First passage time for reaching a wall by diffusion

A small object moves around by diffusion with diffusion coefficient D. It starts out a distance d away from an infinite wall, which we take to be at position $x = 0$. How long will it take to reach the wall? This is called the first passage time and we'll call it T, remembering that it is a random quantity. We would like to know the probability distribution of T, or even just its mean value.

$$\begin{aligned} \rho_T(t) &= ? \\ \langle T \rangle &= ? \end{aligned}$$

Guessing

Whatever $\langle T \rangle$ is, it should be determined by the distance d (units of meters) to the wall and the diffusion coefficient D (units of meters^2/second). The larger the distance, the longer we expect the mean first passage time to be. The larger the diffusion coefficient, the smaller the mean first passage time. So a good guess, with the correct units, is

$$\langle T \rangle \propto \frac{d^2}{D}$$

Figuring it out

In order to calculate the distribution of the first passage time, we need to be mathematically able to express events such as "before time t, the diffusing object has not yet touched the wall." At first sight this appears difficult to express in terms of the probability distribution $\rho(x,t)$ of the object's position, since the position tells us nothing about the object's past; knowing that the object is near the wall does not tell us whether it has already bounced off it, or not. The solution is to seek, instead, the *average density of objects that have not yet touched the wall,* which we will call $\rho_{\text{pre}}(x,t)$. Here is the key fact that makes this a useful thing to do: away from the wall, $\rho_{\text{pre}}(x,t)$ obeys the same diffusion equation as the probability density $\rho(x,t)$ does:

$$\frac{\partial \rho_{\text{pre}}(x,t)}{\partial t} = D \frac{\partial^2 \rho_{\text{pre}}}{\partial x^2} \tag{1}$$

The only difference is in the boundary condition at $x = 0$. While diffusing objects are reflected off of the wall, by definition "diffusing objects that have not yet touched the wall" *disappear* when they hit the wall. This is taken into account by making $x = 0$ an absorbing surface, where we maintain the boundary condition

$$\rho_{\text{pre}}(0,t) = 0 \tag{2}$$

Here's the part where I cheat and write down the answer:

$$\rho_{\text{pre}}(x,t) = \Phi(x-d,t) - \Phi(x+d,t), \tag{3}$$

where $\Phi(x,t)$ is the probability distribution of the position of a freely diffusing object that starts out perfectly localized[1]:

$$\Phi(x,t) = \frac{1}{\sqrt{4\pi Dt}} \cdot \exp\left(-\frac{x^2}{4Dt}\right) \tag{4}$$

You can easily verify that Eqn. (3) gives a solution of the diffusion equation (1), and that it obeys the boundary conditions. Indeed, it's a solution of the diffusion equation because it is a sum of terms, each of which is a solution – and the diffusion equation is linear. As for the boundary conditions, by construction

$$\rho_{\text{pre}}(0,t) = \Phi(-d,t) - \Phi(d,t) = 0 \tag{5}$$

Now we have $\rho_{\text{pre}}(x,t)$, which is the average spatial density of objects that have not yet hit the wall. This makes sense only for $x > 0$, of course! As soon as the objects hit the wall at $x = 0$, they "leak out" and are no longer considered. At time t, the probability that the object has not yet hit the wall is

$$\begin{aligned}
\text{Prob}(T > t) &= \int_0^\infty \rho_{\text{pre}}(x,t)dx \\
&= \int_0^\infty \Phi(x-d,t)dx - \int_0^\infty \Phi(x+d,t)dx \\
&= \int_{-d}^\infty \Phi(x,t)dx - \int_d^\infty \Phi(x,t)dx \\
&= \int_{-d}^d \Phi(x,t)dx = 2\int_0^d \Phi(x,t)dx = \text{erf}\left(\frac{d}{\sqrt{4Dt}}\right), \qquad (6)
\end{aligned}$$

where we have used the error function

$$\text{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du \tag{7}$$

Now you must convince yourself[2] that

$$\rho_T(t) = -\frac{\partial}{\partial t}\text{Prob}(T > t) \tag{9}$$

[1] In other words, Φ is the Green's function for the diffusion equation.

[2] Fine then, I will convince you. For a very small number dt,

$$\rho_T(t)dt = \text{Prob}(T > t) - \text{Prob}(T > t + dt), \tag{8}$$

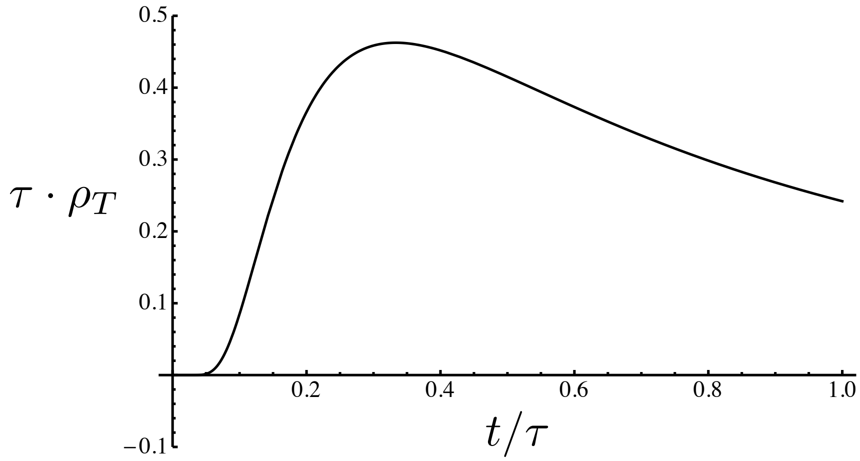

Figure 1: Close-up of probability distribution of first passage time, highlighting the essential singularity at $t = 0$. Here $\tau = d^2/2D$.

Then, the probability distribution of the first passage time is

$$\begin{aligned} \rho_T(t) &= -\frac{\partial}{\partial t}\text{Prob}(T > t) \\ &= -\text{erf}'\left(\frac{d}{\sqrt{4Dt}}\right) \cdot \frac{d}{\sqrt{4D}} \cdot (-\frac{1}{2})t^{-3/2} \\ &= \frac{d}{\sqrt{4\pi D}} \cdot t^{-3/2} \exp\left(-\frac{d^2}{4Dt}\right) \end{aligned} \tag{10}$$

Remember that this is the probability distribution for t and consider where t shows up in it! What you see in the exponential is called an "essential singularity" at $t = 0$.

Let's define a characteristic time

$$\tau \equiv \frac{d^2}{2D}$$

Then

$$\tau \cdot \rho_T(t) = \frac{1}{\sqrt{2\pi}} \cdot \left(\frac{\tau}{t}\right)^{3/2} \cdot \exp\left(-\frac{\tau}{2t}\right) \tag{11}$$

There are interesting things happening at both large and small t. We have already commented on the essential singularity at $t = 0$, whose effects can be seen in Fig. 1.

For large t, the exponential factor $\exp(-\tau/2t)$ becomes equal to 1, and the distribution falls off as a power law:

$$\rho_T(t) \propto t^{-3/2} \qquad \text{(Large } t\text{)} \tag{12}$$

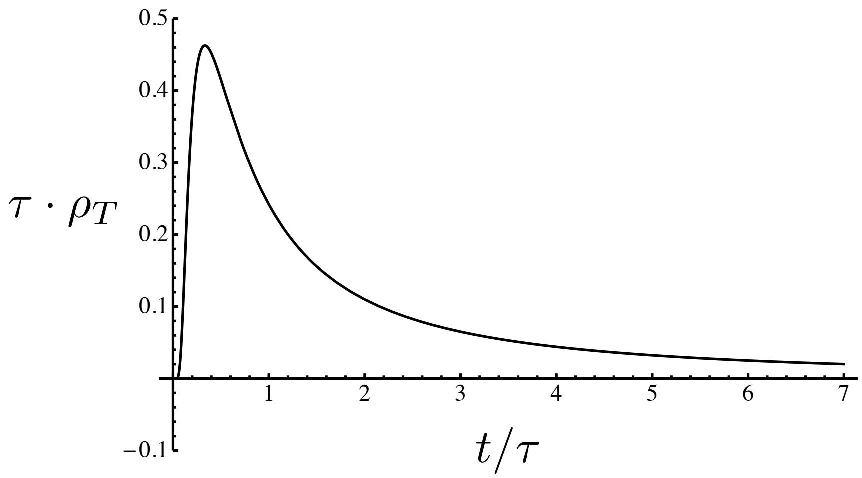

Figure 2: Probability distribution of first passage time to a wall. Here $\tau = d^2/2D$.

The tail of the distribution is "heavy" in the sense that it has a significant probability. Numerically, one finds that the probability that $T > 7 \cdot \tau$ is about 30 percent; by no means has the curve in Fig. 2 finished decaying to zero. An important consequence of this heavy tail is that the mean first passage time diverges!

$$\langle T \rangle = \int_0^\infty t \cdot \rho_T(t) dt \propto \int_0^\infty \frac{1}{\sqrt{t}} \cdot dt = \infty \tag{13}$$

So I guess my initial guess, that $\langle T \rangle \approx d^2/D$ was off. Off by infinity. This first passage time is one of those strange beasts among random variables. It is always well-defined, in the sense that the object will *always* eventually hit the wall. However, the mean time it takes to do so does not exist.[3]

[3]The median of the distribution of first passage times is, however, well-defined. It is about $2.2 \cdot \tau$.