Surface area of the domain visited by a spherical Brownian particle

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A spatial domain swept out by a spherical particle, whose center follows a Wiener trajectory, is referred to as a Wiener sausage. The present study focuses on the surface area of the Wiener sausage. Using intuitive arguments we derive the mean and variance of the surface area, as well as the asymptotic behavior of its probability density in the limits when the area tends to zero and infinity. [doi:10.1063/1.3665090]

Wiener sausage is defined as the spatial domain swept out by a spherical particle executing Brownian motion.¹⁻³ As the motion is stochastic, the main parameters describing a Wiener sausage are random variables. The necessity to determine statistical properties of these parameters, which are important for applications, raises several interesting mathematical issues. In the present work, we obtain (i) the mean of the surface area of the Wiener sausage, (ii) the variance of the surface area, and (iii) the asymptotic behavior of its probability density.

I. INTRODUCTION

For a spherical particle of radius R , the Wiener sausage is the R -vicinity of its Wiener trajectory W_t which is followed by the center of the particle, where the subscript t indicates the observation time. One of the important characteristics of a Wiener sausage is its volume. Being a functional of the Wiener trajectory, this volume is a random variable. A calculation of the complete distribution of the volume of a Wiener sausage poses rather formidable mathematical problems except in one dimension where all calculations can be carried out exactly because the volume can be identified as a span of diffusion process.^{4,5} Calculations of the first moment for all values of the time as well as the long time asymptotic behavior of the second moment and variance of this random variable are given in Ref. 6.

Another characteristic of a Wiener sausage is its surface area. The mean surface area was recently rigorously calculated in Refs. 7 and 8 using sophisticated formalisms of the theory of stochastic processes. Here, in Sec. II, we present a back-of-the-envelope derivation of the mean surface area in three dimensions based on intuitive arguments. In addition, in Sec. III, we derive the variance of this random variable. In the concluding Sec. IV, we discuss asymptotic behavior of the probability density of the Wiener sausage area in the limiting cases when the area is much smaller and much larger than the mean value.

One can think about the surface of a Wiener sausage from a different perspective. Consider a spherical particle of radius R , which touches a Wiener trajectory without inter-

secting. Wiener sausages are R -vicinities of Wiener trajectories. Therefore, the surface of a Wiener sausage is the locus of positions of the center of the particle touching the trajectory, as illustrated in Figure 1. This makes our results to be of potential importance to the problems in biology and polymer physics that deal with polymer accessibility for bulky enzymes.

II. MEAN SURFACE AREA OF THE WIENER SAUSAGE

Let $\mathbf{X}_t$ be an arbitrary trajectory of the center of a spherical particle of radius R in three-dimensional space, where subscript t indicates the time during which the trajectory has been observed. The volume of the domain visited by the particle, $v_R(\mathbf{X}_t)$, can be written in terms of the indicator function $I_R(\mathbf{r}|\mathbf{X}_t)$ defined as

$$I_R(\mathbf{r}|\mathbf{X}_t) = \begin{cases} 0, & \text{if the distance from } \mathbf{r} \text{ to the trajectory} \\ & \mathbf{X}_t \text{ is larger than } R \\ 1, & \text{if otherwise} \end{cases}. \quad (2.1)$$

This volume is the volume of the R -vicinity of the trajectory given by

$$v_R(\mathbf{X}_t) = \int I_R(\mathbf{r}|\mathbf{X}_t) d\mathbf{r}. \quad (2.2)$$

To define the surface area of the domain visited by the particle, $A_R(\mathbf{X}_t)$, consider a spherical particle of radius $R + \Delta R$ whose center moves along the same trajectory $\mathbf{X}_t$. When $\Delta R \rightarrow 0$, the difference $v_{R+\Delta R}(\mathbf{X}_t) - v_R(\mathbf{X}_t)$ is equal to the product $A_R(\mathbf{X}_t)\Delta R$. Then,

$$A_R(\mathbf{X}_t) = \lim_{\Delta R \rightarrow 0} \frac{v_{R+\Delta R}(\mathbf{X}_t) - v_R(\mathbf{X}_t)}{\Delta R} = \frac{\partial v_R(\mathbf{X}_t)}{\partial R}. \quad (2.3)$$

When there is a set of random trajectories $\mathbf{X}_t$, one can define the mean domain area, $\langle A_R(t) \rangle$, by averaging the area $A_R(\mathbf{X}_t)$, Eq. (2.3), over realizations of the trajectory,

$$\langle A_R(t) \rangle = \langle A_R(\mathbf{X}_t) \rangle = \frac{\partial \langle v_R(\mathbf{X}_t) \rangle}{\partial R}, \quad (2.4)$$

FIG. 1. (Color online) The surface of the domain visited by a spherical Brownian particle is also the locus of positions of the center of another spherical particle of the same radius, which touches the Wiener trajectory (depicted as the solid curve) without intersecting. Three examples of such contacts are illustrated by “spheres” shown by dotted circles with the crosses at their centers. The properties of the contact surface are of importance in problems of biology and polymer physics, wherein polymer chain interactions with bulky enzymes are considered.

where $\langle v_R(\mathbf{X}_t) \rangle$ is the mean volume of the domain. When the particle center moves along a Wiener trajectory, W_t , the domain is the Wiener sausage, and $\langle v_R(\mathbf{X}_t) \rangle = \langle v_R(t) \rangle$ is the mean Wiener sausage volume given by⁶

$$\langle v_R(t) \rangle = 4\pi R D t + 8\sqrt{\pi} R^2 \sqrt{D t} + \frac{4}{3} \pi R^3, \quad (2.5)$$

where D is the particle diffusion coefficient. Then the mean surface area of the Wiener sausage observed for time t is

$$\langle A_R(t) \rangle = 4\pi D t + 16\sqrt{\pi} R \sqrt{D t} + 4\pi R^2. \quad (2.6)$$

One can find detailed discussion of averaging over Wiener trajectories in Refs. 9 and 10.

At $t = 0$, $\langle A_R(t) \rangle$ in Eq. (2.6) reduces to the surface area of the sphere of radius R , $4\pi R^2$, as it must be. The first two terms in Eq. (2.6) describe the Wiener sausage surface area at large t , when $\sqrt{D t} \gg R$. These terms have a transparent interpretation based on the fact that the fractal dimension of the Wiener trajectories equals two.³ This implies that the trajectories densely cover two-dimensional manifolds in the three-dimensional space. Therefore, the Wiener sausages can be thought of as “pancake”-like objects of thickness $2R$.¹¹ The first term in Eq. (2.6), which is independent of R , is the mean area of the pancake of zero thickness that is, on average, proportional to $D t$. The second term in Eq. (2.6) is the contribution to the surface area due to the finite thickness of the pancake. Therefore, this term is a product of the thickness, $2R$, and the pancake perimeter, which is, on average, proportional to $\sqrt{D t}$.

III. VARIANCE OF THE SURFACE AREA OF THE WIENER SAUSAGE

The variance, $\sigma_{A_R}^2(t)$, of the surface area of the Wiener sausage is defined as

$$\sigma_{A_R}^2(t) = \langle [A_R(W_t)]^2 \rangle - \langle A_R(t) \rangle^2. \quad (3.1)$$

Here $\langle [A_R(W_t)]^2 \rangle$ is the second moment of the surface area given by

$$\begin{aligned} \langle [A_R(W_t)]^2 \rangle &= \left\langle \left[\frac{\partial v_R(W_t)}{\partial R} \right]^2 \right\rangle \\ &= \lim_{R_1 \rightarrow R} \frac{\partial^2}{\partial R \partial R_1} \langle v_R(W_t) v_{R_1}(W_t) \rangle. \end{aligned} \quad (3.2)$$

Using the relation

$$\langle A_R(t) \rangle^2 = \left[\frac{\partial \langle v_R(t) \rangle}{\partial R} \right]^2 = \lim_{R_1 \rightarrow R} \frac{\partial^2}{\partial R \partial R_1} (\langle v_R(t) \rangle \langle v_{R_1}(t) \rangle), \quad (3.3)$$

we can write the variance, Eq. (3.1), as

$$\sigma_{A_R}^2(t) = \lim_{R_1 \rightarrow R} \frac{\partial^2}{\partial R \partial R_1} K_{11}(t), \quad (3.4)$$

where $K_{11}(t)$ is

$$K_{11}(t) = \langle v_R(W_t) v_{R_1}(W_t) \rangle - \langle v_R(t) \rangle \langle v_{R_1}(t) \rangle. \quad (3.5)$$

The long-time asymptotic behavior of this function has been found in Ref. 12,

$$K_{11}(t) = (4\pi R R_1)^2 D t \ln \left(\frac{D t}{R^2} \right), \quad D t \gg R^2. \quad (3.6)$$

This allows us to find the long-time asymptotic behavior of the variance

$$\sigma_{A_R}^2(t) \simeq 64\pi^2 R^2 D t \ln \left(\frac{D t}{R^2} \right), \quad D t \gg R^2, \quad (3.7)$$

which is the main result of this section.

The relation between the mean surface area of the Wiener sausage and its mean volume is given by the relation in Eq. (2.4), with $\langle v_R(\mathbf{X}_t) \rangle = \langle v_R(t) \rangle$. This relation is exact at all times. To establish a similar relation between the variances of these random variables we use the results in Eq. (3.7) and the expression for the variance of the Wiener sausage volume, $\sigma_{v_R}^2(t)$, obtained in Ref. 6,

$$\sigma_{v_R}^2(t) \simeq 16\pi^2 R^4 D t \ln \left(\frac{D t}{R^2} \right), \quad D t \gg R^2. \quad (3.8)$$

Using Eqs. (3.7) and (3.8), we find

$$\sigma_{A_R}^2(t) \simeq \frac{1}{3} \frac{\partial^2}{\partial R^2} \sigma_{v_R}^2(t), \quad D t \gg R^2. \quad (3.9)$$

This relation is valid only at long times, $D t \gg R^2$.

Finally we note that the variance of a stochastic process with independent stationary increments is proportional to time. It is obvious that the surface area of the Wiener sausage is not such a process. This is the reason why the variance $\sigma_{A_R}^2(t)$, Eq. (3.7), is a non-linear function of time.

IV. CONCLUDING REMARKS

Using intuitive arguments we have derived the mean surface area of the Wiener sausage, Eq. (2.6), and its variance, Eq. (3.7). Now we discuss the asymptotic behavior of the probability density of the surface area, A_R , in two limits when the area tends to zero and infinity. (Of course, the surface area cannot be smaller than the surface area of the sphere, $4\pi R^2$. So, when saying that $A_R \rightarrow 0$, we mean that A_R is much smaller than the mean value $\langle A_R(t) \rangle$, but still much larger than $4\pi R^2$).

The probability density of A_R at time t , $\varphi(A_R|t)$, is formally defined as

$$\varphi(A_R|t) = \langle \delta(A_R - A_R(W_t)) \rangle, \quad (4.1)$$

where $\delta(z)$ is the Dirac delta-function. The probability density is a bell-shaped function that vanishes as $A_R \rightarrow \infty$ and $A_R \rightarrow 0$, having a maximum inbetween (Fig. 2). At intermediate values of A_R (not too large and not too small), Wiener sausages of a given surface area can be of very different shapes. The situation is different when $A_R \rightarrow \infty$ and $A_R \rightarrow 0$ that allows evaluation of the asymptotic behavior of $\varphi(A_R|t)$.

Trajectories that are responsible for Wiener sausages of very large A_R are almost straight lines. Therefore, such Wiener sausages are very long cylinders of radius R and length l , with the surface area $A_R \simeq 2\pi Rl$, where l is the displacement of the center of the Brownian particle in time t , $l \gg \sqrt{Dt} \gg R$. The probability density of l , $\varphi(l|t)$, is given by the Green's function,

$$\varphi(l|t) \simeq \frac{4\pi l^2}{(4\pi Dt)^{3/2}} \exp\left(-\frac{l^2}{4Dt}\right), \quad l \gg \sqrt{Dt}. \quad (4.2)$$

Since A_R is proportional to l we can find the asymptotic behavior of $\varphi(A_R|t)$ at $A_R \rightarrow \infty$ using $\varphi(l|t)$ in Eq. (4.2). The result is

$$\varphi(A_R|t) \simeq \frac{4\pi A_R^2}{(16\pi^3 R^2 Dt)^{3/2}} \exp\left(-\frac{A_R^2}{16\pi^2 R^2 Dt}\right), \quad A_R \gg Dt. \quad (4.3)$$

This describes how $\varphi(A_R|t)$ approaches zero as $A_R \rightarrow \infty$.

Realizations of the Wiener trajectory, which are responsible for the small- A_R asymptotic behavior of $\varphi(A_R|t)$ have a distinctive feature: They spend all time t in spherical

domains, radii of which are much smaller than the mean displacement $\sqrt{6Dt}$. Such trajectories densely fill in the domains. Therefore, corresponding Wiener sausages are spheres of the radii identical to the domain radii.

The probability $P(r|t)$ that a diffusing particle does not escape from a sphere of radius r , centered at the particle initial position, in time t , $R \ll r \ll \sqrt{Dt}$, is given by

$$P(r|t) \simeq 2 \exp\left(-\frac{\pi^2 Dt}{r^2}\right), \quad r^2 \ll Dt. \quad (4.4)$$

Therefore, the probability density of the maximum deviation r of the trajectory from its starting point in time t , $\varphi(r|t)$, on condition that this deviation is small compared to the mean displacement $\sqrt{6Dt}$, is given by

$$\varphi(r|t) = \frac{\partial P(r|t)}{\partial r} \simeq \frac{4\pi^2 Dt}{r^3} \exp\left(-\frac{\pi^2 Dt}{r^2}\right), \quad r^2 \ll Dt. \quad (4.5)$$

Wiener sausage of a trajectory with maximum deviation from its starting point in time t equal r , $R \ll r \ll \sqrt{Dt}$, is a sphere of radius r , with the surface area $A_R = 4\pi r^2$. We use this to find the small- A_R asymptotic behavior of $\varphi(A_R|t)$,

$$\begin{aligned} \varphi(A_R|t) &= \left[\frac{1}{dA_R/dr} \varphi(r|t) \right] \Big|_{r=\sqrt{A_R/(4\pi)}} \\ &\simeq \frac{16\pi^3 Dt}{A_R^2} \exp\left(-\frac{4\pi^3 Dt}{A_R}\right), \\ &A_R \ll Dt. \end{aligned} \quad (4.6)$$

This shows how $\varphi(A_R|t)$ approaches zero as $A_R \rightarrow 0$.

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FIG. 2. Schematic representation of the probability density $\varphi(A_R|t)$ of the surface area A_R of the Wiener sausage at different moments of time, $t_1 < t_2$. As time increases, the distribution shifts to larger A_R and becomes wider.

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