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The Two-State Random Walk

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We develop asymptotic results for the two-state random walk, which can be regarded as a generalization of the continuous-time random walk. The two-state random walk is one in which a particle can be in one of two states for random periods of time, each of the states having different spatial transition probabilities. When the sojourn times in each of the states and the second moments of transition probabilities are finite, the state probabilities have an asymptotic Gaussian form. Several known asymptotic results are reproduced, such as the Gaussian form for the probability density of position in continuous-time random walks, the time spent in one of these states, and the diffusion constant of a two-state diffusing particle.

KEY WORDS: Random walks; Markov processes; Markov renewal processes; asymptotic distributions.

The theory of the continuous-time random walk (CTRW), first discussed by Montroll and Weiss,[1] has been applied to calculate the transport properties of disordered solids.[2–4] The CTRW can be formulated as a two-state process, in which a random walker is either at rest or in motion. A single sojourn in the rest state takes a random amount of time, at the conclusion of which the random walker moves to another position, with infinite speed (i.e., the transition time is zero). In this paper we point out that an appropriate generalization of the CTRW is a two-state random walk with different parameters appropriate to the two states. The diffusion analog to such random walks has been discussed by Bak[5] as a model for certain types of electrophoresis experiments, by Meiboom[5] in the context of NMR measurements, by Friedman and Ben-Naim[7] in the calculation of transport coefficients in electrolyte solutions, and by Giddings and Eyring and others[8–14] as a model for chromatographic processes. More recently the two-state random walk has been used by Lindenberg and Cukier[15] to study molecular rotational

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motion. Other recent applications of the ideas of the two-state walk have been made by Bedeaux *et al.*[16] and Kenkre *et al.*[17] The mathematical theory of the two-state process is summarized by Cox[18] based on the work of Smith.[19,20] In the present paper we apply Smith's results to calculate asymptotic properties of two-state random walks.

Let the probability density for a single sojourn in state i be $\psi_i(t)$, $i = 1, 2$, and let the transition densities be denoted by $p_i(\mathbf{r}, t)$, i.e., $p_i(\mathbf{r}, t)\, d^n\mathbf{r}$ is the probability that a random walker in state i makes a (vector) transition to a volume element $d^n\mathbf{r}$ centered at r in time. Our present development is for continuous random walks; the specialization to lattice random walks will be summarized later. The probability density for a displacement r during a single complete sojourn in state i of duration t will be denoted by $f_i(\mathbf{r}, t)$ and is given by

$$f_i(\mathbf{r}, t) = p_i(\mathbf{r}, t)\psi_i(t) \tag{1}$$

The CTRW discussed by earlier authors is subsumed under our more generalized model by making the particular choice

$$f_1(\mathbf{r}, t) = \delta(\mathbf{r})\, \psi(t), \qquad f_2(\mathbf{r}, t) = p(\mathbf{r})\, \delta(t) \tag{2}$$

where $p(\mathbf{r})$ is the single-step transition probability density and $\psi(t)$ is the waiting time density.

We present an exact expression for the Laplace–Fourier transform for the probability density of the position of the random walker at time t. For this expression it will be possible to derive asymptotic results for the moments, which can then be used in an application of the central limit theorem to specify the complete asymptotic distribution. Let α_i be the probability of being in state i at $t = 0$. Let $\gamma_i(t)$ be the probability density for the duration of the sojourn time of the state that starts at $t = 0$ if that state is i. This definition is necessary since if one observes a random walk that has been going on for some time in the past and the observation takes place at $t = 0$, then this time does not necessarily coincide with the beginning of a sojourn. It is known[18] that $\gamma_i(t)$ is given by

$$\gamma_i(t) = \int_t^\infty \psi_i(\tau)\, d\tau \Big/ \int_0^\infty \psi_i(\tau)\, d\tau \tag{3}$$

Similarly the conditional densities $p_i(\mathbf{r}, t)$ must be replaced by different ones for the first sojourn, but properties of these new functions will not influence asymptotic properties, so we simply denote the new conditional densities by $q_i(\mathbf{r}, t)$ without specifying them more exactly. For convenience we also define the functions

$$F_i(\mathbf{r}, t) = p_i(\mathbf{r}, t) \int_t^\infty \psi_i(\tau)\, d\tau$$
$$Q_i(\mathbf{r}, t) = q_i(\mathbf{r}, t) \int_t^\infty \gamma_i(\tau)\, d\tau \tag{4}$$

These are the conditional densities for the transition in space in time t and state i, conditional on the sojourn time being longer than t.

Let $P(\mathbf{r}, t)$ be the probability density for position at time t. We can decompose this as $P = P_1 + P_2$, where $P_i(\mathbf{r}, t)\, d^n\mathbf{r}$ is the probability that the random walker is in volume $d^n\mathbf{r}$ centered at $\mathbf{r}$ at time t in state i. Let $\omega_i(\mathbf{r}, t)\, dt$ be the probability that a sojourn in state i ends with the random walker in the volume $d^n\mathbf{r}$ during the time interval $(\tau, \tau + d\tau)$. Then P_1, for example, satisfies the integral equation

$$P_1(\mathbf{r}, t) = \alpha_1 Q_1(\mathbf{r}, t) + \int_0^t d\tau \int_{-\infty}^\infty \omega_2(\boldsymbol{\rho}, \tau) F_1(\mathbf{r} - \boldsymbol{\rho}, t - \tau)\, d^n\boldsymbol{\rho} \tag{5}$$

and $P_2(\mathbf{r}, t)$ satisfies an analogous equation. These equations contain the $\omega_i(\mathbf{r}, t)$. We can write similar equations for the $\omega_i(\mathbf{r}, t)$. For example, ω_1 satisfies

$$\omega_1(\mathbf{r}, t) = \alpha_1 k_1(\mathbf{r}, t) + \int_0^t d\tau \int_{-\infty}^\infty \omega_2(\boldsymbol{\rho}, \tau) f_1(\mathbf{r} - \boldsymbol{\rho}, t - \tau)\, d^n\boldsymbol{\rho} \tag{6}$$

where $k_i(\mathbf{r}, t)$ is $q_i(\mathbf{r}, t)\gamma_i(t)$. A similar equation is satisfied by $\omega_2(\mathbf{r}, t)$. The form of Eqs. (5) and (6) suggests the use of the Laplace–Fourier transform. Let an arbitrary function $h(\mathbf{r}, t)$ have a Laplace–Fourier transform

$$h^*(\boldsymbol{\omega}, s) = \int_0^\infty [\exp(-st)]\, dt \int_{-\infty}^{\infty} \cdots \int h(\mathbf{r}, t) \exp(i\boldsymbol{\omega} \cdot \mathbf{r})\, d^n\mathbf{r} \tag{7}$$

Then Eqs. (5) and (6), when transformed, become algebraic equations, from which it is possible to find $P^*(\boldsymbol{\omega}, s)$ in the form

$$P^*(\boldsymbol{\omega}, s) = \alpha_1 Q_1^* + \alpha_2 Q_2^* + \frac{1}{1 - f_1^* f_2^*} [\alpha_1 k_1^*(F_2^* + F_1^* f_2^*)$$
$$+ \alpha_2 k_2^*(F_1^* + F_2^* f_1^*)] \tag{8}$$

One can verify, after some algebra, that $P^*(0, s) = 1/s$.

The expression in Eq. (8) is exact, involving no approximations. When the moments of the $\psi_i(t)$ and $p_i(\mathbf{r}, t)$ and $q_i(\mathbf{r}, t)$ are finite, then $P(\mathbf{r}, t)$ must be asymptotically Gaussian in space for sufficiently large t, by an argument making use of the central limit theorem. The asymptotic form of the moments can be calculated from Eq. (8) by differentiation and the application of appropriate Tauberian arguments.

Since $P(\mathbf{r}, t)$ is asymptotically Gaussian, we need only give the first and second moments and covariance functions to specify the form completely. For simplicity we first consider the first two moments corresponding to a random walk in one spatial dimension. In order to express the results we need some notation. The moments of a function $\lambda(\mathbf{r}, t)$ with respect to $f_i(\mathbf{r}, t)$ is defined in the usual manner and will be denoted by $\langle\lambda_i\rangle$. Notice that it follows from the definition in Eq. (1) that if λ is a function *only* of t, then

$$\langle\lambda(t)\rangle_i = \int_0^\infty \lambda(t)\psi_i(t)\,dt \tag{9}$$

since the space integral is just equal to 1. We define the quantities

$$\begin{aligned}
&\langle t\rangle = \langle t\rangle_1 + \langle t\rangle_2, \qquad &&\langle x\rangle = \langle x\rangle_1 + \langle x\rangle_2 \\
&\sigma_{x,i}^2 = \langle x^2\rangle_i - \langle x\rangle_i^2, \qquad &&\sigma_x^2 = \sigma_{x,1}^2 + \sigma_{x,2}^2 \\
&\sigma_{T,i}^2 = \langle t^2\rangle_i - \langle t\rangle_i^2, \qquad &&\sigma_T^2 = \sigma_{T,1}^2 + \sigma_{T,2}^2 \\
&\rho_{XT} = \sum_{i=1}^{2} (\langle xt\rangle_i - \langle x\rangle_i\langle t\rangle_i)
\end{aligned} \tag{10}$$

The first two moments are, in the limit of $t/\langle t\rangle \to \infty$,

$$\langle x(t)\rangle \sim \langle x\rangle(t/\langle t\rangle)$$

$$\sigma^2(t) = \langle x^2(t)\rangle - \langle x(t)\rangle^2 \sim \left[\sigma_x^2 + \sigma_T^2\left(\frac{\langle x\rangle}{\langle t\rangle}\right)^2 - 2\frac{\langle x\rangle}{\langle t\rangle}\rho_{XT}\right]\frac{t}{\langle t\rangle} \tag{11}$$

It is interesting to note that in addition to the pure spatial and temporal moments, the mixed time–space correlation ρ_{XT} appears in the expression for the asymptotic variance.

As a first example of the application of this theory we calculate the mean and variance of the CTRW for which the $f_i(x, t)$ are specified in Eq. (2). For this model one can easily find that

$$\begin{gathered}
\langle x\rangle_1 = \langle x^2\rangle_1 = \langle t\rangle_2 = \langle t^2\rangle_2 = 0 \\
\langle x\rangle_2 = \langle x\rangle, \qquad \langle t\rangle_1 = \langle t\rangle, \qquad \langle x^2\rangle_2 - \langle x\rangle_2^2 = \sigma_X^2 \\
\langle t^2\rangle_1 - \langle t\rangle_1^2 = \sigma_T^2, \qquad \rho_{XT,1} = \rho_{XT,2} = 0
\end{gathered} \tag{12}$$

so that Eq. (11) implies that

$$\begin{aligned}
&\langle x(t)\rangle \sim \langle x\rangle(t/\langle t\rangle) \\
&\sigma^2(t) \sim [\sigma_x^2 + \sigma_T^2(\langle x\rangle/\langle t\rangle)^2](t/\langle t\rangle)
\end{aligned} \tag{13}$$

which are just the results given by Schlesinger[21] in a slightly different notation. A second application of the general formulas in Eq. (11) is to the calculation of statistical properties of the time spent in one of the two states. For this problem the space variable is replaced by the time spent in state 1. We can take this into account by setting

$$f_1(x, t) = \delta(x - t)\psi_1(t), \qquad f_2(x, t) = \delta(x)\psi_2(t) \tag{14}$$

Both the spatial and temporal moments corresponding to these transition densities can be expressed in terms of the moments of $\psi_1(t)$ and $\psi_2(t)$. A calculation of the relevant quantities leads to the asymptotic expressions

$$\begin{aligned} \langle x(t)\rangle &\sim \langle t\rangle_1(t/\langle t\rangle) \\ \sigma^2(t) &\sim [(\sigma_1{}^2\langle t\rangle_2{}^2 + \sigma_2{}^2\langle t\rangle_1{}^2)/\langle t\rangle^3]t \end{aligned} \tag{15}$$

with a Gaussian density. These results were first given by Takacs.[22] A final application of the general results is to the calculation of the distribution of displacement of a two-state Brownian particle in a constant field. This is a slight generalization of Giddings and Eyring's model for a molecule in a chromatographic column.[8] They assumed that one phase was stationary, i.e., the molecule was temporarily trapped, and the second was a mobile phase, in which the molecule moves at constant speed for a random time. We will assume that the transition densities are

$$f_i(x, t) = \frac{1}{(4\pi D_i t)^{1/2}} \exp\left[-\frac{(x - v_i t)^2}{4D_i t}\right] \psi_i(t), \qquad i = 1, 2 \tag{16}$$

which are characterized by two (constant) average speeds v_i and two diffusion constants D_i. For this model the general results in Eq. (11) imply in particular that

$$\begin{aligned} \langle x(t)\rangle &\sim \bar{v}t \\ \sigma^2(t) &\sim 2\bar{D}t + [\sigma_1{}^2(v_1 - \bar{v})^2 + \sigma_2{}^2(v_2 - \bar{v})^2](t/\langle t\rangle) \end{aligned} \tag{17}$$

in which $\bar{v}$ and $\bar{D}$ are defined by

$$\bar{v} = (v_1\langle t\rangle_1 + v_2\langle t\rangle_2)/\langle t\rangle, \qquad \bar{D} = (D_1\langle t\rangle_1 + D_2\langle t\rangle_2)/\langle t\rangle \tag{18}$$

and the $\sigma_1{}^2$ are variances with respect to the $\psi_i(t)$. Thus, one can define an effective diffusion constant by

$$D_{\text{eff}} = \bar{D} + (1/2)[\sigma_1{}^2(v_1 - \bar{v})^2 + \sigma_2{}^2(v_2 - \bar{v})^2]/\langle t\rangle \tag{19}$$

There are two contributions to D_{eff}; the first is a weighted average of the two diffusion constants. The second can occur even in the absence of diffusion in either of the two phases, and is due to the time in each phase being random and to a difference in convective speeds. Notice that although we have chosen the $p_i(x, t)$ to be Gaussian to obtain the results in Eqs. (17) and (19), all that is really required is that the moments be of the form

$$\int_{-\infty}^{\infty} xp_i(x, t)\, dx = v_i t, \qquad \int_{-\infty}^{\infty} x^2 p_i(x, t)\, dx = v_i^2 t^2 + 2D_i t \tag{20}$$

It is simple to generalize the preceding analysis to the multidimensional case starting from Eq. (11). When the first moments of the $\psi_i(t)$ are finite, a Tauberian argument allows us to derive the following expressions for the asymptotic values of the first two moments and covariances:

$$\begin{aligned}
&\langle x_j(t)\rangle \sim \langle x\rangle_j (t/\langle t\rangle_j)\\
&\langle x_j(t) x_l(t)\rangle - \langle x_j(t)\rangle\langle x_l(t)\rangle\\
&\quad \sim \left[\langle x_j x_l\rangle - \langle x_j\rangle\langle x_l\rangle + \sigma_T^2 \frac{\langle x_j\rangle\langle x_l\rangle}{\langle t\rangle^2} - \frac{1}{\langle t\rangle}(\langle x_j\rangle \rho_{x_l T} + \langle x_l\rangle \rho_{x_j T})\right]\frac{t}{\langle t\rangle}
\end{aligned} \tag{21}$$

generalizing Eq. (11). Both of Eqs. (11) and (21) are valid under the assumptions that the average sojourn times are finite as well as the indicated spatial averages.

Analogs of these results exist for lattice random walks both in discrete and continuous time. Let us consider the former case. Let $p_j(\mathbf{r}; n)$ be the probability of a displacement $\mathbf{r}$ in n steps in state j, and let $\psi_i(n)$ be the probability that a given sojourn in state i will consist of exactly n steps. Then the joint probability that a sojourn in state j will be of duration n, leading to a displacement $\mathbf{r}$, is $f_j(\mathbf{r}; n) = p_j(\mathbf{r}; n)\psi_i(n)$, analogous to Eq. (1). We may also define the analogs to Eq. (4) as

$$F_j(\mathbf{r}; n) = p_j(\mathbf{r}; n) \sum_{m=n}^{\infty} \psi_j(m), \qquad G_j(\mathbf{r}; n) = g_j(\mathbf{r}; n) \sum_{m=n}^{\infty} \gamma_j(m) \tag{22}$$

It will prove convenient later to define single-step transition probabilities $q_j(\mathbf{r})$ and $h_j(\mathbf{r})$ corresponding to the n-step probabilities $p_j(\mathbf{r}; n)$ and $g_j(\mathbf{r}; n)$, respectively, together with the generating functions

$$\begin{aligned}
q_j^*(\boldsymbol{\theta}) &= \sum_{r_1} \cdots \sum_{r_n} q_j(\mathbf{r}) \exp(i\mathbf{r}\cdot\boldsymbol{\theta})\\
h_j^*(\boldsymbol{\theta}) &= \sum_{r_1} \cdots \sum_{r_n} h_j(\mathbf{r}) \exp(i\mathbf{r}\cdot\boldsymbol{\theta})
\end{aligned} \tag{23}$$

It is well known that these allow us to express the $p_j(\mathbf{r}; n)$ as

$$p_j(\mathbf{r}; m) = \frac{1}{(2\pi)^n} \int_{-\pi}^{\pi} \cdots \int [q_j^*(\boldsymbol{\theta})]^m \exp(-i\mathbf{r}\cdot\boldsymbol{\theta})\, d^n\boldsymbol{\theta} \tag{24}$$

with a similar expression for the $g_j(\mathbf{r}; n)$. Rather than working with Fourier–Laplace transforms as we have earlier, we use the joint generating functions

$$a^*(\boldsymbol{\theta}; z) = \sum_{r_1=-\infty}^{\infty} \cdots \sum_{r_n=-\infty}^{\infty} \sum_{m=0}^{\infty} a(\mathbf{r}; m) z^m \exp(i\mathbf{r}\cdot\boldsymbol{\theta}) \tag{25}$$

The joint generating function is then given by $P^*(\boldsymbol{\theta}; z)$, which is expressed in terms of the component functions as in Eq. (8) except that the continuous transforms there are replaced by generating functions. In particular, if we know the generating function corresponding to the $\psi_i(n)$, i.e.,

$$\Psi_j(z) = \sum_{m=0}^{\infty} \psi_j(m) z^m \tag{26}$$

then $f_j^*(\boldsymbol{\theta}; z)$ is just

$$f_j^*(\boldsymbol{\theta}; z) = \Psi_j(zq_j^*(\boldsymbol{\theta})) \tag{27}$$

This identity is derived by combining Eqs. (23)–(26).

The asymptotic results in Eq. (11) are valid also for lattice random walks, as can be verified by an analysis similar to that given for the continuous case. However, we can also derive results of specific interest in the theory of lattice random walks. Any asymptotic properties of the random walk will depend only on properties of the integral

$$Q(\mathbf{r}; z) = \frac{1}{(2\pi)^n} \int_{-\pi}^{\pi} \cdots \int \frac{\alpha_1 k_1^*(F_2^* + \Psi_2^* F_1^*) + \alpha_2 k_2^*(F_1^* + \Psi_1^* F_2^*)}{1 - \Psi_1^* \Psi_2^*} \times \exp(-i\boldsymbol{\theta}\cdot\mathbf{r})\, d^n\boldsymbol{\theta} \tag{28}$$

where

$$F_j^* = \frac{1 - zq_j^*(\boldsymbol{\theta})\Psi_j(zq_j^*(\boldsymbol{\theta}))}{1 - zq_j^*(\boldsymbol{\theta})}$$

$$k_j^* = \sum_{\mathbf{r}} \sum_{m=0}^{\infty} g_j(\mathbf{r}; m)\gamma_j(m) z^m \exp(i\mathbf{r}\cdot\boldsymbol{\theta}) \tag{29}$$

Equation (28) is the discrete analog of the inverse to Eq. (8), except for the first two terms, which do not contribute to any asymptotic properties when the $\gamma_i(n)$ have finite first moments. The probability that a random walk starting from the origin will eventually return to the origin is equal to one when

$$\lim_{z=1} Q^*(\mathbf{0}, z) = \infty \tag{30}$$

and is less than one otherwise. The integrand in Eq. (28) is or is not integrable depending on the dimension d and the singularity at $\boldsymbol{\theta} = 0, z = 1$.

We make the assumptions that the $q_j(\mathbf{r})$ are symmetric about $\mathbf{r} = \mathbf{0}$ since otherwise the question of return to the origin is not an interesting one. We also assume that the moments $\sigma_l^2(j) = \sum_{r_1} \cdots \sum_{r_n} r_l^2 q_j(\mathbf{r})$ are finite and that the two mean sojourn times $\langle m \rangle_1$ and $\langle m \rangle_2$ are finite. When these two conditions are fulfilled we can expand $\Psi_i^*(u)$ around $u = 1$ as

$$\Psi_i^*(u) = 1 - \langle m \rangle_i (1 - u) + O[(1 - u)] \tag{31}$$

and $q_j^*(\boldsymbol{\theta})$ as

$$q_j^*(\boldsymbol{\theta}) = 1 - \tfrac{1}{2} \sum_l \sigma_l^2(j) \theta_l^2 + O(|\boldsymbol{\theta}|^2) \tag{32}$$

Hence an expansion of the denominator in Eq. (28) yields

$$1 - \Psi_1^* \Psi_2^* \sim \langle m \rangle \Big(1 - z + \tfrac{1}{2} \sum_{l=1}^{n} \overline{\sigma_l^2} \theta_l^2\Big) \tag{33}$$

where

$$\langle m \rangle = \langle m \rangle_1 + \langle m \rangle_2, \qquad \overline{\sigma_l^2} = [\langle m \rangle_1 \sigma_l^2(1) + \langle m \rangle_2 \sigma_l^2(2)]/\langle m \rangle \tag{34}$$

But the expression in Eq. (33) is of the same form as that for the single-state random walk, so that for the two-state random walk return to the origin is certain in one and two dimensions, and occurs with some probability less than one in three or more dimensions. It also follows that for this case the dependence of such quantities as the average number of points visited and the average number of times a given lattice point is visited in an m-step walk is the same as for a single-state random walk, except that the quantity σ_l^2 that appears in formulas for these quantities in the one-state random walk is to be replaced by $\overline{\sigma^2}$ as defined in Eq. (34).

Two generalizations of this work suggest themselves. The first, a relatively simple one that leads to a complicated algebraic development, allows for the possibility of $n \geqslant 3$ states. This generalization can be set up in terms of Markov renewal processes[23] in which one describes the transitions between states by a Markov chain. The two-state problem allows only the transition matrix

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

but the formalism to allow for more general transition matrices is easily developed. A second generalization is one in which the sojourn time densities have infinite first moments so that the asymptotic results given in Eq. (11) are not valid.

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