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Volume of the Domain Visited by N Spherical Brownian Particles

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The average value and variance of the volume of the domain visited in time t by N spherical Brownian particles starting initially at the same point are presented as quadratures of the solutions of simple diffusion problems of the survival of a point Brownian particle in the presence of one and two spherical traps. As an illustration, explicit time dependences are obtained for the average volume in one and three dimensions.

KEY WORDS: Brownian motion; Wiener sausage.

The number of distinct sites visited by a random walker after n steps is one of the most important properties of a random walk.[1,2] Recently the problem has been generalized to the case of N identical walkers starting simultaneously from the same lattice site.[3-6] These problems are of great interest because the number of distinct sites plays a central role in theoretical models of different phenomena in physics and chemistry, ecology, and metallurgy (detailed references can be found in refs. 1–7). In the present work we study a continuous version of the problem. We consider a spatial domain visited in time t by N identical spherical Brownian particles starting initially at the same point which we choose to be the origin. The quantity of interest is the volume of the domain, which is the analog of the number of distinct sites in the lattice random walk. The volume is random due to the uncertainty in the Wiener trajectories chosen by the particles in their Brownian motion. We estimate the average value and the variance of the domain volume and show how these quantities can be represented in

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terms of quadratures of the solutions of the simple diffusive problems. As an illustration, explicit time dependences are obtained for the average volume in one and three dimensions.

The estimation method used below is a generalization of the method suggested in ref. 8 to calculate the average value and the dispersion of the volume of the domain visited by a single spherical Brownian particle. In the case of a single Brownian particle such a domain is known as the Wiener sausage.[9-11] To define its volume we use the indicator $\chi(\mathbf{r} \mid W_t)$, which is a function of the position $\mathbf{r}$ of the point in d-dimensional space and a functional of the Wiener trajectory W_t of the particle center observed during time t,

$$\chi(\mathbf{r} \mid W_t) = \begin{cases} 1 & \text{if } \min |\mathbf{r} - \mathbf{r}_{W_t}| \leqslant b \\ 0 & \text{if } \min |\mathbf{r} - \mathbf{r}_{W_t}| \geqslant b \end{cases} \tag{1}$$

where b is the radius of the particle and $\mathbf{r}_{W_t} \in W_t$. The Wiener sausage volume corresponding to a given trajectory W_t is

$$v(W_t) = \int \chi(\mathbf{r} \mid W_t)\, d\mathbf{r} \tag{2}$$

This volume is random and is distributed according to the probability density

$$F(v, t) = \langle \delta(v - v(W_t)) \rangle \tag{3}$$

where $\delta(z)$ is the Dirac delta function and the symbol $\langle \cdots \rangle$ stands for the average over the Wiener trajectories.[11,12]

The average volume of the Wiener sausage is

$$\bar{v}(t) = \int vF(v, t)\, dv = \langle v(W_t) \rangle = \int \langle \chi(\mathbf{r} \mid W_t) \rangle\, d\mathbf{r} \tag{4}$$

The quantity $\langle \chi(\mathbf{r} \mid W_t) \rangle = q(t \mid \mathbf{r})$ is the fraction of the trajectories which visit the b vicinity of the point $\mathbf{r}$ in time t at least once. This quantity equals the probability that a point Brownian particle is trapped in time t in the sink of radius b centered at the point $\mathbf{r}$. To calculate this trapping probability one needs to solve the diffusion equation with the sink term, which leads to

$$q(t \mid \mathbf{r}) = H(b - r) + H(r - b)\, u(r, t) \tag{5}$$

Here $H(z)$ is the Heaviside step function and

$$u(r,t)=u\left(x=\frac{r}{b};\tau=\frac{Dt}{b^2}\right)$$
$$=\frac{2}{\pi x^{\nu}}\int_0^{\infty}\frac{1-\exp(-\tau y)}{y}\,\frac{J_\nu(y)\,N_\nu(xy)-J_\nu(xy)\,N_\nu(y)}{J_\nu^2(y)+N_\nu^2(y)}\,dy \tag{6}$$

where D is the diffusion coefficient, $\nu=(d-2)/2$, and $J_\nu(z)$ and $N_\nu(z)$ are Bessel functions of the first and second kinds of the order ν.[13] Substitution of Eq. (5) into Eq. (4) and subsequent integration leads to[8]

$$\bar{v}(r,t)=v_b\left\{1+d\left[\tau(d-2)\,\theta(d-2)+\frac{4}{\pi^2}\int_0^{\infty}\frac{1-\exp(-\tau y^2)}{J_\nu^2(y)+N_\nu^2(y)}\frac{dy}{y^3}\right]\right\} \tag{7}$$

where v_b is the volume of the Brownian particle. In one and three dimensions Eqs. (6) and (7) have simple forms. When $d=1$, $v_b=2b$, and

$$u(x,\tau)=\operatorname{erfc}\left(\frac{x-1}{2\sqrt{\tau}}\right) \tag{8}$$

and

$$\bar{v}(t)=2b+\frac{4}{\sqrt{\pi}}(Dt)^{1/2} \tag{9}$$

where $\operatorname{erfc}(z)$ is the complementary error function.[13] When $d=3$, $v_b=4\pi b^3/3$,

$$u(x,\tau)=\frac{1}{x}\operatorname{erfc}\left(\frac{x-1}{2\sqrt{\tau}}\right) \tag{10}$$

and

$$\bar{v}(t)=\tfrac{4}{3}\pi b^3+8\sqrt{\pi}\,b^2(Dt)^{1/2}+4\pi bDt \tag{11}$$

To write down a formal definition of the volume of the spatial domain visited by N identical spherical Brownian particles which start from the same point, we introduce the indicator $\chi_N(\mathbf{r}\,|\,\{W_t^{(j)}\})$, $j=1,2,\dots,N$, which is a generalization of the indicator

$$\chi_N(\mathbf{r}\,|\,\{W_t^{(j)}\})=\left\{1-\prod_{j=1}^{N}\left[1-\chi(\mathbf{r}\,|\,W_t^{(j)})\right]\right\} \tag{12}$$

where $W_t^{(j)}$ is the Wiener trajectory of the jth Brownian particle observed during time t. The indicator in Eq. (12) is equal to 1 if the b vicinity of the point $\mathbf{r}$ (the sink area) is visited by at least one of the trajectories, and equal to 0 if none of the trajectories visits the b vicinity. The domain visited by N Brownian particles is a unification of N Wiener sausages corresponding to the trajectories $W_t^{(j)}$. Its volume is given by the equation

$$\begin{aligned} v_N(\{W_t^{(j)}\}) &= \int \chi_N(\mathbf{r} \mid \{W_t^{(j)}\})\, d\mathbf{r} \\ &= \int \left\{1 - \prod_{j=1}^{N} [1 - \chi(\mathbf{r} \mid W_t^{(j)})]\right\} d\mathbf{r} \end{aligned} \tag{13}$$

The volume $v_N(\{W_t^{(j)}\})$ is a random quantity and its probability density is given by

$$F_N(v, t) = \langle \delta(v - v_N(\{W_t^{(j)}\})) \rangle_N \tag{14}$$

where $\langle \cdots \rangle_N$ is the notation for the average over the Wiener trajectories of N Brownian particles. Hence, the average volume is

$$\begin{aligned} \overline{v_N(t)} &= \int v F_N(v, t)\, dv = \langle v_N(\{W_t^{(j)}\}) \rangle_N \\ &= \int \left\{1 - \left\langle \prod_{j=1}^{N} [1 - \chi(\mathbf{r} \mid W_t^{(j)})] \right\rangle_N \right\} d\mathbf{r} \end{aligned} \tag{15}$$

In carrying out the averaging step we have assumed that particles can overlap. This means that Wiener trajectories of different particles are independent and hence in Eq. (15) the average of the product is equal to the product of the averages. Thus,

$$\overline{v_N(t)} = \int \{1 - [1 - q(t \mid \mathbf{r})]^N\}\, d\mathbf{r} = \int \{1 - [p(t \mid \mathbf{r})]^N\}\, d\mathbf{r} \tag{16}$$

where $p(t \mid \mathbf{r}) = 1 - q(t \mid \mathbf{r})$ is the survival probability of the Brownian particle during time t when there is a single sink of radius b located at the $\mathbf{r}$ point. Making use of Eq. (5), one can write down the volume $\overline{v_N(t)}$ as

$$\overline{v_N(t)} = v_b + \int_{b \leqslant r} \{1 - [1 - u(r, t)]^N\}\, d\mathbf{r} \tag{17}$$

For $N = 1$, Eqs. (16) and (17) reduce to Eqs. (4) and (7), respectively.

The dispersion $\sigma_N(t)$ of the domain volume is

$$\sigma_N^2(t) = \langle [v_N(\{W_t^j\})]^2 \rangle_N - \langle v_N(\{W_t^j\}) \rangle_N^2 \tag{18}$$

According to the definition of the domain volume, Eq. (13), the average value of the square of this quantity is

$$\begin{aligned} \langle [v_N(\{W_t^j\})]^2 \rangle_N &= \overline{v_N^2(t)} \\ &= \left\langle \int \left\{ 1 - \prod_{j=1}^{N} [1 - \chi(\mathbf{r}_1 \mid W_t^{(j)})] \right\} \right. \\ &\quad \left. \times \left\{ 1 - \prod_{j'=1}^{N} \left[1 - \chi(\mathbf{r}_2 \mid W_t^{(j')}) \right] \right\} d\mathbf{r}_1 \, d\mathbf{r}_2 \right\rangle_N \end{aligned} \tag{19}$$

When the terms in curly brackets are multiplied and use is made of the independence of Wiener trajectories of different particles, one can write $\overline{v_N^2(t)}$ as

$$\begin{aligned} \overline{v_N^2(t)} = \int \{ & 1 - [1 - \langle \chi(\mathbf{r}_1 \mid W_t) \rangle]^N - [1 - \langle \chi(\mathbf{r}_2 \mid W_t) \rangle]^N \\ & + [1 - \langle \chi(\mathbf{r}_1 \mid W_t) \rangle - \langle \chi(\mathbf{r}_2 \mid W_t) \rangle \\ & + \langle \chi(\mathbf{r}_1 \mid W_t) \rangle \langle \chi(\mathbf{r}_2 \mid W_t) \rangle]^{N(N-1)} \\ & \times [1 - \langle \chi(\mathbf{r}_1 \mid W_t) \rangle - \langle \chi(\mathbf{r}_2 \mid W_t) \rangle \\ & + \langle \chi(\mathbf{r}_1 \mid W_t) \, \chi(\mathbf{r}_2 \mid W_t) \rangle]^N \} \, d\mathbf{r}_1 \, d\mathbf{r}_2 \end{aligned} \tag{20}$$

If we denote the survival probability of the Brownian particle in time t in the presence of two spherical traps around the points $\mathbf{r}_1$ and $\mathbf{r}_2$ by $p(t \mid \mathbf{r}_1, \mathbf{r}_2)$, the average $\langle \chi(\mathbf{r}_1 \mid W_t) \, \chi(\mathbf{r}_2 \mid W_t) \rangle$ can be written as

$$\begin{aligned} & \langle \chi(\mathbf{r}_1 \mid W_t) \, \chi(\mathbf{r}_2 \mid W_t) \rangle \\ & \quad = \{ 1 - [1 - \langle \chi(\mathbf{r}_1 \mid W_t) \rangle] \} \{ 1 - [1 - \langle \chi(\mathbf{r}_2 \mid W_t) \rangle] \} \\ & \quad = 1 - p(t \mid \mathbf{r}_1) - p(t \mid \mathbf{r}_2) + p(t \mid \mathbf{r}_1, \mathbf{r}_2) \end{aligned} \tag{21}$$

Hence we have

$$\begin{aligned} \overline{v_N^2(t)} = \int \{ & 1 - [p(t \mid \mathbf{r}_1)]^N - [p(t \mid \mathbf{r}_2)]^N + [p(t \mid \mathbf{r}_1) \, p(t \mid \mathbf{r}_2)]^{N(N-1)} \\ & \times [p(t \mid \mathbf{r}_1, \mathbf{r}_2)]^N \} \, d\mathbf{r}_1 \, d\mathbf{r}_2 \end{aligned} \tag{22}$$

On substituting Eqs. (16) and (22) into Eq. (18), one obtains

$$\sigma_N^2(t) = \int [p(t|\mathbf{r}_1)\, p(t|\mathbf{r}_2)]^{N(N-1)} \{[p(t|\mathbf{r}_1, \mathbf{r}_2)]^N - [p(t|\mathbf{r}_1)\, p(t|\mathbf{r}_2)]^N\}\, d\mathbf{r}_1\, d\mathbf{r}_2 \tag{23}$$

Both the survival probabilities $p(t|\mathbf{r})$ and $p(t|\mathbf{r}_1, \mathbf{r}_2)$ are found from the solution of the diffusion equation with one and two sinks, respectively. While for the case of one sink the survival probability can be found exactly, for the case of two sinks the exact solution is known in one dimension only. In refs. 8, 14, and 15 an approximate solution of the problem is suggested that is correct in the multidimensional case for most trap configurations. In ref. 8 this solution is used to evaluate the variance of the volume of the Wiener sausage. This variance is a special case of that given by Eq. (23) for $N=1$.

We consider two illustrative examples which show how the equations just derived lead to the explicit dependence on time of the quantities under study. Let us start with the average volume in one dimension. In this particular case Eq. (17) can be written as

$$\overline{v_N(t)} = 2b + \frac{4}{\sqrt{\pi}} (Dt)^{1/2} I_N \tag{24}$$

where

$$I_N = \sqrt{\pi} \int_0^\infty \{1 - [\operatorname{erf}(y)]^N\}\, dy \tag{25}$$

Note that the factor I_N depends on the number of particles only and is independent of both time and the particle size. The simple equation for $\overline{v_N(t)}$ [decomposition of $\overline{v_N(t)}$ into factors depending on N, t, and b] is possible because of specific features of geometry in one dimension. The point is that in this case there exists a trivial relation between the length $L_N(\{W_t^{(j)}\})$ of the interval visited by N particles of the size $2b$ and the length $l_N(\{W_t^{(j)}\})$ of the interval visited by the particle centers

$$L_N(\{W_t^{(j)}\}) = 2b + l_N(\{W_t^{(j)}\}) \tag{26}$$

The integral I_N, Eq. (25), can be estimated in the following manner. For $N=1$ it is equal to unity and Eq. (24) is reduced to Eq. (9). For $N=2$ the integral is equal to $\sqrt{2}$. When $N \gg 1$ an approximate expression can be obtained as follows: First consider the difference

$$I_{N+1} - I_N = \frac{1}{\sqrt{\pi}} \int_0^\infty \operatorname{erfc}(y) \operatorname{erf}^N(y)\, dy \tag{27}$$

The integral in this expression can be evaluated by the steepest descent method, which leads to the estimate

$$I_{N+1} - I_N \approx \frac{1}{(2e)^{1/2} N[\ln(N/\sqrt{\pi})]^{1/2}} \tag{28}$$

If we approximate the difference $I_{N+1} - I_N$ by the first derivative dI_N/dN and solve the differential equation, we obtain

$$I_N \approx \frac{\pi}{e} (2 \ln N)^{1/2} \tag{29}$$

Thus, we have

$$I_N \approx \begin{cases} 1 & \text{for} \quad N = 1 \\ \sqrt{2} & \text{for} \quad N = 2 \\ \dfrac{\pi}{e} (2 \ln N)^{1/2} & \text{for} \quad N \gg 1 \end{cases} \tag{30}$$

Note that the large-N estimate of I_N gives 0.96 of the exact value even for $N = 2$.

Our second example is an estimate of the time dependence of the average volume in three dimensions. In this case, $\overline{v_N(t)}$, Eq. (17), is

$$\overline{v_N(t)} = v_b[1 + 3J_N(\tau)] \tag{31}$$

where

$$J_N(\tau) = \int_1^\infty \left\{1 - \left[1 - \frac{1}{x} \operatorname{erfc}\left(\frac{x-1}{2\sqrt{\tau}}\right)\right]^N\right\} x^2 \, dx \tag{32}$$

For $N = 1$, $J_1(\tau) = \tau + (2/\sqrt{\pi})\sqrt{\tau}$, and Eq. (31) is reduced to Eq. (11). Below we estimate $J_N(\tau)$ for τ, $N \gg 1$, which allows us to neglect the unity in the argument of the complementary error function in Eq. (32). Our estimate is based on the following approximation of the expression in curly brackets in the integrand:

$$\left\{1 - \left[1 - \frac{1}{x} \operatorname{erfc}\left(\frac{x}{2\sqrt{\tau}}\right)\right]^N\right\} \simeq \begin{cases} 1 & \text{for} \quad x < x^* \\ \dfrac{N}{x} \operatorname{erfc}\left(\dfrac{x^*}{2\sqrt{\tau}}\right) & \text{for} \quad x > x^* \end{cases} \tag{33}$$

where x^* is the root of the equation

$$\frac{N}{x^*} \operatorname{erfc}\left(\frac{x^*}{2\sqrt{\tau}}\right) = 1 \tag{34}$$

It is convenient to introduce a new variable $y = x/2\sqrt{\tau}$ and use the approximation (33) to approximate the integral $J_N(\tau)$ as

$$J_N(\tau) = \frac{8}{3}\tau^{3/2}\left[y^{*3} + \frac{3N}{2\sqrt{\tau}}\int_{y^*}^{\infty} y\,\mathrm{erfc}(y)\,dy\right] \tag{35}$$

where y^* is determined from the equation

$$\frac{1}{y^*}\,\mathrm{erfc}(y^*) = \frac{2\sqrt{\tau}}{N} \tag{36}$$

Equations (35) and (36) show that the ratio $\sqrt{\tau}/N$ is a parameter that determines the behavior of $J_N(\tau)$. When $\sqrt{\tau}/N \gg 1$, $y^* \simeq N/2\sqrt{\tau} \ll 1$ and the second term in the square brackets in Eq. (35) is the more significant one. In this case it is found that $J_N(\tau) \simeq N\tau$. In the regime defined by the condition $\sqrt{\tau}/N \ll 1$, Eq. (36) takes the form

$$\frac{1}{\sqrt{\pi}}\frac{1}{y^{*2}}\exp(-y^{*2}) = \frac{2\sqrt{\tau}}{N} \tag{37}$$

which implies that $y^* \simeq \ln[N/2(\pi\tau)^{1/2}] > 1$. In this case the square brackets in Eq. (35) is dominated by the first term and the integral $J_N(\tau)$ has the approximate form

$$J_N(\tau) \simeq \frac{8}{3}\tau^{3/2}\left[\ln\frac{N}{2(\pi\tau)^{1/2}}\right]^{3/2} \tag{38}$$

Thus, we obtain that for τ, $N \gg 1$ the dependence $\overline{v_N(t)}$ has the form

$$\overline{v_N(t)} = \begin{cases} \dfrac{32}{3}\pi(Dt)^{3/2}\left[\ln\dfrac{N}{2(\pi\, Dt/b^2)^{1/2}}\right]^{3/2} & \text{for} \quad Dt \ll N^2b^2 \\ 4\pi b\, DtN & \text{for} \quad Dt \gg N^2b^2 \end{cases} \tag{39}$$

In conclusion, the main results of this analysis are contained in Eqs. (16) and (23). They show how the average value and the dispersion of the domain visited by N spherical Brownian particles starting initially at the same point can be expressed in terms of the survival probability of a single Brownian particle in the presence of one and two traps. The explicit dependences in Eqs. (24), (29), and (39), obtained as a result of applying the general formula (16) to particular cases, are in qualitative agreement with the results obtained in ref. 4 for N random walkers on a lattice.

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