$ by $\psi(t) = -dp/dt$, or $p(t) = 1 - \int_0^t \psi(t')\, dt' = \int_t^\infty \psi(t')\, dt'$.

This is just the gamma distribution with a positive integer parameter M. It arises if we imagine each jump to occur at the end of M fictitious stages, each such intermediate stage being independently, exponentially distributed with probability density $\lambda \exp(-\lambda t)$. The case $M = 1$ yields the original distribution (18), while increasing M implies increasing temporal correlation in the jump process. The holding time distribution corresponding to (20) is found to be

$$p(t) = 1 - \int_0^t \psi(t')\,dt' = \exp(-\lambda t) \sum_{j=0}^{M-1} (\lambda t)^j / j!, \tag{21}$$

while the age-specific jump rate is

$$\phi(t) = \lambda \frac{(\lambda t)^{M-1} / (M-1)!}{\sum_{j=0}^{M-1} (\lambda t)^j / j!}. \tag{22}$$

Figure 1 shows the behaviour of $\phi(t)$ for $M = 1, 2, 3$ and 4.

While a closed expression for $P(\mathrm{m}, t)$ cannot be obtained for general M, a lot can

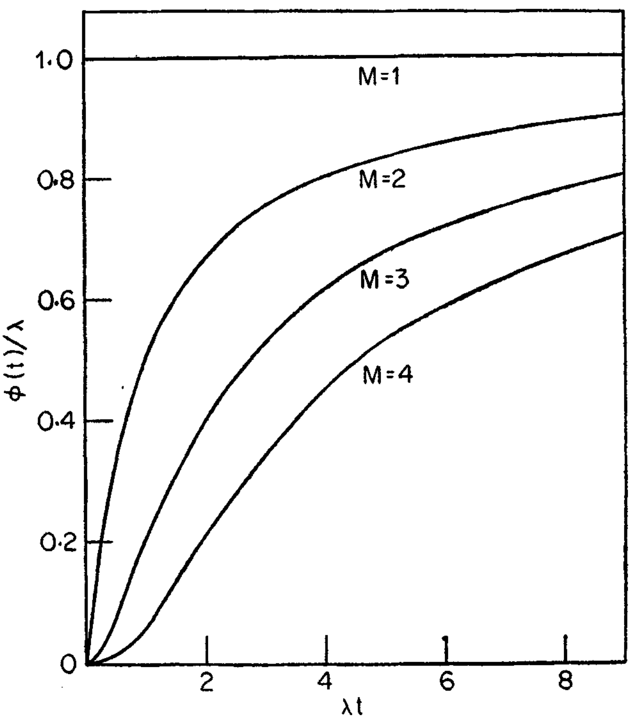

Figure 1. The 'age-specific jump rate' $\phi(t)$ (equation (22)) corresponding to the special Erlangian form (equation (20)) for the distribution $\psi(t)$. $M = 1$ refers to the exponential form for $\psi(t)$, *i.e.*, to an uncorrelated step sequence with a Poisson distribution for $W(n, t)$.

be learnt from the result for (the transform of) the generating function, $\tilde{H}(z, s)$. From (15), (16), (19) and (21) we find

$$\tilde{H}(z, s) = \frac{1}{s} + \frac{\lambda(z-1)}{Ms^2} \frac{(s+\lambda)^M - \lambda^M}{(s+\lambda)^M - z\,\lambda^M}. \tag{23}$$

It is possible to extract a closed expression for $W(n, t)$ from (23), on expanding $\tilde{H}$ in powers of z and inverting the transform. After some algebra, we get

$$W(n, t) = \exp(-\lambda t) \left\{ \sum_{j=(n-1)M}^{nM-1} \frac{(\lambda t)^j}{j!} \left(\frac{j}{M} - n + 1\right) + \sum_{j=nM}^{(n+1)M-1} \frac{(\lambda t)^j}{j!} \left(n + 1 - \frac{j}{M}\right) \right\}. \tag{24}$$

When $n = 0$, only the second sum contributes. Equation (24) is to be compared with the Poisson distribution (2), which is the case $M = 1$. In order to illustrate the effect of the correlations in the jumps (especially at short times), we have numerically calculated for $M = 2$ the quantity $P(\mathbf{m}, t)$ in the special case $d = 1$, $m = 0$, $r = l = \frac{1}{2}$, that is, the probability of finding the diffusing particle back at the origin at time t, for an unbiased one-dimensional random walk. The result is shown in figure 2, along with the variation of the $M = 1$ expression,

$$P(0, t) = I_0(\lambda t) \exp(-\lambda t), \tag{25}$$

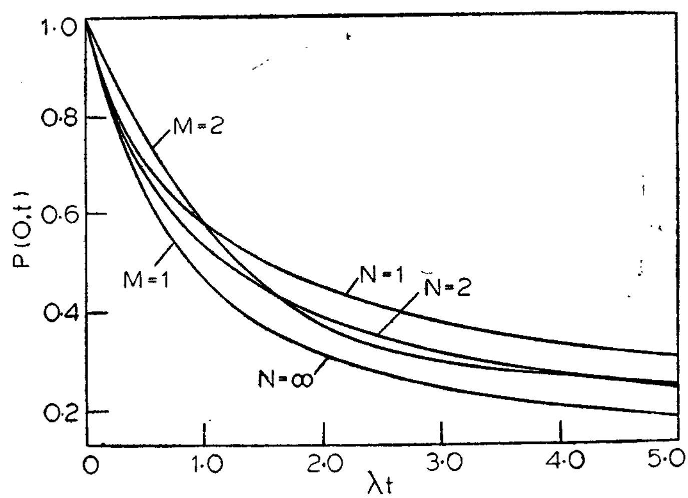

Figure 2. The probability $P(0, t)$ of finding the random walker back at the origin at time t, in the case $d = 1$, $r = l = \frac{1}{2}$. $M = 1, 2$ refer respectively to the exponential distribution and a special Erlangian distribution for the waiting-time distribution $\psi(t)$ (§ 2). $N = 1$, 2 and ∞ correspond respectively to the geometric, a negative bionomial, and the Poisson distribution for $W(n, t)$ (§ 3).

corresponding to an uncorrelated random walk, for comparison.

Another angle which provides some insight into the correlations which exist in the model is the master equation satisfied by P(or, equivalently, the differential equation obeyed by H). For this purpose it is helpful to write

$$\left.\begin{aligned} H(z, t) &= h(z, t) \exp(-\lambda t), \\ \text{or} \qquad \tilde{h}(z, s) &= \tilde{H}(z, s-\lambda). \end{aligned}\right\} \tag{26}$$

Equation (23) then leads to

$$\tilde{h}(z, s) = \frac{1}{(s^M - z\,\lambda^M)} \sum_{j=0}^{M-1} \left[1 - \frac{j}{M}(1-z)\right] s^{M-1-j}\,\lambda^j. \tag{27}$$

It is easily verified from this expression that $h(z, t)$ satisfies the differential equation

$$\partial^M h(z, t)/\partial t^M = z\,\lambda^M h(z, t), \tag{28}$$

in contrast to the first order equation (see (13)) which obtains for $M = 1$. The conventional first-order time derivative on the left-hand side of the master equation (12) for $P(\mathbf{m}, t)$ is therefore replaced, when $M > 1$, by the sum of derivatives

$$\sum_{j=0}^{M-1}{}' \binom{M}{j} \lambda^j \frac{\partial^{M-j}}{\partial t^{M-j}} P(\mathbf{m}, t), \tag{29}$$

while the difference operator on the right of that equation is essentially unchanged. Higher-order time derivatives are of course one way of representing memory effects. " Alternatively, one can consider (see, *e.g.*, Kehr and Haus 1978) the *inhomogeneous* master equation with a memory kernel that is obeyed by the probability $P(\mathbf{m}, t)$ corresponding to every CTRW. This is most easily derived by beginning with (16) written in the form

$$\left[s - (z-1)\frac{s\tilde{\psi}}{(1-\tilde{\psi})}\right] \tilde{H}(z, s) = 1 + (z-1)\frac{(\tilde{\psi}_0 - \tilde{\psi})}{(1-\tilde{\psi})}, \tag{30}$$

and going on to the corresponding equation for $\tilde{L}$, by replacing z with $g(z)$. For the family of distributions (20), the memory kernel of the master equation in the time domain turns out to be the inverse transform of

$$\tilde{K}(s) = s\lambda^M / [(s+\lambda)^M - \lambda^M]\,. \tag{31}$$

This yields $K(t-t') = \lambda\delta\,(t-t')$ for $M=1$, as expected. We find

$$K(t-t') = \begin{cases} \lambda^2 \exp\,[-\,2\lambda\,(t-t')] \quad (M=2)\,, \\ (2\lambda^2/\sqrt{3}) \exp\,[-\,3\,\lambda(t-t')/2]\, \sin\,[\sqrt{3}\lambda\,(t-t')/2] \quad (M=3) \end{cases} \tag{32}$$

and so on.

3. Another class of temporally correlated random walks

3.1 *The distribution* $W(n, t)$

Instead of regarding the jump sequences as realizations of a renewal process and using CTRW theory for $W(n, t)$, let us now explore the solutions obtained for $P(\mathbf{m}, t)$ when certain standard distributions are used as inputs for $W(n, t)$. In particular, we shall concentrate on the family of negative binomial distributions, namely,

$$W(n, t) = \binom{N-1+n}{n} \left(\frac{\lambda t}{N}\right)^n \left(1+\frac{\lambda t}{N}\right)^{-N-n}, \quad N = 1, 2, \ldots \tag{33}$$

In addition to the important reason of analytical tractability, there is another reason for this choice. Among the conventional one-parameter distributions, the Poisson and the geometric distributions represent the two extremes in the degree of correlation between the n pulses (events) described by $W(n, t)$. (Just as, in the case of a continuous random process, a roughly analogous statement may be made with respect to white or $1/f^0$ noise and Brownian or $1/f^2$ noise). The family of distributions (30) provides a natural and convenient interpolation between these two extremes. This enables us, once again, to see the effect of a gradual change in the degree of correlation, as we go from the geometric ($N=1$) to the Poisson ($N\to\infty$) distribution.*

Before taking up the solution $P(\mathbf{m}, t)$ of the diffusion problem associated with the foregoing distributions, let us observe the following. For each given value of N, the expression (33) can be regarded as a *continuous superposition* of the corresponding Poissonian expression, with different mean rates. In other words,

$$W(n, t) = \int_0^\infty d\lambda_1\, \sigma(\lambda_1) \left\{\frac{(\lambda_1 t)^n}{n!} \exp\,(-\lambda_1 t)\right\}, \tag{34}$$

*There is also a physical realization of this family of distributions, in another field. Under suitable experimental conditions, the photon counting statistics pertaining to admixtures of coherent and chaotic (thermal) light can be shown to run the gamut of the negative binomial distributions (Saleh 1978). Indeed, a well-known bunching effect in photon counting arises essentially from the difference between the distribution $\psi(t)$ and the first-waiting-time distribution $\psi_0(t)$, in the language of random processes.

where the (normalized) spectral weight function $\sigma(\lambda_1)$ is easily seen to be

$$\sigma(\lambda_1) = \frac{1}{(N-1)!}\left(\frac{N}{\lambda}\right)\left(\frac{N\lambda_1}{\lambda}\right)^{N-1}\exp\left(-\frac{N\lambda_1}{\lambda}\right). \tag{35}$$

The ' non-analytic ' effects arising from such a continuous spectrum of characteristic times have already been discussed elsewhere (BV; see also Balakrishnan 1980). Prominent among these effects is a deviation from the usual ($\sim t^{-d/2}$) asymptotic behaviour of $P(\mathbf{m}, t)$ for finite $\mathbf{m}$ and large t, as we shall see below.

3.2 *The solution for* $P(\mathbf{m}, t)$

To discover the solution $P(\mathbf{m}, t)$ corresponding to $W(n, t)$ as given by (33) for finite values of N, we use the simple stratagem of writing the step-generating function in the form

$$H(z, t) = \sum_{n=0}^{\infty} W(n, t)\, z^n = \left[1 + (1-z)\frac{\lambda t}{N}\right]^{-N}$$

$$= \frac{1}{(N-1)!}\int_0^\infty d\xi\; \xi^{N-1} \exp\left[-\xi\left\{1 + (1-z)\frac{\lambda t}{N}\right\}\right]. \tag{36}$$

Then, on replacing z by $g(z)$ to obtain L from H (see (5)), we arrive, as in the Poissonian case, at the answer

$$P(\mathbf{m}, t) = \frac{1}{(N-1)!}\int_0^\infty d\xi\; \xi^{N-1} \exp\left\{-\xi\left(1 + \frac{\lambda t}{N}\right)\right\}\prod_{i=1}^{d}(r_i/l_i)^{m_i/2}$$

$$\times\, I_{m_i}\left(2\xi\,\frac{\lambda t}{N}(r_i l_i)^{1/2}\right). \tag{37}$$

This is to be compared with (11). The latter represents the $N \to \infty$ limit of the former.

Let us digress briefly to consider in some further detail the limiting case $N = 1$, *i.e.*, that of the geometric distribution

$$W(n, t)\Big|_{N=1} = \frac{(\lambda t)^n}{(1 + \lambda t)^{n+1}}. \tag{38}$$

Remarkably enough, the integral representation (37) for $P(\mathbf{m}, t)$ with $N = 1$ has the analytic structure of the lattice Green function (or extended Watson integral) for an anisotropic lattice (orthorhombic for $d = 3$, rectangular for $d = 2$), for general values of the bias factors r_i, l_i. A vast literature exists on these Green functions, dealing with their analytic properties, methods for numerical evaluation, etc. (Mannari and Kawabe 1970, and references therein; Katsura *et al* 1971, and references therein). It is amusing to learn, on wading through this literature, that the following analytical results are known. In two dimensions, $P(\mathbf{0}, t)$ can be expressed as a complete elliptic integral of the first kind. For 'diagonal' points ($m_1 = m_2$), $P(\mathbf{m}, t)$ is given by a hypergeometric ($_2F_1$) function. For $m_1 \neq m_2$ but $r_1 l_1 = r_2 l_2$, P is a hypergeometric function of the $_4F_3$ type. In the most general case ($m_1 \neq m_2$, $r_1 l_1 \neq r_2 l_2$), P is expressible in terms of the Appell double hypergeometric function F_4. In three dimensions, very few such analytical results exist. $P(\mathbf{0}, t)$ can be reduced to an integral over a complete elliptic integral of the first kind. A similar statement holds good if $m_1 = m_2 = 0$, but $m_3 \neq 0$, provided $r_1 l_1 = r_2 l_2$. Again, if at least two of the three products $r_i l_i$ are equal, $P(\mathbf{m}, t)$ can be written in terms of Kampé de Fériet functions (generalized hypergeometric functions in two variables). In all cases, power series representations and asymptotic expansions for $P(\mathbf{m}, t)$ are available.

Returning to the solution (37) for general N, let us now examine the asymptotic ($\lambda t \to \infty$) behaviour of the probability $P(\mathbf{m}, t)$. Although the mean square displacement (in the absence of bias) is identical ($=\lambda t$) for all the members of this class of models, differences show up, of course, in various other moments. The asymptotic behaviour of $P(\mathbf{m}, t)$ is a feature which illustrates the peculiarities of each case quite strikingly. The leading large t behaviour of $P(\mathbf{m}, t)$ is deduced by analysing (37) and corroborated, where applicable, by the explicit solutions in the limiting cases $N \to \infty$ and $N = 1$ (respectively, (11) and (43) below). The results are catalogued in table 1. Here $\mathbf{m}$ is a finite point, and

$$b_d = 1 - 2 \sum_{i=1}^{d} (r_i l_i)^{1/2}, \tag{39}$$

is the numerical factor that provides a measure of the anisotropy in the random walk. It vanishes in the isotropic case, when each $r_i = l_i = 1/(2d)$.

We turn now to a closer investigation of the case $d = 1$. Rather convenient closed-form solutions are available in this instance. This facilitates a better understanding of the correlations in the diffusion process originating from the statistics of the jump-causing pulse sequences.

Table 1. Asymptotic behaviour of $P(\mathbf{m}, t)$ for a class of random walks (see Equation (37))

Step number distribution parameter N (see equation (33))	Lattice dimensionality d					
	1		2		3	
	Isotropic	Anisotropic	Isotropic	Anisotropic	Isotropic	Anisotropic
1 (geometric)	$t^{-1/2}$	t^{-1}	$t^{-1} \ln t$	t^{-1}	t^{-1}	t^{-1}
$2 \leqslant N < \infty$ (negative binomial)	$t^{-1/2}$	t^{-N}	t^{-1}	t^{-N}	$t^{-3/2}$	t^{-N}
∞ (Poisson)	$t^{-1/2}$	$t^{-1/2} e^{-b_1 \lambda t}$	t^{-1}	$t^{-1} e^{-b_2 \lambda t}$	$t^{-3/2}$	$t^{-3/2} e^{-b_3 \lambda t}$

3.3 *Jump diffusion on a linear lattice and the continuum limit*

When $d = 1$, the solution (37) essentially reduces to an associated Legendre polynomial. We find (for $m > -N$)

$$P(m, t) = \frac{(m + N - 1)!}{(N - 1)!} (r/l)^{m/2} [A_N(t)]^{-N} P_{N-1}^{-m}\left(\frac{1 + \frac{\lambda t}{N}}{A_N}\right), \tag{40}$$

where the symbol P_β^α on the right side is an associated Legendre function, and

$$A_N(t) = \left[\left(1 + \frac{\lambda t}{N}\right)^2 - 4rl\left(\frac{\lambda t}{N}\right)^2\right]^{1/2} \xrightarrow[r = l = \frac{1}{2}]{} \left(1 + \frac{2\lambda t}{N}\right)^{1/2}. \tag{41}$$

A similar result, in terms of P_{N-1}^{m}, obtains in the case $m < 1 - N$. Thus $P(m, t)$ is an algebraic function for finite N. It may be checked that as $N \to \infty$, one correctly recovers the limit

$$\lim_{N\to\infty} P(m, t) = I_m (2\lambda t(rl)^{1/2}) \exp(-\lambda t). \tag{42}$$

At the other extreme of the geometric distribution (38) for $W(n, t)$, (40) reduces to

$$P(m, t)\Big|_{N=1} = (r/l)^{m/2} [A_1(t)]^{-1/2} \left[\frac{2\lambda t(rl)^{1/2}}{1 + \lambda t + A_1(t)}\right]. \tag{43}$$

In order to illustrate the effect of the correlations in $W(n, t)$ for $N < \infty$, we have again plotted in figure 2 the probability for return to the origin $P(0, t)$, as a function of λt in the cases $N = 1$, 2 and ∞ respectively, for an unbiased random walk. The lowest curve ($N = \infty$) and the topmost curve ($N = 1$) represent, in a sense, the two end-points of uncorrelated and correlated diffusion.

The last statement is reinforced by constructing and looking at the structure of a master equation for the probability density $P(m, t)$ in the case $N = 1$. (For $N \to \infty$, $P(m, t)$ is of course the solution of the standard Markovian master equation (12), with $d = 1$). The generating function for this P is

$$L(z, t) = H(g(z), t) = [1 + \lambda t \{1 - g(z)\}]^{-1}, \tag{44}$$

where $g(z) = rz + lz^{-1}$. Therefore

$$\partial L(z, t) / \partial t = \lambda[g(z) - 1] L^2(z, t). \tag{45}$$

From (45) it is readily deduced that

$$\frac{\partial}{\partial t} P(m, t) = \lambda \sum_{m'=-\infty}^{\infty} P(m-m', t) [r \{P(m' - 1, t) - P(m', t)\}$$

$$+ l \{P(m' + 1, t) - P(m', t)\}], (N = 1), \tag{46}$$

a non-linear master equation. Thus the transition probability per unit time is time-dependent, and is itself dependent on P again, as is evident from the convolution in (46). Finally, let us pass to the continuum limit, in which matters become more transparent. For simplicity, consider the unbiased case ($r = l = \frac{1}{2}$). Re-introducing the lattice constant a, and going over to the limit $a \to 0$, $\lambda \to \infty$ such that

$$\lim \lambda a^2 = 2\, D = \text{finite}, \tag{47}$$

we find that (46) is transformed into

$$\frac{\partial}{\partial t} P(x, t) = D \int_{-\infty}^{\infty} dx' \, P(x - x', t) \frac{\partial^2}{\partial x'^2} P(x', t), \; (N = 1), \tag{48}$$

so that $x(t)$ is very far from being a Markov process. The relevant solution of (48) is

$$P(x, t) = (4Dt)^{-1/2} \exp\,[-|x|/(Dt)^{1/2}], \quad (N = 1) \tag{49}$$

as may be deduced, for instance, by a spatial Fourier transform of (48). This solution can be directly got from (43), on first setting $r = l = \frac{1}{2}$, $m = x/a$, $P(m, t) = aP(x, t)$, and then taking the required limits in a and λ. For the sake of comparison, recall that the corresponding probability density for conventional diffusion is

$$P(x, t) = (4\pi Dt)^{-1/2} \exp\,[-x^2/4Dt], \quad (N \to \infty). \tag{50}$$

While the mean square displacement $\langle x^2(t) \rangle = 2Dt$ in both cases, the higher moments are larger for the exponential distribution than for the Gaussian. It is easy to show that

$$\langle x^{2j} \rangle_{\text{exp}} / \langle x^{2j} \rangle_{\text{Gauss}} = j! \;\; (j = 0, 1, 2, \ldots). \tag{51}$$

Finally, it is very interesting to see precisely how the probability density changes its functional form from the exponential to the Gaussian, as N increases. The continuum limit of (40), again for $r = l = \frac{1}{2}$, answers this question. After some tedious algebra, we arrive at the following suggestive expression: writing

$$(N/Dt)^{1/2}\, |x| = u, \tag{52}$$

we find

$$P(x, t) = \left(\frac{N}{Dt}\right)^{1/2} e^{-u} \sum_{j=0}^{N-1} \frac{1}{(N - 1 - j)!} \binom{N - 1 + j}{j} 2^{-N-j} \, u^{N-1-j}. \tag{53}$$

As an illustration to complement figure 2, we plot in figure 3 the functions $P(x, t)$ for $N = 1$, 2 and ∞ as functions of x, for the same fixed value ($= \frac{1}{2}$) of Dt. It may appear that $P(N = 1)$ alone is singular at $x = 0$, since it has a cusp at that point. This is not so. It is clear from (52) and (53) that $P(x, t)$ is singular at $x = 0$ for all

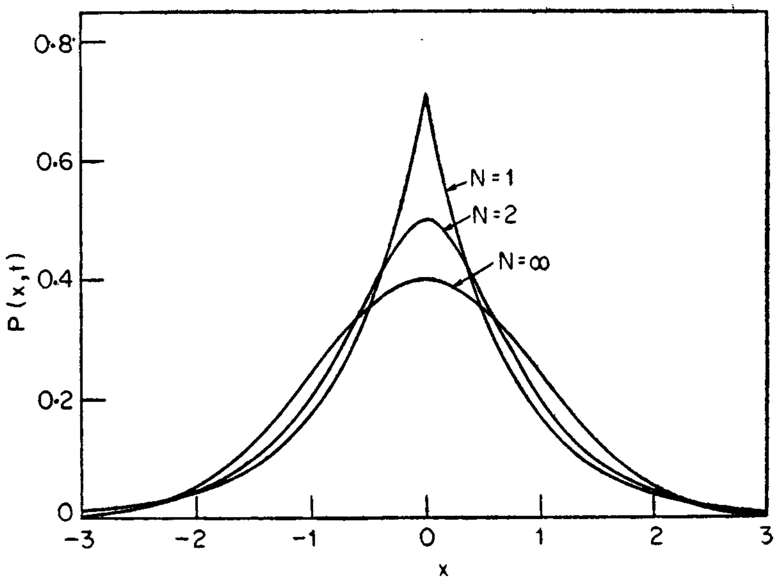

Figure 3. The probability $P(x, t)$ (equation (53)) in the continuum limit (again for $d = 1$ and $r = l = \frac{1}{2}$) at a fixed instant of time, here taken to be given by $2Dt = 1$. The rms displacement is thus unity in each case. While $P(N = 2)$ appears to be smooth at $x = 0$, its third derivative is discontinuous at that point (see text and equation (54)).

finite values of N. The polynomial factor in (53) has the effect of progressively softening the singularity as N increases. For a general value of N, it can be shown that $P(x, t)$ and its first $(2N - 2)$ derivatives are continuous at $x = 0$, while its $(2N - 1)$th derivative is discontinuous at that point. The discontinuity is found to be

$$\left[\partial^{2N-1} P(x, t)/\partial x^{2N-1}\right]_{x=-0}^{x=+0} = (-N/Dt)^N. \tag{54}$$

It is indeed remarkable how, as N increases and the pulse sequence underlying the diffusion becomes more and more uncorrelated, the singularity in the probability density function is pushed out to higher order derivatives—till in the limit $N \to \infty$, it disappears altogether. As $P(x, t)$ for general N can be regarded as a superposition of N gamma density functions (see (50)), a central limit theorem operates. The familiar Gaussian emerges.

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