Occupancy of a single site by many random walkers

M. Boguñá,[1] A. M. Berezhkovskii,[2,*] and G. H. Weiss[1]
[1]*Center for Information Technology, Bethesda, Maryland 20892*
[2]*National Institute of Child Health and Human Development, National Institutes of Health, Bethesda, Maryland 20892*
(Received 12 April 2000)

We consider an infinite number of noninteracting lattice random walkers with the goal of determining statistical properties of the time, out of a total time T, that a single site has been occupied by n random walkers. Initially the random walkers are assumed uniformly distributed on the lattice except for the target site at the origin, which is unoccupied. The random-walk model is taken to be a continuous-time random walk and the pausing-time density at the target site is allowed to differ from the pausing-time density at other sites. We calculate the dependence of the mean time of occupancy by n random walkers as a function of n and the observation time T. We also find the variance for the cumulative time during which the site is unoccupied. The large-T behavior of the variance differs according as the random walk is transient or recurrent. It is shown that the variance is proportional to T at large T in three or more dimensions, it is proportional to $T^{3/2}$ in one dimension and to $T \ln T$ in two dimensions.

PACS number(s): 05.40.Fb, 02.50.−r, 05.40.−a

I. INTRODUCTION

The theory of random walks generally deals with properties of a single random walker. Several more recent studies deal with aspects of the theory for properties of N independent random walkers, in particular outlining the behavior of the expected number of distinct sites visited by a lattice random walker in n steps [1]. The result of these calculations is that, although the random walkers move independently, allowing the use of single-particle propagators to analyze their properties, they nevertheless generate a rich qualitative behavior as a function of the parameters N and the step number. A somewhat similar theory has been developed for the average volume of the Wiener sausage generated by N spherical Brownian particles in Ref. [2]. A calculation of the average volume visited by randomly injected spherical Brownian particles was done in Ref. [3]. While there is no interaction between the random walkers, the kinetic behavior of such systems can still exhibit surprisingly complex collective behavior.

In this paper we analyze another property of multiple random walks on a lattice; the fluctuations in the occupancy of a single site resulting from the motion of an infinite number of lattice random walkers initially uniformly distributed over the entire lattice. This is a crude model that mimics a membrane pore that can be occupied by one or more metabolite molecules that initially diffuse throughout a bathing solution [4]. Since characteristics of the motion of molecules transiting the pore differ from those in solution, the model allows the transition rates at the target point to differ from those in solution. Similar models, based on lattice random walks, have been successfully applied to the study of photons diffusing in a tissue, in which a localized region may have optical properties differing from those of the remaining tissue [5,6].

*Permanent address: Karpov Institute of Physical Chemistry, 10 Vorontsovo Pole Street, 103064 Moscow K-64, Russia.

II. THE MODEL

Our theory is based on a continuous-time random walk on a d-dimensional simple cubic lattice, in which transitions are allowed only to nearest neighbors and in which the probability density for the time between successive jumps starting from any site excluding the origin, is

$$\psi(t) = k e^{-kt}. \tag{1}$$

The corresponding pausing-time density for a random walker at the origin will be denoted by $\psi_0(t) = k_0 e^{-k_0 t}$. These very specific definitions are for convenience only, since the asymptotic behavior for any pausing-time density that has a finite first moment will be essentially the same. We develop the theory for isotropic nearest-neighbor random walks, for which the probability of moving to any specific neighboring point is $1/(2d)$, where d is the dimension.

When all of the sites have the same pausing-time density, the model is exactly solvable for all values of the time t [7,8]. In what follows we will measure rates in terms of the common rate k. This is equivalent to taking t to be a dimensionless time and setting $k=1$. With this understanding the probability that a random walker is at $\mathbf{r}=(l_1,l_2,\ldots,l_d)$ at time t, having been at $\mathbf{r}_0=(l_1(0),l_2(0),\ldots,l_d(0))$ at $t=0$ is

$$p_F(\mathbf{r},t|\mathbf{r}_0) = e^{-t} I_{l_1-l_1(0)}\left(\frac{t}{d}\right) I_{l_2-l_2(0)}\left(\frac{t}{d}\right)\cdots I_{l_d-l_d(0)}\left(\frac{t}{d}\right), \tag{2}$$

where the subscript F indicates that it is a propagator in free space on a homogeneous lattice and the $I_j(u)$ are modified Bessel functions [9]. Since the lattice is translationally invariant the propagator is seen to be a function only of the vector distance $\mathbf{r}-\mathbf{r}_0$.

The initial condition for the ensemble of random walkers is chosen so that the probability of finding n random walkers at a given site is the Poisson

$$\beta_n = \frac{c^n}{n!} e^{-c} \tag{3}$$

whose expected value is equal to the concentration c. In addition it will be assumed that initially there are no random walkers at the origin.

III. CONCENTRATION AT THE ORIGIN

In this section we prove that the time-dependent distribution of the population at the origin is a Poisson, and depends only on the concentration of random walkers at that site at time t. To do so we assume that initially N random walkers are uniformly distributed in a hypercube of volume V. We then pass to the thermodynamic limit $N,V \to \infty$, with $N/V = c$. The probability that a random walker that is initially at $\mathbf{r}_0$ is at the origin at time t, is the propagator $p(\mathbf{0},t|\mathbf{r}_0)$, and the probability that a single random walker is at the origin at time t can be expressed in terms of the propagator by

$$\theta_V(t) = \frac{1}{V-1} \sum_{\mathbf{r}_0 \neq 0} p(\mathbf{0},t|\mathbf{r}_0). \tag{4}$$

Therefore, in the finite system defined above, the probability that there are n random walkers at the origin is

$$Q_{n,N}(t) = \binom{N}{n} [\theta_V(t)]^n [1-\theta_V(t)]^{N-n}, \tag{5}$$

which is a binomial distribution. In the thermodynamic limit as defined earlier, it can be shown that $Q_{n,N}(t)$ goes over into a Poisson distribution [10]. If $Q_n(t)$ is the probability that there are n random walkers at the origin at t, this line of reasoning leads to

$$Q_n(t) = \frac{[c_0(t)]^n}{n!} e^{-c_0(t)}, \tag{6}$$

where $c_0(t)$ is the concentration of random walkers at the origin.

The concentration at the origin can be shown to depend only on the single propagator $p(\mathbf{0},t|\mathbf{0})$. To see this we start from the obvious definition

$$c_0(t) = c \sum_{\mathbf{r}_0 \neq \mathbf{0}} p(\mathbf{0},t|\mathbf{r}_0) \tag{7}$$

and invoke the condition of detailed balance [11] which can be expressed as

$$p(\mathbf{0},t|\mathbf{r}_0) = p(\mathbf{r}_0,t|\mathbf{0})/k_0. \tag{8}$$

This allows us to reexpress $c_0(t)$ as

$$c_0(t) = \frac{c}{k_0}[1-p(\mathbf{0},t|\mathbf{0})] = c_0^{eq}[1-p(\mathbf{0},t|\mathbf{0})], \tag{9}$$

where $c_0^{eq} = c_0(\infty) = c/k_0$. The important point here is that only the propagator for the transition $\mathbf{0} \to \mathbf{0}$ is needed to find the concentration at the origin, and hence, by Eq. (6), the probability $Q_n(t)$.

The reader should notice that the argument we have given to derive the Poisson distribution is quite general, and does not depend on a specific model for the dynamics. The only requirements for the validity of Eq. (6) are that the target region (in the present case, the point at the origin) should be small with respect to the remainder of the space and that the thermodynamic limit be taken.

Equation (6) indicates that the time-dependent concentration at the origin contains all the information required to calculate the probability distribution of the number of random walkers at that site. An exact formula can be derived in the case when all sites have the same pausing-time density $\psi_0(t) = \psi(t)$. In contrast, only the asymptotic behavior can be found when $\psi_0(t) \neq \psi(t)$ since only the Laplace transforms of the relevant functions can be found. When the pausing-time densities are identical we can immediately write

$$\begin{aligned} c_0(t) &= c_0^{eq}[1-p(\mathbf{0},t|\mathbf{0})] \\ &= c_0^{eq}\left[1-e^{-t} I_0^d\left(\frac{t}{d}\right)\right] \\ &\approx c_0^{eq}\left[1-\left(\frac{d}{2\pi t}\right)^{d/2}\right], \quad t \to \infty \end{aligned} \tag{10}$$

so that the higher the dimension, the quicker will be the rate at which the concentration at the origin reaches its equilibrium value c_0^{eq}. We will see that when $k_0 \neq k = 1$ the time dependence of the asymptotic form of $c_0(t)$ remains unchanged but a prefactor appears that depends on $\psi_0(t)$.

As shown in Eq. (9) the concentration at the origin has a simple relation to the propagator $p(\mathbf{0},t|\mathbf{0})$. To keep the presentation self-contained we derive an expression for the Laplace transform of this function in terms of the propagator for the random walk in free space. For this purpose we require the probability density for a random walker that is one lattice site from the origin at $t=0$, to reach the origin for the first time at $t>0$. This function will be denoted by $f(t)$. An elementary argument then allows us to write the following integral equation for $p(\mathbf{0},t|\mathbf{0})$:

$$\begin{aligned} p(\mathbf{0},t|\mathbf{0}) &= e^{-k_0 t} + k_0 \int_0^t e^{-k_0 \tau} d\tau \\ &\quad \times \int_0^{t-\tau} f(\tau') p(\mathbf{0},t-\tau-\tau'|\mathbf{0}) d\tau', \end{aligned} \tag{11}$$

where the integral term accounts for cases in which it has left the origin at least once during $(0, t)$.

A solution to Eq. (11) can be found in terms of Laplace transforms. It is expressed in terms of the Laplace transform of the first-passage time density, $\hat{f}(s)$ as

$$\hat{p}(\mathbf{0},s|\mathbf{0}) = \frac{1}{s + k_0[1-\hat{f}(s)]}. \tag{12}$$

But $\hat{f}(s)$ is, in turn, related to the transform of the probability of moving from a nearest neighboring point to the origin in a time t on a homogeneous lattice [8] by

$$\hat{f}(s)=\frac{\hat{p}_F(\mathbf{0},s|nn)}{\hat{p}_F(\mathbf{0},s|\mathbf{0})}. \tag{13}$$

By $\hat{p}_F(\mathbf{0},s|nn)$ we mean the Laplace transform of the free-space propagator from a nearest-neighboring site to the origin. An expression for the free-space propagator in d dimensions for the nearest-neighbor random walk has been given in Eq. (2). Using this propagator one can see that

$$\begin{aligned} p_F(\mathbf{0},t|nn)&=e^{-t}I_0^{d-1}\left(\frac{t}{d}\right)I_1\left(\frac{t}{d}\right)\\ &=e^{-t}\frac{d}{dt}I_0^d\left(\frac{t}{d}\right)\\ &=\frac{dp_F(\mathbf{0},t|\mathbf{0})}{dt}+p_F(\mathbf{0},t|\mathbf{0}). \end{aligned} \tag{14}$$

In the Laplace domain this means

$$\hat{p}_F(\mathbf{0},s|nn)=(s+1)\hat{p}_F(\mathbf{0},s|\mathbf{0})-1, \tag{15}$$

which provides a relation between $\hat{p}(\mathbf{0},s|\mathbf{0})$ and $\hat{p}_F(\mathbf{0},s|\mathbf{0})$:

$$\hat{p}(\mathbf{0},s|\mathbf{0})=\frac{\hat{p}_F(\mathbf{0},s|\mathbf{0})}{s\hat{p}_F(\mathbf{0},s|\mathbf{0})+k_0[1-s\hat{p}_F(\mathbf{0},s|\mathbf{0})]}. \tag{16}$$

Thus, in the small-s regime we have

$$\hat{p}(\mathbf{0},s|\mathbf{0})\approx\hat{p}_F(\mathbf{0},s|\mathbf{0})/k_0 \tag{17}$$

from which we can infer that at large t

$$p(\mathbf{0},t|\mathbf{0})\approx\frac{1}{k_0}\left(\frac{d}{2\pi t}\right)^{d/2} \tag{18}$$

and

$$c_0(t)\approx c_0^{eq}\left[1-\frac{1}{k_0}\left(\frac{d}{2\pi t}\right)^{d/2}\right]. \tag{19}$$

This asymptotic behavior is equivalent to our earlier assertion that the time dependence of the approach to equilibrium remains unchanged when properties of a single point are modified.

IV. OCCUPANCY TIMES

A. General relations

Another random variable, suggested by the physical problem motivating the present paper, relates to the occupancy time of the site at the origin by n random walkers. By this we will mean the amount of time that the origin has been occupied by n random walkers during a time interval $(0,T)$. We begin by calculating the first moment of this time. This will be denoted by $\langle\tau_n(T)\rangle$, and can be expressed in terms of $Q_n(t)$. The contribution of the time interval $(t,t+dt)$ to $\langle\tau_n(T)\rangle$ is equal to $Q_n(t)dt$. From this observation we infer that

$$\langle\tau_n(T)\rangle=\int_0^T Q_n(t)dt,\quad n=0,1,2\ldots. \tag{20}$$

After inserting the expression for $Q_n(t)$ in Eq. (6) we find the large-T limit of $\langle\tau_n(T)\rangle$:

$$\lim_{T\to\infty}\langle\tau_n(T)\rangle=Q_n(\infty)T=\frac{(c_0^{eq})^n}{n!}e^{-c_0^{eq}}T. \tag{21}$$

In similar fashion we can infer that, if $Q_{nn}(t_1,t_2)$ is the joint probability, that there are n random walkers at the origin at times t_1 and t_2, and the contribution to $\langle\tau_n^2(T)\rangle$ from the pair of intervals (t_1,t_1+dt_1) and (t_2,t_2+dt_2) is equal to $Q_{nn}(t_1,t_2)dt_1dt_2$. Consequently, $\langle\tau_n^2(T)\rangle$ is

$$\langle\tau_n^2(T)\rangle=2\int_0^T dt_2\int_0^{t_2}Q_{nn}(t_2,t_1)dt_1dt_2, \tag{22}$$

where the factor of 2 reflects the symmetry inherent in $Q_{nn}(t_1,t_2)$ with respect to an interchange of t_1 and t_2.

We now proceed to calculate a representation of the function $Q_{00}(t+\tau,t)$ to be used in evaluating the expression for $\langle\tau_0^2(T)\rangle$ in Eq. (22). For convenience of notation we define $p(\mathbf{r}',t+\tau;\mathbf{r},t|\mathbf{r}_0)$ be the probability that a random walker is initially at $\mathbf{r}_0$, then is at $\mathbf{r}$ at time t and at $\mathbf{r}'$ at $t+\tau$. Since the random walk is Markovian, this joint probability can be decomposed into a product of the propagators by the relation

$$p(\mathbf{r}',t+\tau;\mathbf{r},t|\mathbf{r}_0)=p(\mathbf{r}',\tau|\mathbf{r})p(\mathbf{r},t|\mathbf{r}_0). \tag{23}$$

The probability that a single random walker initially at $\mathbf{r}_0$ is not at the origin at both the times t and $t+\tau$ is

$$U(t,t+\tau|\mathbf{r}_0)=\sum_{\mathbf{r}\neq 0}\sum_{\mathbf{r}'\neq 0}p(\mathbf{r}',t+\tau;\mathbf{r},t|\mathbf{r}_0), \tag{24}$$

The joint probability $Q_{00}(t+\tau,t)$ can be written in terms of this function as

$$\begin{aligned} Q_{00}(t+\tau,t)&=e^{-c}\prod_{\mathbf{r}_0\neq 0}\sum_{n=0}^{\infty}\frac{c^n}{n!}U^n(t,t+\tau|\mathbf{r}_0)\\ &=\exp\left[-c\left\{1-\sum_{\mathbf{r}_0\neq 0}U(t,t+\tau|\mathbf{r}_0)\right\}\right] \end{aligned} \tag{25}$$

since $e^{-c}c^n/n!$ is the probability that an arbitrary site (other than at the origin) has n particles initially and $U^n(t,t+\tau|\mathbf{r}_0)$ is the probability that none of them will be at the origin at $t(>0)$ and $t+\tau$. This leaves us only with the task of evaluating the sum over $\mathbf{r}_0$ that appears in the exponential. This is easily done by successively adding in and subtracting out the contributions from $\mathbf{r}=0$ and $\mathbf{r}'=0$ in the definition of Eq. (24), noting that

$$\sum_{\mathbf{r}}\sum_{\mathbf{r}'}p(\mathbf{r}',t+\tau;\mathbf{r},t|\mathbf{r}_0)=1 \tag{26}$$

so that

$$\begin{aligned} Q_{00}(t+\tau,t)=\exp\Big[-c\sum_{\mathbf{r}_0\neq 0}\{&p(\mathbf{0},t+\tau|\mathbf{r}_0)+p(\mathbf{0},t|\mathbf{r}_0)\\ &-p(\mathbf{0},\tau|\mathbf{0})p(\mathbf{0},t|\mathbf{r}_0)\}\Big] \end{aligned} \tag{27}$$

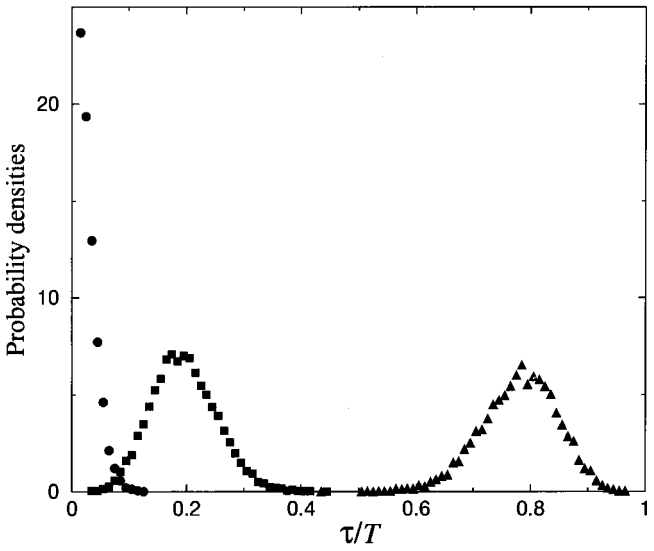

FIG. 1. Plots of the probability densities for the fractional occupation time, $g_n(\tau/T)$, where n is the number of the state. The results are shown for $n=0$, 1, and 2, which are represented by $n=0$ (▲), 1 (■), and 2 (●), respectively. The results shown are for a three-dimensional lattice, with $T=1000(k=1)$ and $k_0=0.1$. The initial concentration here is $18/729\approx 0.025$. The data were generated by randomly placing 18 random walkers in a three-dimensional box of dimensions $9\times 9\times 9$ and with periodic boundaries. Aside from the two peaks centered at $\tau/T\approx 0.19$ and 0.77 there is a large peak at very small τ/T, indicating that the cumulative residence time in the state in which there are two random walkers at the origin, is very close to zero.

where we have made use of Eq. (23). We can invoke detailed balance as expressed in Eq. (8) to write $Q_{00}(t+\tau,t)$ in terms of the single propagator $p(\mathbf{0},t|\mathbf{0})$. This is done by taking account of the relation in Eq. (9) between $c_0(t)$ and $p(\mathbf{0},t|\mathbf{0})$, allowing us to write

$$Q_{00}(t+\tau,t)=\exp\left[-\left\{c_0(t+\tau)+\frac{c_0(t)c_0(\tau)}{c_0^{eq}}\right\}\right]$$
$$=Q_0(t+\tau)\exp[-c_0(t)\{1-p(\mathbf{0},\tau|\mathbf{0})\}]. \tag{28}$$

Having this representation in hand enables us to calculate the mean and variance of the cumulative time during which the origin is unoccupied.

These quantities are of use in the case of low concentrations $c\ll 1$. In this regime it is overwhelmingly likely that the origin will either be occupied by none or a single random walker. Some simulated results for this regime are shown in Fig. 1, for $c=18/729\approx 0.025$ and $T=1000$. The first peak (dark circles) which is identified with the possibility of having two random walkers at the origin, is seen to lie quite close to 0. The dominant feature of the figure is that most of the time the origin is empty or occupied by one random walker, and only rarely by two.

It appears to be quite difficult to solve the occupancy problem for an arbitrary number of random walkers at the origin. However, some progress can be made in finding the large-T behavior of the probability density for the total time that the origin is unoccupied. This follows from the consideration that as $T\to\infty$ there will have been many occasions on which the origin is unoccupied. With this in mind it is reasonable to conjecture that the probability density will be a Gaussian at large T. In order to specify the Gaussian we need the first moment and the variance. The asymptotic form of the first moment is found in Eq. (21) with $n=0$. We therefore proceed to calculate the large-T form of the variance.

B. Asymptotic forms of the variance

1. Transient random walks

The asymptotic dependence of the variance on T differs in one, two, and three or more dimensions, because the underlying random walk is recurrent in one and two dimensions, and transient in three or more dimensions.

A formal expression for the variance, $\sigma_0^2(T)=\langle\tau_0^2(T)\rangle-\langle\tau_0(T)\rangle^2$, is found by combining Eqs. (20) and (22) with $n=0$. On differentiating $\sigma_0^2(T)$ with respect to T we find

$$\frac{d\sigma_0^2(T)}{dT}=2\int_0^T[Q_{00}(T,t)-Q_0(t)Q_0(T)]dt. \tag{29}$$

If we invoke Eq. (28) we can factor $Q_0(T)$ out of the integral transforming this equation to

$$\frac{d\sigma_0^2(T)}{dT}=2Q_0(T)\int_0^T[e^{p(\mathbf{0},T-t|\mathbf{0})c_0(t)}-1]Q_0(t)dt \tag{30}$$

or

$$\sigma_0^2(T)=2\int_0^T Q_0(\xi)d\xi\int_0^{\xi}[e^{p(\mathbf{0},\xi-t|\mathbf{0})c_0(t)}-1]Q_0(t)dt. \tag{31}$$

In the limit $T\to\infty$ we can assert that $c_0(T)\to c_0^{eq}$ and $Q_0(T)\to\exp(-c_0^{eq})$. Further, when $t\to\infty$, $p(\mathbf{0},t|\mathbf{0})$ goes to zero as $t^{-d/2}$ in d dimensions. This, in turn, implies that the integral with respect to t will be finite in the limit $T\to\infty$ for $d\geqslant 3$. Hence the lowest-order term in an asymptotic expansion of $\sigma_0^2(T)$ is

$$\sigma_0^2(T)\approx 2e^{-2c_0^{eq}}T\int_0^{\infty}[e^{p(\mathbf{0},t|\mathbf{0})c_0^{eq}}-1]dt. \tag{32}$$

The integral on the right-hand side converges when the underlying random walk is transient. In the low-concentration limit $\sigma_0^2(T)$ becomes

$$\sigma_0^2(T)\approx 2\frac{c_0^{eq}}{k_0}T\int_0^{\infty}e^{-\rho}I_0^3\left(\frac{\rho}{3}\right)d\rho. \tag{33}$$

A convenient expansion of $\sigma_0^2(T)$ in powers of c can be given for the three-dimensional case when $k_0=1$, i.e., all of the lattice sites have identical properties. In this case Eq. (32) reduces to

$$\sigma_0^2(T)=2e^{-c}T\int_0^{\infty}[e^{-c_0(t)}-e^{-c}]dt. \tag{34}$$

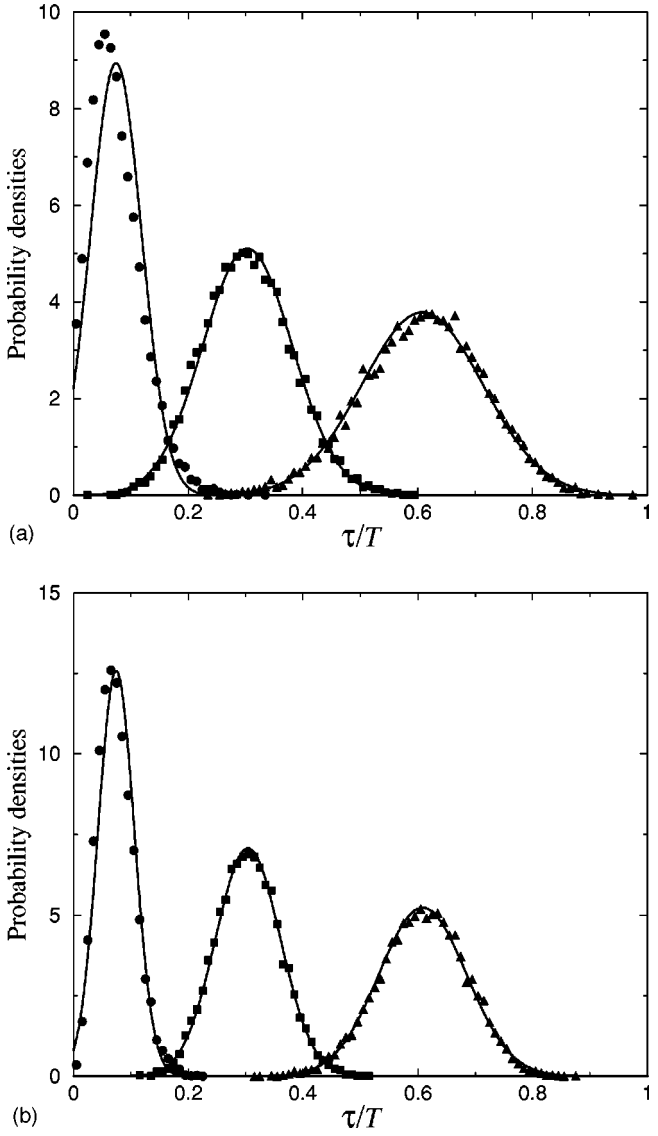

FIG. 2. (a) Plots of the probability densities for the fractional occupation time $g_n(\tau/T)$, where n is the number of random walkers at the origin. The results are shown for $n=0$, 1, and 2 and for $T=500$ steps. The rate constants were taken to be $k=1$ and $k_0=0.1$ so that random walkers tend to remain at the origin longer than on any other site. Ten-thousand trials were used in the simulations and the initial concentration was $36/729\approx 0.05$. The data suggest a Gaussian form for all three values of n. The solid curves represent the Gaussian densities to which the data were fit. (b) Similar data except that here $T=1000$. The trend towards Gaussian behavior is evident.

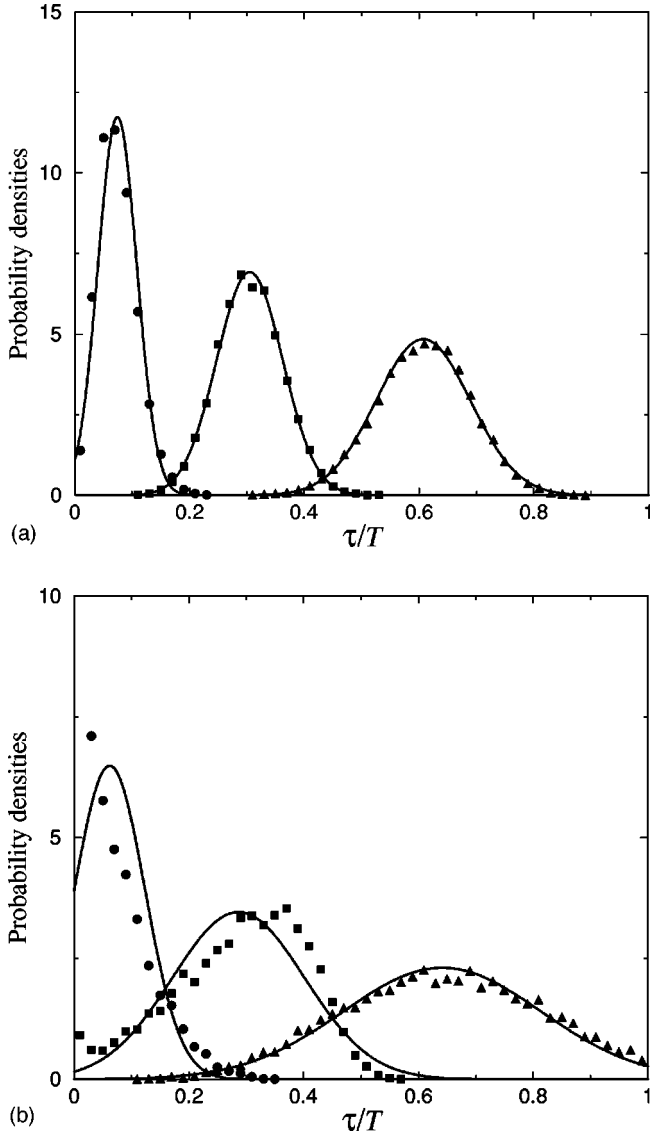

FIG. 3. (a) Simulated data and the Gaussian approximations for a two-dimensional lattice. Here $T=1300$, $c=31/625$, $k=1$, and $k_0=0.1$. The fit is considerably improved over that in the case of one dimension. (b) Simulated data and the associated Gaussian approximations for one dimension. The parameters used to generate the data are $T=2800$, $k=1$, $k_0=0.1$, and $c=25/499\approx 0.0501$.

If the term in brackets in the integral is expanded in powers of c, one arrives at the representation

$$\sigma_0^2(T)=2e^{-c}T\sum_{n=1}^{\infty}\frac{c^n}{n!}\int_0^{\infty}e^{-n\rho}I_0^{3n}\left(\frac{\rho}{3}\right)d\rho$$

$$=2e^{-c}T\sum_{n=1}^{\infty}\frac{c^n}{nn!}\int_0^{\infty}e^{-\rho}I_0^{3n}\left(\frac{\rho}{3n}\right)d\rho. \qquad (35)$$

When $n=1$, the integral is approximately equal to 1.52, when $n=2$ it is approximately equal to 1.1, and with $n\geqslant 3$ the integral is approximately equal to 1, which considerably simplifies the evaluation of the variance.

2. Recurrent random walks

When the random walk is recurrent, that is when $d=1$ or 2, the integral in Eq. (32) diverges as T tends to infinity due to the behavior of the integrand in the neighborhood of $t=T$. In this case, to analyze the large-T behavior of $\sigma_0^2(T)$ we use Eq. (30) to find that, at large T,

$$\frac{d\sigma_0^2(T)}{dT}\approx\frac{2c_0^{eq}e^{-2c_0^{eq}}}{\pi k_0}\begin{cases}\sqrt{2\pi T}, & d=1\\ \ln T, & d=2.\end{cases} \qquad (36)$$

After taking this into account we find the approximations

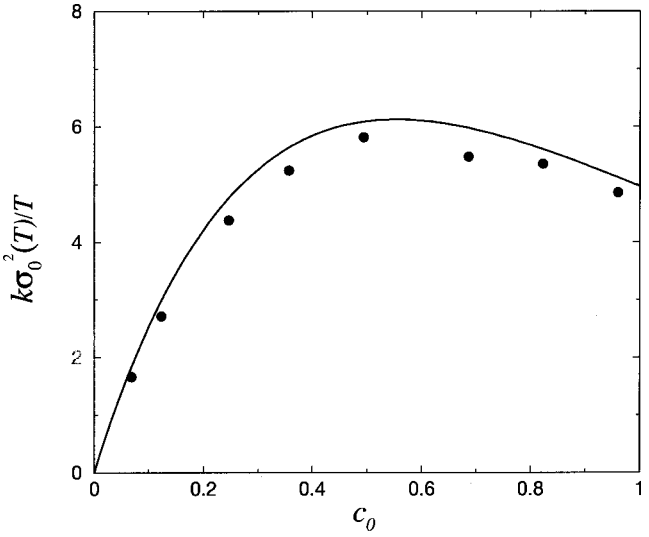

FIG. 4. A plot of the dimensionless variable $k\sigma_0^2(T)/T$ generated by replacing c in Eq. (35) by c/k_0 and replacing k by k_0. The agreement between the calculated and simulated data is seen to be best in the low-concentration limit.

$$\sigma_0^2(T) \approx \frac{2c_0^{eq}e^{-2c_0^{eq}}}{\pi k_0} \begin{cases} \dfrac{2\sqrt{2\pi}}{3} T^{3/2}, & d=1 \\ T \ln T, & d=2. \end{cases} \tag{37}$$

These estimates can also be derived from the general theory of randomly interconverting two-state systems developed in Ref. [12].

V. NUMERICAL RESULTS

To verify some of the results just found, we performed simulations using the parameters $k=1$ and $k_0=0.1$ so that random walkers that arrive at the origin tend to remain there longer than at any other lattice point [13]. In Figs. 2(a) and 2(b) we show plots of the probability density for the fraction of time spent by a three-dimensional system in different states. A concentration of 36/729 (≈ 0.05) was used to generate the figure together with observation times of $T=500$ and $T=1000$, respectively. The generated points indicate that for this choice of parameters the probability densities for both zero and one random walkers occupying the origin tend towards a Gaussian, the approximation improving as T increases. The results summarized in Figs. 2(a) and 2(b) suggest that the probability densities for the times corresponding to any occupancy number are all approximately Gaussian. Figures 3(a) and 3(b) display results for $d=2$ and $d=1$ with $T=1300$ and $T=2800$, respectively. The two sets of simulations are for approximately the same value of initial concentration. One sees an evident tendency towards Gaussian behavior, but the approach to this functional form is clearly much slower in one dimension than in two. This is to be expected from the different behavior of $\sigma_0^2(T)$ in these dimensions. There is good agreement between the theoretical and simulated results. The average value approaches its asymptotic form faster than does the variance.

We have not been able to find a rigorous extension of the result in Eq. (35) for the case $k_0 \neq 1$, but, as a heuristic approximation, we have replaced c in that equation by c/k_0 and k by k_0. The results of doing so are shown in Fig. 4, where one sees good agreement between simulated data and the proposed approximation for low concentrations.

VI. DISCUSSION

This paper, motivated by studies of the kinetics of the transfer of metabolite molecules through membrane pores, [4] analyzes the occupancy of a single lattice site by one or more continuous-time random walkers. The restriction to a single site is done mainly to keep the analysis simple. The analysis can be extended to a set of sites by using formalism developed in Ref. [14], but qualitative aspects of the results would not be changed by doing so. Since, in realistic situations, a molecule tends to move more slowly through a pore than in a bathing medium, we have assumed that the pausing-time density for transitions out of the site representing the pore, can differ from those at other lattice sites. We have addressed the problem of calculating statistics related to the cumulative time during which the origin is unoccupied.

A more complicated problem is that of determining statistical properties of the fraction of time that the origin is occupied by one or more random walkers. This is related to the local time, which is an important property of diffusion processes [15]. An argument based on the central-limit theorem predicts that the probability density for the fraction of time that the origin is occupied by n random walker over a long period T should also be Gaussian centered at $\langle \tau_n(T) \rangle$ given in Eq. (21). This agrees with findings based on simulations. The results depend on whether the random walks are transient or recurrent. A more difficult problem in this class is posed if one is interested in first-passage time densities, e.g., the probability density for the first time that the origin is occupied by n random walkers. We have obtained partial results in this area, and will present them at a later time.

[1] S. Havlin, H. Larralde, J. E. Kiefer, H. E. Stanley, and G. H. Weiss, Phys. Rev. A **46**, R1717 (1992); H. Larralde, G. H. Weiss, and H. E. Stanley, Physica A **209**, 368 (1994); S. B. Yuste, Phys. Rev. Lett. **79**, 3565 (1997); Phys. Rev. E **57**, 6327 (1998); G. Berkolaiko, S. Havlin, H. Larralde, and G. H. Weiss, *ibid.* **53**, 5774 (1996); G. Berkolaiko, and S. Havlin, *ibid.* **55**, 1395 (1997); **57**, 2549 (1998); S. B. Yuste, and L. Acedo, *ibid.* **60**, R3459 (1999); **61**, 2340 (2000).

[2] A. M. Berezhkovskii, J. Stat. Phys. **76**, 1089 (1994).

[3] A. M. Berezhkovskii and G. H. Weiss, Phys. Rev. E **54**, 92 (1996).

[4] S. M. Bezrukov, I. Vodyanoy, and V. A. Parsegian, Nature (London) **370**, 279 (1994); S. M. Bezrukov, J. Membr. Biol. **174**, 1 (2000).

[5] A. H. Gandjbakhche and G. H. Weiss, Prog. Opt. **34**, 333 (1995).

[6] G. H. Weiss and P. P. Calabrese, Physica A **234**, 443 (1996).

[7] E. W. Montroll and G. H. Weiss, J. Math. Phys. **6**, 167 (1965).

[8] G. H. Weiss, *Aspects and Applications of the Random Walk* (North-Holland, Amsterdam, 1994).
[9] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972) reprint.
[10] W. Feller, *An Introduction to Probability Theory and its Applications* (Wiley, New York, 1970).
[11] C. W. Gardiner, *Handbook of Stochastic Methods*, 2nd ed. (Springer-Verlag, Berlin, 1985).
[12] M. Boguñá, A. M. Berezhkovskii, and G. H. Weiss, Physica A **282**, 475 (2000).
[13] G. Doetsch, *Theorie und Anwendung der Laplace-Transformation* (Dover, New York, 1943).
[14] R. J. Rubin and G. H. Weiss, J. Math. Phys. **23**, 250 (1982).
[15] S. Karlin and H. M. Taylor, *A Second Course in Stochastic Processes* (Academic Press, New York, 1981).