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Discrete versus Continuous-Time Random Walks

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The results obtained on the basis of discrete and continuous-time random walk models on a finite chain are compared with one another in problems such as longitudinal dispersion and the spectrum of a random oscillator. In these applications, discrete and continuous-time models cannot be used interchangeably.

KEY WORDS: Random walk; dispersion; spectrum.

1. INTRODUCTION

The theory of random walks has a long history, starting with the pioneering work of Einstein on Brownian motion.[1] Different descriptions of Brownian motion have been put forward, depending on whether time and/or space are treated as discrete or continuous variables.[2,3] This choice is often made on the basis of convenience, e.g., discrete models are conceptually simpler, possibly more transparent, and more suitable for numerical calculation, whereas the analytic results for continuous models are often considerably simpler.

In this paper we discuss the differences that may show up (and prevail, even in the long-time limit) between discrete and continuous-time random walks on a finite chain in applications such as longitudinal dispersion and the spectrum of a random oscillator. In these applications, both discrete and continuous-time models have been used. These models do not give the same results because fluctuations play an important if not dominant role in the above examples. The purpose of this paper is to calculate these differences in an explicit way. To do so, we consider a discrete-time random walk that encompasses both the case of fixed residence times and

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exponentially distributed ones as limiting cases, namely one in which the residence time between jumps is a binomial distribution. On this basis the differences between discrete and continuous time can be easily discussed. Most of the results for the continuous-time case have been given in previous papers[4–6] and are recovered in the appropriate limit.

The discussion of a discrete-time model is, apart from its academic interest and relevance to numerical experiments, also of direct importance in applications where the "time variable" is essentially discrete. An application of this type from polymer physics illustrates this point.

The paper is organized as follows. The general mathematical setup is presented in Section 2, while the specific applications, dispersion and the random oscillator, are discussed in Sections 3 and 4, respectively. All these results are valid asymptotically for large times. Some results valid for all time are derived in Section 5 and an application to polymer physics is given.

2. PRESENTATION OF THE PROBLEM

We will formulate the problem in the context of the so-called "generalized Taylor dispersion"[7] or "composite stochastic processes."[8] We consider a system with N internal states i, $i = 1,..., N$, and an external real coordinate x. The time evolution of the external variable is, for simplicity, taken to be deterministic, but monitored by the internal state:

$$\partial_t x = u_i \tag{1}$$

u_i is the rate of change of x while in the state i. At the same time and independently, the system performs a random walk over its internal states. As far as the modeling of these internal states is concerned, we will restrict ourselves to a linear set of N states i, $i = 1,..., N$, between which nearest neighbor transitions occur. The system stays a fixed time step Δt in a site i, after which it jumps with probabilities $\alpha_i^{\pm}$ to the sites $i \pm 1$, or it stays for another time step Δt in the same site with probability

$$\alpha_i^0 = 1 - \alpha_i^+ - \alpha_i^- \tag{2}$$

The residence time per visit of a state is then a binomial probability distribution. The cumulative probability is a step function of the form

$$P(t_{\text{residence}} > n\,\Delta t) = [1 - (k_i^+ + k_i^-)\,\Delta t]^n \tag{3}$$

where we introduced the transition rates $k_i^{\pm} = \alpha_i^{\pm}/\Delta t$. The average residence time in site i is found to be $(k_i^+ + k_i^-)^{-1}$. In the limit $\Delta t \to 0$, an exponential residence time distribution is recovered.

The equation of evolution for the probability $P(x, i, n)$ to be at the position x in site i at the end of the nth time step (i.e., at time $t = n\,\Delta t$) reads

$$\begin{aligned} P(x, i, n) = {} & P(x - u_i\,\Delta t, i, n-1)(1 - \alpha_i^+ - \alpha_i^-) \\ & + P(x - u_i\,\Delta t, i-1, n-1)\,\alpha_{i-1}^+ \\ & + P(x - u_i\,\Delta t, i+1, n-1)\,\alpha_{i+1}^- \end{aligned} \tag{4}$$

The particular case $\alpha_i^0 = 1 - \alpha_i^+ - \alpha_i^- = 0$ covers the situation of the usual discrete-time random walk in which the system always spends a fixed time Δt between two jumps. On the other hand, a continuous-time random walk, with exponential residence times between the jumps, is obtained in the following limit:

$$n \to \infty,\ \Delta t \to 0,\ \alpha_i^\pm \to 0 \qquad \text{with} \qquad n\,\Delta t = t,\ \alpha_i^\pm / \Delta t = k_i^\pm \text{ fixed} \tag{5}$$

In this limit, the evolution equation (4) becomes

$$\begin{aligned} \partial_t P(x, i, t) = {} & -\frac{\partial}{\partial x} u_i P(x, i, t) + k_{i-1}^+ P(x, i-1, t) \\ & + k_{i+1}^- P(x, i+1, t) - (k_i^+ + k_i^-)\,P(x, i, t) \end{aligned} \tag{6}$$

Let us now discuss the quantities of interest in the physical applications. In the dispersion problem, we are interested in the reduced probability

$$P(x, n) = \sum_{i=1}^{N} P(x, i, n) \tag{7}$$

It will be shown that $P(x, n)$ is asymptotically (i.e., in the long-time, large-n limit) Gaussian. The two important quantities to be evaluated are then the average value $\langle x(t) \rangle$ and the dispersion $\langle [x(t) - \langle x(t) \rangle]^2 \rangle = \langle \delta x^2(t) \rangle$.

In the random oscillator problem, the x variable plays the role of the phase of the oscillator. Each internal state i corresponds to a site with different rotation frequency u_i. The oscillators are started in phase at the initial time, say $x(t=0) \equiv 0$. Since each oscillator performs another realization of the random walk over the internal states, this phase coherence gradually gets lost. This depolarization is described by the following average[9,10]:

$$\phi(t) = \langle \exp[ix(t)] \rangle \tag{8}$$

Again, this average can be evaluated in the long-time limit. This limit covers effectively a large, if not the entire time domain in the case of fast modulation.

The solution to the above problems in the continuous-time case has been given for reflecting boundary conditions in Ref. 4 (dispersion) and Ref. 5 (random oscillator). Periodic boundary conditions are discussed in Ref. 6. All these results will be recovered in the continuous-time limit.

3. LONGITUDINAL DISPERSION

In longitudinal dispersion the velocity of a particle is determined by its internal state. As the particle wanders over these states, it loses memory of its previous visits, hence of its previous velocity. Consequently, the velocity correlation function decays to zero and, on a sufficiently long time scale, the particle's motion in the x direction can be thought of as the result of a large number of uncorrelated displacements. In view of the central limit theorem, it is thus no surprise to find that x is asymptotically a Gaussian random variable. The proof of the Gaussian nature of x for large time is along lines similar to that for the continuous-time case[4] and will be omitted here. The first two moments $\langle x \rangle$ and $\langle \delta x^2 \rangle$ are most easily expressed in terms of the steady state distributions p_i^{st}. These are the steady-state probabilities to find a particle in state i. For simplicity, we will assume that the latter obey the detailed balance condition:

$$k_i^+ p_i^{\mathrm{st}} = k_{i+1}^- p_{i+1}^{\mathrm{st}} \tag{9}$$

where the transition rates $k_i^{\pm}$ are defined in (5).

Note that this condition is automatically satisfied in the case of reflecting boundary conditions. In general, it implies the following relation between forward and backward rates[11]:

$$\prod_{i=1}^{N} k_i^+ = \prod_{i=1}^{N} k_i^- \tag{10}$$

The explicit expression for the steady-state probabilities then reads

$$p_i^{\mathrm{st}} = Z k_1^+ \cdots k_{i-1}^+ k_{i+1}^- \cdots k_N^- \tag{11}$$

with Z a normalization constant.

Let us now state the results. We have (cf. Appendix)

$$\lim_{n \to \infty} \frac{\langle x(n) \rangle}{n \, \Delta t} = \bar{u} \tag{12}$$

$$\lim_{n \to \infty} \frac{\langle \delta x^2(n) \rangle}{2n \, \Delta t} = K \tag{13}$$

with

$$\bar{u} = \sum_{i=1}^{N} u_i p_i^{st} \tag{14}$$

and

$$K = \frac{\sum_{r=1}^{N} \sum_{s=1}^{N} \{[\sum_{i=1}^{r} (u_i - \bar{u}) p_i^{st} - \sum_{j=1}^{s} (u_j - \bar{u}) p_j^{st}]^2 / k_r^+ p_r^{st} k_s^+ p_s^{st}\}}{2 \sum_{q=1}^{N} (1/k_q^+ p_q^{st})}$$

$$+ \frac{\Delta t}{2} \sum_{i=1}^{N} (\bar{u}^2 - u_i^2) p_i^{st} \tag{15}$$

Equation (15) is one of the central results of this paper. The effective dispersion coefficient is the sum of two terms. The first term is identical to the expression for the dispersion coefficient in the continuous-time case. The second term is a negative contribution, which is due to the discrete nature of the time process. Dispersion is thus smaller in a discrete-time random walk then in the continuous-time case. Note that this contribution persists even though we are considering here asymptotic time properties.

As was already discussed in detail in Ref. 6, the case of a reflecting boundary (at the states $i = 1$ and $i = N$) can be obtained by letting k_1^- and k_N^+ go to zero with constant ratio:

$$k_1^- p_1^{st} / k_N^+ p_N^{st} = 1 \tag{16}$$

In this limit, we obtain[6]

$$K = \sum_{r=1}^{N-1} \frac{[\sum_{i=1}^{r} (u_i - \bar{u}) p_i^{st}]^2}{k_r^+ p_r^{st}} + \frac{\Delta t}{2} \sum_{i=1}^{N} (\bar{u}^2 - u_i^2) p_i^{st}$$

(reflecting boundary conditions) (17)

In order to evaluate the importance of the term proportional to Δt, we consider the simple $N = 2$ model that has been proposed as a model for chromatography.[12] For

$$p_1^{st} = \frac{k_2}{k_1 + k_2}, \qquad p_2^{st} = \frac{k_1}{k_1 + k_2} \tag{18}$$

we obtain from (17)

$$K = \frac{k_1 k_2 (u_1 - u_2)^2}{(k_1 + k_2)^3} \left[1 - \frac{1}{2} (k_1 + k_2) \Delta t \right] \tag{19}$$

We conclude that the effect of time discreteness is small when Δt is smaller then the typical time $(k_1+k_2)^{-1}$ of the transitions between the states. On the other hand, the dispersion becomes zero for $\alpha_1 = k_1/\Delta t = 1$ and $\alpha_2 = k_2/\Delta t = 1$.

An alternative way for writing the results (15) is as follows:

$$K = \sum_{i=1}^{N} \sum_{j=1}^{N} M_{ij} u_i u_j \tag{20}$$

with

$$M_{ij} = \left[\sum_{r=1}^{N} \sum_{s=1}^{r-1} \frac{\sum_{k=s+1}^{r} \sum_{l=s+1}^{r} (p_i^{\mathrm{st}} - \delta_{ik})(p_j^{\mathrm{st}} - \delta_{jl})\, p_k^{\mathrm{st}}\, p_l^{\mathrm{st}}}{k_r^+\, p_r^{\mathrm{st}} k_s^+\, p_s^{\mathrm{st}}} \right] \times \left(\sum_{q=1}^{N} \frac{1}{k_q^+\, p_q^{\mathrm{st}}} \right)^{-1} + \frac{\Delta t}{2} (p_i^{\mathrm{st}}\, p_j^{\mathrm{st}} - \delta_{ij}\, p_j^{\mathrm{st}}) \tag{21}$$

The advantage of this way of writing K becomes clear by noticing that [for $x(0) = 0$]

$$x(n) = \sum_{i=1}^{N} \tau_i(t) u_i \tag{22}$$

where $\tau_i(t)$ is the accumulated resdence time in state i. From (22), we conclude that

$$\langle x(n) \rangle = \sum_{i=1}^{N} \langle \tau_i(t) \rangle u_i \tag{23}$$

and

$$\langle \delta x^2(n) \rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} \langle \delta\tau_i(t)\, \delta\tau_j(t) \rangle\, u_i u_j \tag{24}$$

By comparison with (14) and (21) it follows that

$$\lim_{n \to \infty} \frac{\langle \tau_i(t) \rangle}{n\, \Delta t} = p_i^{\mathrm{st}} \tag{25}$$

$$\lim_{n \to \infty} \frac{\langle \delta\tau_i(t)\, \delta\tau_j(t) \rangle}{2n\, \Delta t} = M_{ij} \tag{26}$$

Note also that the property $\sum_{i=1}^{N} \delta\tau_i = 0$ implies that

$$\sum_{i=1}^{N} M_{ij} = 0 \tag{27}$$

For the particular case $k_i^{\pm} \equiv k$ and $p_i^{\mathrm{st}} = 1/N$ we have

$$M_{ij} = \frac{1}{6kN^2}\left[\frac{N^2-1}{2} + 3(i-j)^2 - 3N|i-j|\right] + \frac{\Delta t}{2N^2}(1 - N\delta_{ij}) \tag{28}$$

For reflecting boundary conditions ($k_i^{\pm} \equiv k$ except for $k_1^- = k_N^+ = 0$), one finds

$$M_{ij} = \frac{1}{6kN^2}\left[(N+1)(2N+1) + 3(i^2+j^2) - 3(N+1)(i+j) - 3N|i-j|\right] + \frac{\Delta t}{2N^2}(1 - N\delta_{ij}) \tag{29}$$

These results can be used to discuss the random oscillator problem.

4. THE RANDOM OSCILLATOR

In order to evaluate the depolarization function (8), we rewrite it in terms of the random variables $\tau_k(t)$ introduced in the previous section, as follows[13]:

$$\phi(t) = \left\langle \exp\left[i \sum_{k=1}^{N} \tau_k(t)\, u_k \right] \right\rangle \tag{30}$$

Furthermore, we will assume, not unreaistically,[13] that the frequencies u_k are independent Gaussian random variables with average value taken to be zero and dispersion ω_F^2:

$$\langle u_k u_l \rangle_F = \omega_F^2\, \delta_{k,l}^{\mathrm{Kr}} \tag{31}$$

The average brackets in (30) thus have to be understood as a double average, one over the paths of the random walk of the oscillator, denoted by $\langle \cdot \rangle_P$, and another over the frequencies, $\langle \cdot \rangle_F$. The average over the frequencies can be performed exactly, and we obtain

$$\begin{aligned} \phi(t) &= \left\langle \left\langle \exp\left[i \sum_{k=1}^{N} \tau_k(t)\, u_k \right] \right\rangle_F \right\rangle_P \\ &= \left\langle \exp\left[-\frac{1}{2}\omega_F^2 \sum_{k=1}^{N} \tau_k^2(t) \right] \right\rangle_P \end{aligned} \tag{32}$$

A heuristic argument that allows one to calculate the average over the paths runs as follows. The cumulated residence time $\tau_k(t)$ is expected to follow the law of large numbers, i.e., we expect that these random variables are equal to their average value $\langle \tau_k(t) \rangle$ plus fluctuations that are comparatively small in the long-time limit. For the case that all sites are on the average visited equally often (i.e., all the rates $k_i^{\pm}$ are equal), we thus expect

$$\tau_k(t) = t/N + \text{fluctuations of order } \sqrt{t} \tag{33}$$

A mean field type of argument is then to boldly replace τ_k in (32) by its average value. We thus obtain

$$\phi(t) \approx \exp(-\omega_F^2 t^2/2N) \tag{34}$$

To go beyond the mean field argument given above, we will now perform the double average in the inverse order. Since $x(t)$ is asymptotically Gaussian, we obtain

$$\begin{aligned} \phi(t) &= \langle\langle \exp[ix(t)] \rangle_P \rangle_F \\ &\approx \left\langle \exp\left[i\langle x(t)\rangle_P - \frac{1}{2}\langle \delta x^2(t)\rangle_P \right] \right\rangle_F \\ &\approx \left\langle \exp\left[i \sum_{k=1}^{N} u_k p_k^{\mathrm{st}} t - Kt \right] \right\rangle_F \end{aligned} \tag{35}$$

The dispersion coefficient is given by (20)–(21). The average over the frequencies can be performed if we restrict ourselves to the case of equal and symmetric jump rates $k_i^{\pm} \equiv k$. This average over these Gaussian independent random variables u_k can be performed following the same procedure as explained in Appendix B of Ref. 5. We obtain (periodic boundary conditions)

$$\phi(t) \approx \left(\frac{2kN}{\omega_F^2 t} \right)^{(N-1)/2} N \left| \frac{\sinh^N \phi}{\sinh N\phi} \right| \exp\left(-\frac{\omega_F^2 t^2}{2N} \right) \tag{36}$$

with

$$\sinh^{-2}\phi = \frac{2kN}{\omega_F^2 t}\left(1 - \frac{\omega_F^2 t\, \Delta t}{N} \right) \tag{37}$$

In (35), we have used the asymptotic time properties for $x(t)$, hence we expect that (36) will only be valid in the time regime $t \gg N^2 k^{-1}$. For those who worry about the exchange of the long-time limit with the average over the frequencies, we mention that the same result, though with a little more effort, can be obtained directly from (32).

To illustrate the effect of a nonzero value for Δt, we plot $\phi(t)$ for

various values of $k\,\Delta t$ in Fig. 1 for the case $N=16$ and $\omega_F k^{-1}=1$. Our conclusion corroborates the results given in Ref. 13: the depolarization decay $\phi(t)$ is faster for the continuous-time model.

5. TIME DEPENDENCE OF THE SECOND MOMENT

In the case of a symmetric, translationally invariant walk ($k_i^{\pm}=k$, $\alpha_i^{\pm}=\alpha$, and $\alpha=k\,\Delta t$), it is possible to go a little further and to obtain results for the moments $\langle x(t)\rangle$ and $\langle \delta x^2(t)\rangle$ that are valid for all times. By the same token, it is possible to discuss the limit $N\to\infty$, i.e., the case of infinite one-dimensional systems.

Calculations similar to those of Ref. 6 for the continuous-time case lead to the following result for the dispersion [for the initial condition $P(x, i, n=0)=\delta(x)/N$ and for periodic boundary conditions]:

$$\begin{aligned}\langle \delta\tilde{x}^2(s)\rangle &= \sum_{n=0}^{\infty} s^n \langle \delta x^2(n)\rangle \\ &= \frac{\Delta t}{N}\frac{1}{(1-s)^2}\sum_{i,j=1}^{N}(u_i-\bar{u})\frac{\cosh\beta(|i-j|-N/2)}{k\sinh\beta\sinh(N\beta/2)}(u_j-\bar{u}) \\ &\quad + \frac{\Delta t^2}{N}\frac{s}{(1-s)^2}\sum_{i=1}^{N}(\bar{u}^2-u_i^2) \end{aligned} \tag{38}$$

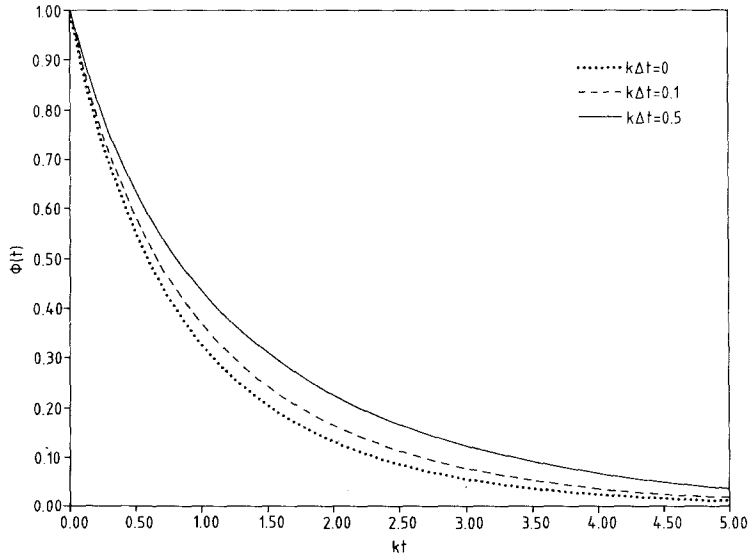

Fig. 1. The correlation function $\phi(t)$ for a random oscillator jumping between $N=16$ sites with modulation parameter $\omega_F k^{-1}=1$. Curves are for (top to bottom) $k\,\Delta t=0.5$, 0.1, and 0, illustrating the effect of a discrete-time model as compared to a continuous-time model ($\Delta t=0$).

with

$$\cosh \beta = 1 + \frac{1-s}{2sk\,\Delta t} \tag{39}$$

Equations (38)–(39) allow one to discuss particular cases or limits. First, the long-time limit can be obtained from the following relationship:

$$K = \lim_{n\to\infty} \frac{\langle \delta x^2(n)\rangle}{2n\,\Delta t} = \lim_{s\to 1} \frac{(s-1)^2\langle \delta \tilde{x}^2(s)\rangle}{2\,\Delta t} \tag{40}$$

and leads to the result (13) and (15) for $k_i^{\pm} \equiv k$.

As a direct application of the result (38), we consider the following two-dimensional free rotation polymer model.[14] The polymer consists of segments of fixed length b in the xy plane. A given segment has the same orientation as a previous one with probability α^0 or makes a fixed bond angle with it with probability $2\alpha = 1-\alpha^0$. For simplicity, we will suppose that this bond angle is equal to $2\pi/N$, with $N \geqslant 2$. The N allowed orientations of the segments thus make the following angles with the x axis:

$$\theta_i = \theta_1 + \frac{2\pi}{N}(i-1), \qquad i = 1,\ldots, N \tag{41}$$

A segment oriented in the θ_i direction leads to the following increase of the x coordinate of the end-to-end distance:

$$\Delta x = b\cos\theta_i = u_i \tag{42}$$

This relation defines the value of u_i. Since the variable n now refers to the number of segments of the polymer, and not to a time variable, we have set $\Delta t = 1$. We have thus mapped the polymer problem onto the discrete-time dispersion problem. The x component of the mean square end-to-end distance is then obtained by inserting (41) and (42) into (38) [note that $\alpha_i^{\pm} = \alpha = (1-\alpha^0)/2$]. In the polymer problem, the angle θ_1 of the orientation $i=1$ with the x axis is itself a random variable with a uniform distribution in $[0, 2\pi[$. By performing this second average, we finally obtain

$$\langle\langle \delta \tilde{x}^2(s)\rangle\rangle = \langle\langle \tilde{x}^2(s)\rangle\rangle = \frac{1}{2}\frac{b^2 s}{(1-s)^2}\frac{1+sC}{1-sC} \tag{43}$$

with

$$C = \alpha^0 + (1-\alpha^0)\cos(2\pi/N) \tag{44}$$

This result can be inverted to obtain $\langle\langle x^2(n)\rangle\rangle$ and the mean square end-to-end distance follows by invoking orientational isotropy. One finds

$$\begin{aligned}\langle R^2(n)\rangle &= \langle\langle x^2(n)\rangle\rangle + \langle\langle y^2(n)\rangle\rangle \\ &= 2\langle\langle x^2(n)\rangle\rangle \\ &= nb^2\frac{1+C}{1-C} - 2b^2C\frac{1-C^n}{(1-C)^2}\end{aligned} \tag{45}$$

This result is in agreement with the general result for the mean square end-to-end distance for polymer models with first-order correlation.[15] Finally, we consider a one-dimensional random walk with persistence. The random walker starts at the origin and moves with equal probability one step of length b to the right or left. At each subsequent step he has a probability p to take another step in the same direction as the previous one, and a probability $q=1-p$ to go in the other direction. This process can be modeled by a two-site discrete-time model, $N=2$, with velocities $u_1=-u_2=b$ and probability $\alpha^0=p=1-2\alpha$ or $2\alpha=1-p$. For this case, we obtain again result (45) with $C=2p-1$, in agreement with the result first given by Taylor.[16]

6. DISCUSSION

We have calculated asymptotic time properties of systems with an internal coordinate that undergoes a nearest neighbor random walk. If a discrete-time description with time step Δt is chosen, corrections arise when compared to the continuous-time case. We have given the long-time analytic form of these corrections for a few problems. These results are also of interest in the case of problems that are intrinsically of the discrete-time type, such as the polymer problem discussed in Section 5.

APPENDIX

We give a short outline of the derivation of Eqs. (12) and (13). Define the vectors $\mathbf{p}(n)$ and $\mathbf{g}(n)$ with components

$$p_i(n)=\int_{-\infty}^{+\infty} P(x, i, n)\,dx \tag{A1}$$

$$g_i(n)=\int_{-\infty}^{+\infty} xP(x, i, n)\,dx \tag{A2}$$

One assumes that $p_i(0)=p_i^{\mathrm{st}}$, then for all n, $p_i(n)=p_i^{\mathrm{st}}$; furthermore, $g_i(0)=0$.

Integration of the basic master equation (4) gives us the following equation for $\mathbf{g}(n)$:

$$\mathbf{g}(n) = \mathsf{T}\mathbf{g}(n-1) + \mathbf{b} \tag{A3}$$

The matrix T has the following elements:

$$T_{ij} = \alpha_{i-1}^{+}\,\delta_{i-1,j} + (1 - \alpha_i^{+} - \alpha_i^{-})\,\delta_{ij} + \alpha_{i+1}^{-}\,\delta_{i+1,j} \tag{A4}$$

while the components of the vector $\mathbf{b}$ are given by

$$b_i = u_i\, p_i^{\mathrm{st}}\, \Delta t \tag{A5}$$

The first two moments can be expressed in terms of the quantities $g_i(n)$ as follows. Obviously, one has

$$\langle x(n) \rangle = \sum_i g_i(n) \tag{A6}$$

The equation for the second moment $\langle x^2(n) \rangle$ follows by multiplying (4) with x^2 and subsequent summation over i and integration over x. After some simple algebra, this equation can be rewritten as follows:

$$\langle \delta x^2(n) \rangle - \langle \delta x^2(n-1) \rangle = 2\,\Delta t \sum_i \sum_j u_i T_{ij}\, g_j(n-1) - 2(n-1)\,\Delta t^2 \bar{u}^2 + \Delta t^2 \sum_i u_i (u_i - \bar{u})\, p_i^{\mathrm{st}} \tag{A7}$$

The problem is thus reduced to solving (A3). By iteration, one finds

$$\mathbf{g}(n) = \sum_{m=0}^{n-1} \mathsf{T}^m \cdot \mathbf{b} \tag{A8}$$

Let X and Y be the right and left eigenvector matrices of T with eigenvalue matrix Λ. The steady-state solutions $X_{i1} = p_i^{\mathrm{st}}$ correspond to the eigenvalue $\lambda_1 = 1$, and right and left eigenvectors are related by

$$Y_{\alpha i} = X_{i\alpha} / p_i^{\mathrm{st}} \tag{A9}$$

We can then write the long-time limit of $\mathbf{g}(n)$ as

$$g_i(n) \underset{n \text{ large}}{\approx} p_i^{\mathrm{st}} g_i^{*} + \bar{u} n p_i^{\mathrm{st}}\, \Delta t \tag{A10}$$

with

$$g_i^{*} = \sum_{l=1}^{N} \sum_{r=2}^{N} \frac{Y_{ri} Y_{rl}}{1 - \lambda_r} b_l \tag{A11}$$

We conclude from (A6), (A7), and (A10) that for large values of n

$$\langle x(n)\rangle \approx \bar{u} n\, \Delta t \tag{A12}$$

$$2K\,\Delta t \approx 2\,\Delta t \sum_i \sum_j u_i T_{ij} g_j^* p_j^{\mathrm{st}} + \Delta t^2 \sum_i u_i (u_i - \bar{u})\, p_i^{\mathrm{st}} \tag{A13}$$

Even though we do not know X, Y, and Λ explicitly, we can calculate g_i^* as follows. By iteration of the eigenvalue equation $(\mathsf{T}\cdot\mathsf{X})_{i,r} = (\mathsf{X}\cdot\Lambda)_{i,r}$, one obtains

$$\alpha_{i+1}^- X_{i+1,r} - \alpha_i^+ X_{i,r} = \sum_{j=1}^{i} (\lambda_r - 1)\, X_{j,r} + \alpha_1^- X_{1,r} - \alpha_N^+ X_{N,r} \tag{A14}$$

Using (A11), (A14), detailed balance, and the orthonormality relation $\mathsf{X}\cdot\mathsf{Y} = 1$, we can construct a recursion relation for g_i^*:

$$g_{i+1}^* - g_i^* = \frac{\alpha_1^-\, p_1^{\mathrm{st}} (g_1^* - g_N^*)}{\alpha_{i+1}^-\, p_{i+1}^{\mathrm{st}}} - \frac{1}{\alpha_{i+1}^-\, p_{i+1}^{\mathrm{st}}} \sum_{j=1}^{i} \left[b_j - p_j^{\mathrm{st}} \sum_{l=1}^{N} b_l \right] \tag{A15}$$

Iterating the last expression gives us g_i^* in terms of g_1^* and g_N^*. We find g_N^* by putting $i = N$, while g_1^* follows from the property

$$(\lambda_r - 1) \sum_{i=1}^{N} X_{i,r} = 0$$

which implies

$$\sum_{i=1}^{N} g_i^* p_i^{\mathrm{st}} = 0 \tag{A16}$$

By the above procedure we get explicit expressions for g_i^*, $i = 1,\ldots, N$. Insertion into (A13) gives us the result (15) of the text.

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REFERENCES

1. A. Einstein, *Investigations on the Theory of Brownian Movement* (Dover, New York, 1956).
2. D. R. Cox and H. D. Miller, *The Theory of Stochastic Processes* (Chapman and Hall, London, 1965).
3. G. H. Weiss and R. J. Rubin, *Adv. Chem. Phys.* **52**:363 (1983).

4. C. Van den Broeck and R. M. Mazo, *Phys. Rev. Lett.* **51**:1309 (1983); *J. Chem. Phys.* **81**:3624 (1984).
5. R. M. Mazo and C. Van den Broeck, *Phys. Rev. A* **34**:2364 (1986).
6. R. M. Mazo and C. Van den Broeck, *J. Chem. Phys.* **86**:545 (1987).
7. H. Brenner, *Phys. Chem. Hydr.* **1**:91 (1980).
8. N. G. Van Kampen, *Physica* **96A**:435 (1979).
9. R. G. Gordon, *Adv. Mag. Reson.* **3**:1 (1967).
10. M. Lax, *Rev. Mod. Phys.* **38**:359 (1966).
11. L. Onsager, *Phys. Rev.* **37**:405 (1931).
12. J. C. Giddings and H. Eyring, *J. Phys. Chem.* **59**:416 (1955).
13. R. Czech and K. W. Kehr, Depolarization of rotating spins by random walks on lattices, preprint.
14. H. Yamakawa, *Modern Theory of Polymer Solutions* (Harper and Row, New York, 1970).
15. C. M. Chen, *J. Chem. Phys.* **20**:214 (1952).
16. G. I. Taylor, *Proc. Lond. Math. Soc.* **20**:196 (1921).