Region visited by a spherical Brownian particle in the presence of an absorbing boundary

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We calculate the time dependence of the average volume of a Wiener sausage in the presence of an absorbing boundary in one and three dimensions. In one dimension it is shown that the presence of an absorbing point reduces the time dependence of the average span from being proportional to $\sqrt{t}$ in an unbounded space, to being proportional to $\ln(t)$ at long times. In three dimensions the average volume increases as $\sqrt{t}$ at long times rather than being proportional to t as in free space.

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I. INTRODUCTION

The number of distinct sites visited by a lattice random walk in time t and its continuous counterpart, the volume of the region swept out by a spherical Brownian particle, have been used to model a variety of chemical and physical phenomena. For example, properties of these and related models have been analyzed to generalize the Smoluchowski theory of diffusion-limited reactions [1–3]. Another potential application of these ideas is the use of random walk models to interpret data from optical imaging techniques in biomedicine. These are based on laser injected photons that move through the tissue and gather information related to optical parameters that may be used for diagnostic purposes, [4,5]. In these applications it is important to be able to estimate the amount and location of tissue interrogated by the photons.

In modeling such experiments an important component in formulating the physical problem is the existence of an interface between the tissue and the exterior space, since data in these experiments consists of measurements of light intensity on the surface. To a good approximation the interface can be taken to be an absorbing plane, [6]. A crude estimate of the tissue interrogated in continuous-wave experiments has been described in [7]. A possibly more accurate estimate can be based on the expected number of distinct sites visited by a random walker before being trapped by the absorbing boundary. This motivates the analysis in the present paper.

The random variables described earlier have been analyzed when the random walk or Brownian motion occurs in an unbounded space, [8–12]. However, the existence of an absorbing boundary is a significant feature of the underlying physical phenomenon. It is, therefore, of interest to understand how constraints are able to influence statistical properties of the random variables. In the present paper we study the average volume of the Wiener sausage in the presence of an absorbing boundary in one and three dimensions. It is evident from physical considerations that boundary effects manifest themselves at times of the order of, and longer than, a characteristic time for the diffusing particle to reach the boundary. On this time scale the rate at which the volume increases is significantly smaller than in free space. In $d=1$ dimension the $t^{1/2}$ dependence in free space will be shown to be replaced by a $\ln(t)$ dependence in the limit $t\to\infty$, and in $d=3$ proportionality to t is replaced by a proportionality to $t^{1/2}$.

All of the following analysis will be based on a general formalism for calculating the average volume of a Wiener sausage discussed in Sec. II. In Secs. III and IV these general results will be applied in one and three dimensions.

II. AVERAGE VOLUME OF THE WIENER SAUSAGE

Let $W_t(\mathbf{r}_0)$ be the trajectory followed by the center of a sphere of radius R, initially at $\mathbf{r}_0$, that moves as a Brownian particle for a time t. The position of the center at time $\tau\leqslant t$ will be denoted by $\mathbf{r}_{W_t}(\tau)$ (to simplify the notation the argument $\mathbf{r}_0$ in the subscript is omitted). The region swept out by the sphere is the Wiener sausage, and its volume will be denoted by $v(W_t(\mathbf{r}_0))$. Since translational invariance of the space is destroyed by the presence of a boundary, it is important to retain the dependence on initial position.

A formal expression for the volume can be written in terms of an indicator function $I(\mathbf{r}|W_t)$ that is equal to 1 when the distance between W_t and the point $\mathbf{r}$ has been smaller than R and equal to 0 otherwise. With this definition the volume of the Wiener sausage is

$$v(W_t(\mathbf{r}_0))=\int I(r|W_t(\mathbf{r}_0))d\mathbf{r}. \tag{1}$$

To calculate the average value of $v(W_t(\mathbf{r}_0))$, therefore, requires finding the average of the indicator function. This functional, $\langle I(\mathbf{r}|W_t(\mathbf{r}_0))\rangle$, is the fraction of trajectories that have, at least once, during the time t visited a spherical domain of radius R centered at $\mathbf{r}$. Thus $\langle I(\mathbf{r}|W_t(\mathbf{r}_0))\rangle$ is the probability that a point Brownian particle, originally at $\mathbf{r}_0$, has been absorbed in time t by a spherical trap of radius R centered at $\mathbf{r}$. To simplify the notation we set $q(t|\mathbf{r}|\mathbf{r}_0)=\langle I(\mathbf{r}|W_t(\mathbf{r}_0))\rangle$. Then the average volume is

$$\langle v(W_t(\mathbf{r}_0))\rangle=\int \langle I(\mathbf{r}|W_t(\mathbf{r}_0))\rangle d\mathbf{r}=\int q(t|\mathbf{r}|\mathbf{r}_0)d\mathbf{r}. \tag{2}$$

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Thus, to find the average volume we need to derive the trapping probability $q(t|\mathbf{r}|\mathbf{r}_0)$.

The span and volume in an unbounded space

An exact solution for the average volume of the Wiener sausage in a d-dimensional free space valid for all values of the time has been calculated in [12]. A more general formulation of the problem has been proposed and analyzed in [8–10]. Because of the generality of that formulation only results in the $t\to\infty$ limit were found. Here we sumarize results in one and three dimensions derived in [12] that will be used for comparison in further discussions. In one dimension the Wiener sausage is the sum of the particle size and the span generated by the center of the particle. Hence all of the information of interest is encapsulated in the span. In one dimension the probability that a particle, initially at x_0, is absorbed by a trap at x by time t is

$$q(t|x|x_0)=\mathrm{erfc}\left(\frac{|x-x_0|}{2\sqrt{Dt}}\right), \tag{3}$$

in which D is the diffusion constant and erfc(z) is the complementary error function, [13]. The average span on an unbounded line is readily found to be

$$\langle L(t)\rangle=\int_{-\infty}^{\infty}q(t|x|x_0)dx=4\sqrt{\frac{Dt}{\pi}}. \tag{4}$$

In 3D the volume of the Wiener sausage at time t is to be calculated rather than a span. The trapping probability in free space is

$$q(t|\mathbf{r}|\mathbf{r}_0)=q(t||\mathbf{r}-\mathbf{r}_0|)=H(R-|\mathbf{r}-\mathbf{r}_0|)+\frac{R}{|\mathbf{r}-\mathbf{r}_0|}\mathrm{erfc}\left(\frac{|\mathbf{r}-\mathbf{r}_0|-R}{2\sqrt{Dt}}\right)H(|\mathbf{r}-\mathbf{r}_0|-R), \tag{5}$$

where $H(z)$ is the heaviside step function. To calculate $\langle v(t)\rangle$ requires integrating this expression over all space, in which case one finds,

$$\langle v(t)\rangle=\frac{4\pi}{3}R^3+8R^2\sqrt{\pi Dt}+4\pi RDt. \tag{6}$$

III. THE 1D SPAN WITH A TRAPPING POINT

In this calculation we set the trap at $x=0$ and the initial position of the particle at $x_0>0$. Then the average span is given by

$$\langle L(t|x_0)\rangle=\int_0^{\infty}q(t|x|x_0)dx \tag{7}$$

and its Laplace transform with respect to t is

$$\langle\hat{L}(s|x_0)\rangle=\int_0^{\infty}\hat{q}(s|x|x_0)dx. \tag{8}$$

Solving the diffusion equation one finds the Laplace transform of the trapping probability to be

$$\hat{q}(s|x|x_0)=\frac{1}{s}\left[e^{-(x_0-x)\sqrt{s/D}}H(x_0-x)+\frac{\sinh\left(x_0\sqrt{\frac{s}{D}}\right)}{\sinh\left(x\sqrt{\frac{s}{D}}\right)}H(x-x_0)\right]. \tag{9}$$

This leads to a representation of the Laplace transform of the span as

$$\langle\hat{L}(s|x_0)\rangle=\sqrt{\frac{D}{s^3}}\left\{1-e^{-x_0\sqrt{s/D}}+\sinh\left(x_0\sqrt{\frac{s}{D}}\right)\ln\left(\frac{1+e^{-x_0\sqrt{s/D}}}{1-e^{-x_0\sqrt{s/D}}}\right)\right\}. \tag{10}$$

The long-time behavior of $\langle\hat{L}(s|x_0)\rangle$ can be inferred from the small-s behavior of this expression. If desired it can also be inverted explicitly in terms of an infinite series from which its behavior can be found for all values of the time.

The long- and short-time behaviors of $\langle L(t|x_0)\rangle$ can be estimated from the small- and large-s behaviors of Eq. (10) and are found to be

$$\langle L(t|x_0)\rangle\approx\begin{cases}4\sqrt{\frac{Dt}{\pi}}, & t\ll x_0^2/D\\ x_0\left[1+\frac{\gamma}{2}+\ln\left(\sqrt{\frac{4Dt}{x_0^2}}\right)\right], & t\gg x_0^2/D.\end{cases} \tag{11}$$

where $\gamma\approx0.6$ is Catalan's constant. The early-time behavior in this equation is exactly that in Eq. (4), which is to be expected since the probability that the diffusing particle reaches the absorbing boundary at $x=0$ is low at the earliest times. At long times there is a good chance that the particle has been trapped, with the result that the growth rate of the average span is dramatically slowed. Finally, we mention that the two limiting time-dependent behaviors in Eq. (11) are the same as those for the expected number of distinct sites visited by a lattice random walk when the time t is replaced by the number of steps n and the multiplicative constant is changed to one appropriate to the random walk picture.

IV. AVERAGE 3D VOLUME

In this section we calculate the behavior in time of the average volume generated by a sphere of radius R moving as a Brownian particle in the presence of an absorbing plane at $z=0$. The particle will be assumed to move in the half-space $z>0$. The initial position of the particle is taken to be $\mathbf{r}_0$

$=(0,0,z_0)$ with the obvious restriction that $z_0>R$. It will be assumed that the particle is absorbed as soon as its center comes into contact with the wall. The general expression for the average volume in this case takes the form

$$\langle v(t|z_0)\rangle=\int_{z>0} q(g|\mathbf{r}|\mathbf{r}_0)d\mathbf{r}. \tag{12}$$

The method of images will be used to guarantee satisfaction of the trapping boundary condition. Hence we consider the diffusion problem for a point particle in the presence of two absorbing spheres of radius R, centered at $\mathbf{r}=(x,y,z)$ and $\mathbf{r}'=(x,y,-z)$, respectively. The trapping probability $q(t|\mathbf{r}|\mathbf{r}_0)$ in the presence of the absorbing plane can be expressed in terms of two trapping probabilities, $q_1^{(2)}(t|\mathbf{r}|\mathbf{r}_0)$ and $q_2^{(2)}(t|\mathbf{r}'|\mathbf{r}_0)$ found by solving the two-trap problem in free space. These are the probabilities that the particle, initially at $\mathbf{r}_0$, has been trapped by time t by the first and second trap, respectively. The expression for $q(t|\mathbf{r}|\mathbf{r}_0)$ is

$$q(t|\mathbf{r}|\mathbf{r}_0)=q_1^{(2)}(t|\mathbf{r}|\mathbf{r}_0)-q_2^{(2)}(t|\mathbf{r}'|\mathbf{r}_0). \tag{13}$$

We make the further assumption that $z_0\gg R$. In this case the main contribution to the value of the integral in Eq. (12) comes from configurations in which the distance between the trap and plane is much larger than the radius of the sphere, $z\gg R$. For such configurations the two trapping probabilities on the right-hand side of Eq. (13) can be approximated by the expression given in Eq. (5). This leads to

$$q_2(t|\mathbf{r}|\mathbf{r}_0)\approx q[t|\sqrt{\rho^2+(z-z_0)^2}]-q[t|\sqrt{\rho^2+(z+z_0)^2}], \tag{14}$$

in which ρ is the radial coordinate $\rho^2=x^2+y^2$. The average volume of the Wiener sausage in this approximation is, therefore, given by

$$\langle v(t|z_0)\rangle\approx 4\pi\int_0^{z_0}dz\int_0^{\infty}q(t|\sqrt{\rho^2+z^2})\rho\, d\rho. \tag{15}$$

Since our interest is the time dependence of the average volume for times t that satisfy $t\gg R^2/D$ we use a simplified version of the expression for $q(t||\mathbf{r}-\mathbf{r}_0|)$ given in Eq. (5)

$$q(t|r)\approx\frac{R}{r}\operatorname{erfc}\left(\frac{r}{\sqrt{4Dt}}\right). \tag{16}$$

The resulting integral is difficult to deal with in the time domain, but its Laplace transform with respect to t is readily evaluated. This function, $\langle\hat{v}(s|z_0)\rangle$, is

$$\langle\hat{v}(s|z_0)\rangle\approx\frac{2\pi R}{s}\int_0^{z_0}dz\int_0^{\infty}\frac{\exp[\sqrt{(s/D)(\xi+z^2)}]}{\sqrt{\xi+z^2}}d\xi$$
$$=\frac{4\pi RD}{s^2}[1-\exp(-z_0\sqrt{s/D})]. \tag{17}$$

The inverse transform of this function of s can be evaluated exactly, leading to the final expression,

$$\langle v(t|z_0)\rangle\approx 4\pi RD\int_0^t\operatorname{erf}\left(\frac{z_0}{2\sqrt{D\tau}}\right)d\tau$$
$$=4\pi RDt\left\{\frac{2\lambda e^{-\lambda^2}}{\sqrt{\pi}}+2\lambda^2\operatorname{erfc}(\lambda)+\operatorname{erf}(\lambda)\right\}, \tag{18}$$

in which $\lambda=z_0/\sqrt{4Dt}$.

The expression in Eq. (18) shows that $\langle v(t|z_0)\rangle$ grows linearly with time at times smaller than z_0^2/D, but at longer times the growth rate decreases and the average volume is proportional to $\sqrt{t}$,

$$\langle v(t|z_0)\rangle\approx\begin{cases}4\pi RDt, & t\ll z_0^2/D\\ 8z_0R\sqrt{\pi Dt} & t\gg z_0^2/D.\end{cases} \tag{19}$$

Again, the t dependence of this result can be replaced by an n dependence in the context of the average distinct number of sites visited by a lattice random walk.

In summary, the main results in this paper are the expressions for the average span in one dimension and the average volume of the Wiener sausage in three dimensions, given in Eqs. (11) and (19). They show how the presence of an absorbing boundary slows the growth of these variables as a function of time as compared to the growth in free space.

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