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Isotropization time for non-Markovian CTRWs

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Abstract

We calculate the mean-squared displacement, $\langle r^2(t)\rangle$, for a CTRW taking into account effects of anisotropic turn angles. When the pausing-time density is a negative exponential one finds a simple expression for $\langle r^2(t)\rangle$ which allows an exact determination of the transition time from ballistic to diffusive motion. In the non-Markovian case an exact expression is obtained for the Laplace transform of $\langle r^2(t)\rangle$. The results are useful in the analysis of photon migration in a turbid medium.

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1. Introduction

One phenomenological theory that accounts for a number of properties of material transport in a disordered medium is based on the continuous-time random walk (CTRW) [1,2]. Over the years many useful properties and appplications have been developed for the simplest formulation of these random walks when successive steps of the walk are uncorrelated. However, applications to the theory of photon transport in turbid media suggest that the standard CTRW model should be extended to incorporate anisotropic scattering and, in particular, to determine the times at which anisotropy becomes unimportant so that the much simpler diffusion model can be used. An analysis of CTRWs with persistence was first given in the context of a model for bacterial motion on a surface [3]. The general problem of the anisotropic CTRW has been discussed by Gandjbakhche et al. [4] for discrete time models and by Weiss et al. [5] for a continuous time model, [5]. Both of these treatments examined points related to models for the migration of photons in turbid media with applications to determining optical properties of human tissue [6]. The isotropization problem is amenable to

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analysis because one need only consider the behavior of the second moment of displacement, and determine the time at which the mean-squared displacement $\langle \mathbf{r}(t)\cdot\mathbf{r}(t)\rangle$ makes a transition from ballistic behavior (in which it is proportional to t^2) to diffusive behavior in which it is proportional to t. Ref. [5] was flawed in not properly accounting for correlations in passing from discrete to continuous time. In this note we correct this error as well as discuss the behavior of the second moment for a more general class of CTRWs in which the pausing-time density is asymptotically proportional to a stable-law density.

2. Analysis

We discuss a model in which a random walker moves along straight lines until interrupted by scattering events at times t_1, t_1+t_2, $t_1+t_2+t_3$, etc. At each scattering event the walker changes the direction in which it is moving according to a specified probability density. Our analysis will be restricted to a situation in which the first direction in which the walker moves in d dimensions is uniformly distributed over the d-dimensional unit sphere. We will show from a calculation of the mean-squared displacement that the only function needed to characterize persistence is $g \equiv \langle \cos\theta \rangle$ where θ is the turn angle in a single step, and where the average is taken with respect to a probability density of turn angles, $p(\theta)$. When the random walk is isotropic this average is equal to zero. Rotations around a single step will be assumed to be uniformly distributed, thus being equivalent to the standard Markov model of polymer configurations [7], except that we here consider the CTRW in d dimensions and that the step lengths are not necessarily equal as they are in most polymer models. The pausing-time density or probability density for the times between successive scattering events will be denoted by $\psi(t)$ with $\hat{\psi}(s) = \int_0^\infty e^{-st}\psi(t)\,dt$. The probability density for the time to the nth scattering event will be denoted by $\psi_n(t)$. Motion along any straight line segment will be assumed made with a constant velocity, which we set equal to 1. An argument that is standard in random walk theory shows that $\mathscr{L}\{\psi_n(t)\} = \hat{\psi}^n(s)$ and $\mathscr{L}\{\Psi(t)\} = [1-\hat{\psi}(s)]/s$. These results will be used in our later analysis.

The assumptions made so far allow us simplify all calculations by considering only the behavior of the projection along a single axis which we shall take to be the x-axis. Because of the assumed initial isotropy we can assert that $\langle x(t)\rangle = 0$ and $\langle r^2(t)\rangle = d\,\langle x^2(t)\rangle$ which means that we can restrict our analysis to a calculation of $\langle x^2(t)\rangle$. Let $\langle x^2(t|m,\tau)\rangle$ be the mean-squared displacement in time t conditioned on the number of turns made being equal to m and on the duration of the interval between the time of the last scattering event before time t. The time of this scattering event will be denoted by τ. The unconditional mean-squared displacement can then be expressed as

$$\langle x^2(t)\rangle = \sum_{m=1}^{\infty}\int_0^t \langle x^2(t|m,\tau)\rangle\,\psi_{m-1}(\tau)\Psi(t-\tau)\,d\tau\,, \qquad (1)$$

where, by convention, $\psi_0(t) = \delta(t)$. The random variable $x(t|m,\tau)$ can be written as the sum

$$x(t|m,\tau) = \sum_{i=1}^{m-1} x_i(t_i) + x_m(t-\tau)\,, \tag{2}$$

where $x_i(t_i)$ is the displacement along the x-axis between the $(i-1)$st and ith turn, and where $x_m(t-\tau)$ is the final displacement between the mth turning point, τ, and time t. When $m=1$ the sum in Eq. (2) is set equal to 0. The last interval, $t-\tau$, is treated differently from the remaining ones since it is not terminated by a scattering event. Therefore, $x_m(t-\tau)$ is distributed differently from the remaining $x_i(t_i)$ except in the case of the negative exponential pausing time density $\psi(t) = T^{-1}\exp(-t/T)$. In the analysis to follow we refer to $x_i(t_i)$ as x_i where the argument t_i is implied.

The conditional mean-squared displacement $\langle x^2(t|m,\tau)\rangle$ will be calculated by squaring the sum in Eq.(2). Our exposition is couched in the language of the two-dimensional CTRW for simplicity of notation, but an elementary geometric argument leads to the same results in higher dimensions. The projection along the x-axis in step i is $x_i = t_i\cos(\phi_1+\beta_i)$ in which ϕ_1 is the angle made by the first step with the x-axis, and $\beta_1 = 0$, $\beta_i = \theta_1+\theta_2+\cdots+\theta_{i-1}$ $(i\geqslant 2)$ is the sum of the angles between successive straight-line segments of the random walk. By our assumption that the initial condition is isotropic the angle ϕ_1 is uniformly distributed in $(-\pi,\pi)$ while the θ's take on values according to the probability density $p(\theta)$. In calculating individual components of $\langle x^2(t|m)\rangle$, we will need to distinguish between correlations of the form $\langle x_i x_j\rangle$ where $i,j\neq m$ and cases in which one or both of them do refer to the final step of the random walk.

In writing the detailed expression for $\langle x^2(t|m,\tau)\rangle$ in terms of its components we will initially treat m and τ as fixed, and, at the final step, average over these variables. Denote $\cos(\phi_1+\beta_i)$ by c_i. The relation between individual steps of the random walk and $\langle x^2(t|m,\tau)\rangle$ can be written in terms of these variables as

$$\begin{aligned}\langle x^2(t|m,\tau)\rangle &= \sum_{i=1}^{m-1}\langle t_i^2(m,\tau)\rangle\langle c_i^2\rangle + 2\sum_{i=1}^{m-1}\sum_{j<i}\langle t_i(m,\tau)t_j(m,\tau)\rangle\langle c_i c_j\rangle \\ &\quad + \tau^2\langle c_m^2\rangle + 2\tau\sum_{i=1}^{m-1}\langle t_i(m,\tau)\rangle\langle c_i c_m\rangle\,.\end{aligned} \tag{3}$$

The time averages are to be made with respect to the appropriate modification of $\psi(t)$ and the averages of the c's are to be taken with respect to $p(\theta)$ and the uniform distribution of ϕ_1. Specific expressions for the angular averages are readily found to be

$$\langle c_i^2\rangle = \tfrac{1}{2},\quad \sum_{i=1}^{m-1}\sum_{j<i}\langle c_i c_j\rangle = \frac{g}{2(1-g)}\left(m - \frac{1-g^m}{1-g}\right), \tag{4}$$

$$\langle c_i c_m\rangle = \frac{g(1-g^m)}{2(1-g)}\,.$$

The calculation of $\langle x^2(t|m,\tau)\rangle$ requires not only finding averages over the set of angles but also averages over time as indicated in Eq. (3). Observe that the $\langle t_i(m,\tau)t_j(m,\tau)\rangle$ do not depend on i and j, and let $C(m,\tau)$ be the correlation function $\langle t_i(m,\tau)t_j(m,\tau)\rangle$ when $i \neq j$. The expression for the conditioned mean-squared displacement in terms of these variables is

$$\begin{aligned}\langle x^2(t|m,\tau)\rangle = \frac{m}{2}\langle t^2(m,\tau)\rangle + C(m,\tau)\frac{g}{1-g}\left(m - \frac{1-g^m}{1-g}\right) \\ +\frac{\tau^2}{2} + \langle t(m,\tau)\rangle \tau g\left(\frac{1-g^m}{1-g}\right).\end{aligned} \tag{5}$$

The conditional time averages that appear in this equation are calculated in terms of inverse transforms of the $\hat{\psi}_n(s)$ and their derivatives. Detailed derivations are given in the appendix. Define the transforms

$$\hat{f}_n(s) = [\hat{\psi}(s)]^{n-2}[\hat{\psi}'(s)]^2, \qquad \hat{h}_n(s) = [\hat{\psi}(s)]^{n-1}(s)\hat{\psi}''(s), \tag{6}$$

where the primes indicate derivatives with respect to s with inverse transforms $h_n(t)$ and $f_n(t)$, respectively. One then finds

$$\begin{aligned}&\langle t(m,\tau)\rangle = (t-\tau)/m, \ \langle t^2(m,\tau)\rangle = h_m(t-\tau)/\psi_m(t-\tau), \\ &C(m,\tau) = f_m(t-\tau)/\psi_m(t-\tau),\end{aligned} \tag{7}$$

which are to be incorporated into Eq. (5).

As mentioned, the most convenient approach to calculating properties of the unconditional mean-squared displacement, $\langle x^2(t)\rangle$, is in terms of Laplace transforms since the transforms $\hat{\psi}_n(s)$, $\hat{h}_n(s)$, and $\hat{f}_n(s)$ are proportional to the powers of $\hat{\psi}(s)$ and its derivatives. On substituting Eq. (7) into Eq. (5) and the result into Eq. (3) one finds that the Laplace transform of the sum can be evaluated in closed form since it reduces to the evaluation of geometric sums. The final result for the transform $\mathscr{L}\{\langle x^2(t)\rangle\}$ is

$$\mathscr{L}\{\langle x^2(t)\rangle\} = \frac{1}{s^3} + \frac{\hat{\psi}'(s)}{s^2}\left\{\frac{1}{1-\hat{\psi}(s)} - \frac{g}{1-g\hat{\psi}(s)}\right\}. \tag{8}$$

If the sums in the denominators in the bracketed terms are again expanded then the transform can be inverted to yield a formal expansion having the form

$$\begin{aligned}\langle x^2(t)\rangle &= \frac{t^2}{2} - \sum_{n=1}^{\infty}\frac{1-g^n}{n}\int_0^t (t-\tau)\tau\psi_n(\tau)\,d\tau \\ &= \langle x^2(t)\rangle_0 + \sum_{n=1}^{\infty}\frac{g^n}{n}\int_0^t (t-\tau)\tau\psi_n(\tau)\,d\tau,\end{aligned} \tag{9}$$

where $\langle x^2(t)\rangle_0$ is the mean-squared displacement with $g = 0$. The form of the last line of Eq. (9) confirms the obvious requirement that when $g > 0$, $\langle x^2(t)\rangle$ should be greater than $\langle x^2(t)\rangle_0$. When $\psi(t)$ is the negative exponential $\psi(t) = (1/T)\exp(-t/T)$ so that $\hat{\psi}(s) = (1+sT)^{-1}$ the transform in Eq. (8) can be inverted, yielding

$$\langle x^2(t)\rangle = \frac{2T^2}{d(1-g)^2}\left\{(1-g)\frac{t}{T} - 1 + e^{-(1-g)t/T}\right\}, \tag{10}$$

where d is the number of dimensions. This also follows from the formal expansion in Eq. (9). Because of the preferential scattering the short time behavior of $\langle x^2(t)\rangle$ is proportional to t^2 which is ballistic motion, and at later times there is a transition to diffusive motion. The cross-over time is of the order of $T/(1-g)$. The formula given in Eq. (10) reduces to the two-dimensional result found in [8] for a model in which the turn-angle density $p(\theta)$ was chosen to be

$$p(\theta) = \frac{1}{2\pi} + 2\varepsilon\cos\theta, \quad |\varepsilon| \leqslant \frac{1}{4\pi} \tag{11}$$

so that $g = 2\pi\varepsilon$.

Since Eq. (8) is exact we can use it to derive the behavior of $\langle x^2(t)\rangle$ at long times in terms of moments of $\psi(t)$. If the first two moments of this density are finite–the mean T and the variance, σ^2–then the long-time form for $\langle x^2(t)\rangle$ is found to be

$$\langle x^2(t)\rangle \approx \frac{(1+g)T^2 + (1-g)\sigma^2}{d(1-g)}\frac{t}{T}. \tag{12}$$

When $\psi(t)$ has an asymptotic stable-law form the effects of persistence are secondary to those induced by the pausing-time density. For example, in one dimension if $\psi(t)$ has the asymptotic property $\psi(t) \approx t^{-(2+\alpha)}$with $0 < \alpha < 1$ it follows that as $s \to 0$, [2],

$$\hat{\psi}(s) \approx 1 - sT + (s\mu)^{\alpha+1}, \tag{13}$$

where T and μ are constants with the dimensions of time. This, together with Eq. (8), implies that at long times

$$\langle x^2(t)\rangle \approx \frac{\alpha\mu^3}{\Gamma(3-\alpha)T}\left(\frac{t}{\mu}\right)^{2-\alpha} \tag{14}$$

which is the same as found in [9] and clearly independent of g. Similarly, if $\psi(t) \approx t^{-(1+\alpha)}$ at long times one obtains a result for $\langle x^2(t)\rangle$ that is approximately equal to $(1-\alpha)t^2/2$ which is independent of g.

We have also carried out similar calculations to derive an expression for the fourth moment, but because of its complicated form do not present it here. It differs from the result for the second moment in requiring $\langle\cos 2\theta\rangle$ in addition to the parameter g.

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Appendix. Calculation of the correlation functions

To find the form of correlation functions for the scattering times we first calculate the joint probability densities for two arbitrary interscattering intervals t_i and t_j $(j > i)$ under the conditions specified in the text. The indicated function will be denoted by $p(t_i, t_j, \tau; m)$. Knowing this function allows us to calculate the conditional densities $p(t_i, t_j|\tau, m)$ from which we can find the correlation functions that appear in Eq. (3) above.

For the purpose of calculating $p(t_i, t_j, \tau; m)$ we will define two times T and T' where T is the time till the ith scattering event, i.e., $T = t_1 + t_2 + \cdots + t_{i-1}$ and T' is the time between the ith and the jth scattering event. It follows from these definitions that the duration of the interval between the time of the scattering event immediately preceding time t and time t itself satisfies the inequality

$$t - \tau \leqslant t - (T + T' + t_i + t_j)\,. \tag{A.1}$$

Remembering that $\psi_n(t)$ is the probability density for the sum of n steps, and that the interscattering times are identically distributed, we can write an expression for $p(t_i, t_j, \tau; m)$ in terms of these functions as

$$p(t_i, t_j, \tau; m) = \psi(t_i)\psi(t_j)\psi_{m-2}(t - \tau - t_i - t_j)\Psi(\tau)\,. \tag{A.2}$$

Hence, as a consequence of the identity

$$\int_0^{t-\tau} dt_i \int_0^{t-\tau-t_i} dt_j\, p(t_i, t_j, \tau; m) = \psi_m(t - \tau)\Psi(\tau) \tag{A.3}$$

it follows that

$$p(t_i, t_j|\tau, m) = \psi(t_i)\psi(t_j)\frac{\psi_{m-2}(t - \tau - t_i - t_j)}{\psi_m(t - \tau)}\,. \tag{A.4}$$

The conditional density describing a single interscattering time is similarly found to be

$$p(t_i|\tau, n) = \psi(t_i)\frac{\psi_{n-1}(t - \tau - t_i)}{\psi_n(t - \tau)}\,. \tag{A.4}$$

The results in Eqs. (A.4) and (A.5) can be utilized to find the conditional correlation $C(m, \tau)$ appearing in Eq. (5). We find for this function

$$C(m, \tau) = \int_0^{t-\tau} t_i\, dt_i \int_0^{t-\tau-t_i} t_j\, p(t_i, t_j|\tau, m)\, dt_j\,. \tag{A.6}$$

If the formula in Eq. (A.4) is substituted into this equation and use is made of the identity

$$\int_0^\infty t\psi(t)e^{-st}\,dt = -\hat{\psi}'(s)\,, \tag{A.7}$$

one finds that

$$\mathscr{L}\{f_n(t)\} = \hat{\psi}_{n-2}(s)[\hat{\psi}'(s)]^2 \tag{A.8}$$

as given in Eq. (6). A similar calculation based on Eq. (A.5) yields the second part of Eq. (6). Finally, since the t_i, $i < m$, are identically distributed random variables we can immediately assert that

$$\langle t(m,\tau)\rangle = \frac{t-\tau}{m}\,. \tag{A.9}$$

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