One dimensional diffusion equation with absorbing boundary condition.

Consider the problem where a Brownian particle gets absorbed once it reaches the position x_a. We want to solve for the probability distribution $P_a(x,t)$ in the presence of the absorbing boundary. Thus we need to solve the diffusion equation:

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

with the *boundary* condition

$$P_a(x = x_a, t) = 0 \tag{2}$$

and *initial* condition

$$P_a(x, t = 0) = \delta(x). \tag{3}$$

We first expand $P_a(x,t)$ using a basis set of functions $\{\phi_k(x)\}$ which satisfy the following equation and boundary condition (corresponding to Eq. 2) :

$$\frac{\partial^2 \phi_k}{\partial^2 x} = -k^2\phi_k \quad \text{with} \quad \phi_k(x = x_a) = 0.$$

One easily gets the following solution:

$$\phi_k(x) = (\frac{2}{\pi})^{1/2}\sin k(x - x_a)$$

and these satisfy the orthonormality condition $\int_{-\infty}^{x_a} dx\phi_k(x)\phi_{k'}(x) = \delta(k - k')$. Note that k is restricted to positive values only. Thus we get the following expansion and inverse transform:

$$P_a(x,t) = \int_0^\infty dk\tilde{P}_a(k,t)\phi_k(x) \tag{4}$$

$$\tilde{P}_a(k,t) = \int_{-\infty}^{x_a} dx P_a(x,t)\phi_k(x) \tag{5}$$

Substituting the expansion Eq. 4 in Eq. 1 we get the following equation for $\tilde{P}_a(k,t)$:

$$\frac{\partial \tilde{P}_a(k,t)}{\partial t} = -Dk^2\tilde{P}_a(k,t)$$

which is a simple differential equation of the form $dy/dt = -ay$ and has the solution $\tilde{P}_a(k,t) = \tilde{P}_a(k,0)e^{-Dk^2t}$. We can determine $\tilde{P}_a(k,0)$ from Eq. 5 and the initial condition $P_a(x,t=0) = \delta(x)$. This gives $\tilde{P}_a(k,0) = \phi_k(x_a) = -(2/\pi)^{1/2}\sin kx_a$. We thus finally get the following solution:

$$\begin{aligned} P_a(x,t) &= -\int_0^\infty dk\frac{2}{\pi}\sin kx_a \sin k(x - x_a)e^{-Dk^2t} \\ &= \frac{1}{2\pi}\int_{-\infty}^\infty dk[\cos kx - \cos k(2x_a - x)]e^{-Dk^2t} \\ &= P(x,t) - P(2x_a - x, t) \end{aligned} \tag{6}$$

where $P(x) = e^{-x^2/(4Dt)}/(4\pi Dt)^{1/2}$ is the usual solution of the diffusion equation without any boundary conditions. Note that $P(2x_a - x, t)$ is also a solution of the diffusion equation but with the Brownian particle initially located at the *i*mage point $2x_a$. You can thus directly verify that Eq. 6 is a solution of the diffusion equation and satisfies the boundary and initial conditions.

Note: When we think of the solution $P(x,t)$ of the diffusion equation, we can either think of it as giving the probability of a single random walker to be between x and $x+dx$ at time t, OR, alternatively we can imagine a gas of noninteracting brownian particles and then $P(x)dx$ gives the fraction of particles in dx. Both viewpoints are valid and useful.

Survival probaility of a particle. Since particles get continually absorbed at the boundary at x_a, the total probability is not conserved and the quantity

$$P_s(t) = \int_{-\infty}^{x_a} dx P_a(x,t) \tag{7}$$

infact gives the fraction of particles that have not been absorbed till time t. Also one can think of $P_s(t)$ as the probability that a diffusing particle, starting from the origin, has not hit the wall at x_a (and got killed!). Hence it is referred to as the survival probability of a random walker. After some simple manipulations we get:

$$P_s(t) = 2\int_0^{x_a} P(x)dx = \frac{2}{(4\pi Dt)^{1/2}}\int_0^{x_a} e^{-\frac{x^2}{4Dt}}dx = \frac{2}{\pi^{1/2}}\int_0^{\frac{x_a}{(4Dt)^{1/2}}} e^{-u^2}du \tag{8}$$

From the definition of the error function $erf(z) = (2/\sqrt{\pi})\int_0^z e^{-u^2}du$ we then finally get:

$$P_s(t) = erf(\frac{x_a}{(4Dt)^{1/2}}) \sim \frac{1}{t^{1/2}} \qquad \text{at large times} \tag{9}$$

Next let us ask the question "what is the probability $F(t)dt$ that a particle gets absorbed (at x_a) between times t and $t+dt$?" By definition: $F(t)dt = P_s(t) - P_s(t+dt)$. Thus

$$F(t) = -\frac{dP_s(t)}{dt} = \frac{x_a}{t}\frac{1}{(4\pi Dt)^{1/2}}e^{-\frac{x_a^2}{4Dt}} \sim \frac{1}{t^{3/2}} \qquad \text{at large times.} \tag{10}$$

A more direct way to obtain $F(t)$ is to note that it also gives the fraction of particles that get absorbed per unit time and so is simply the particle current evaluated at x_a. Thus

$$F(t) = -D\frac{\partial P_a}{\partial x}|_{x=x_a} \tag{11}$$

Finally note that $F(t)$ also gives the first passage probability, *i*.e., the probability that a particle, starting from the origin, reaches the point x_a for the first time between times t and $t+dt$. We can then ask "What is the probability that a random walker, starting from the origin, ever reaches the point x_a ?". This is simply given by $\int_0^\infty dtF(t)$ and evaluation of the integral gives the value one. Thus in one dimension, a random walker will eventually reach any given point. This is also true in two dimensions but not so in higher dimensions !!(This result is known as Polya's theorem).

One dimensional random walker in the presence of a reflecting barrier.

Supposing that we have a hard wall at the point $x = x_r$ and particles cannot penetrate through it. A brownian particle reaching this point gets reflected from it. Thus we now need to solve the diffusion equation with the boundary condition that the particle current at the point x_r is zero, *i.e*

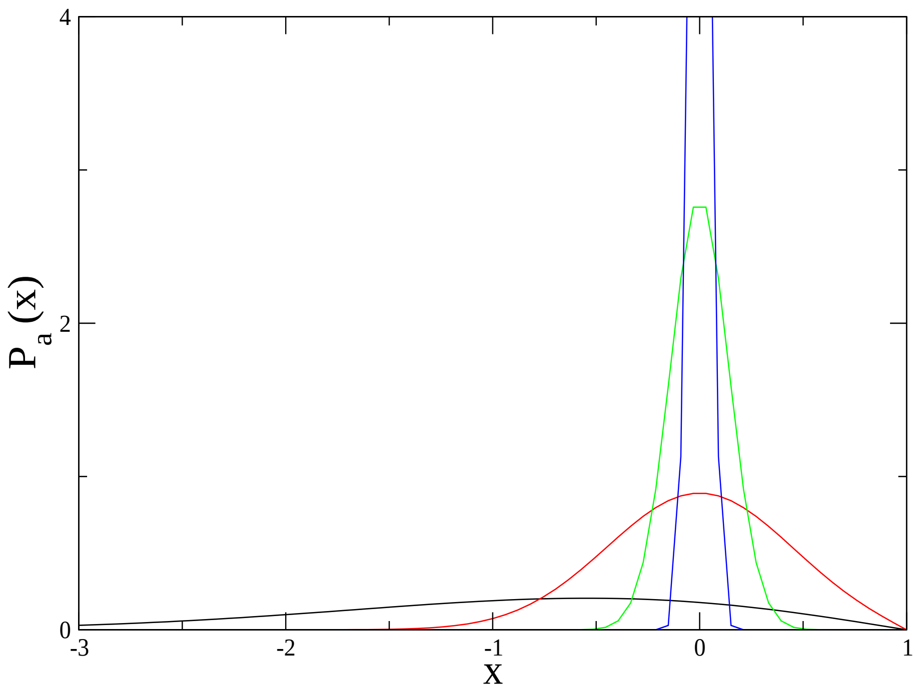
$$-D\frac{\partial P_r(x)}{\partial x} \mid_{x=x_r} = 0. \tag{12}$$

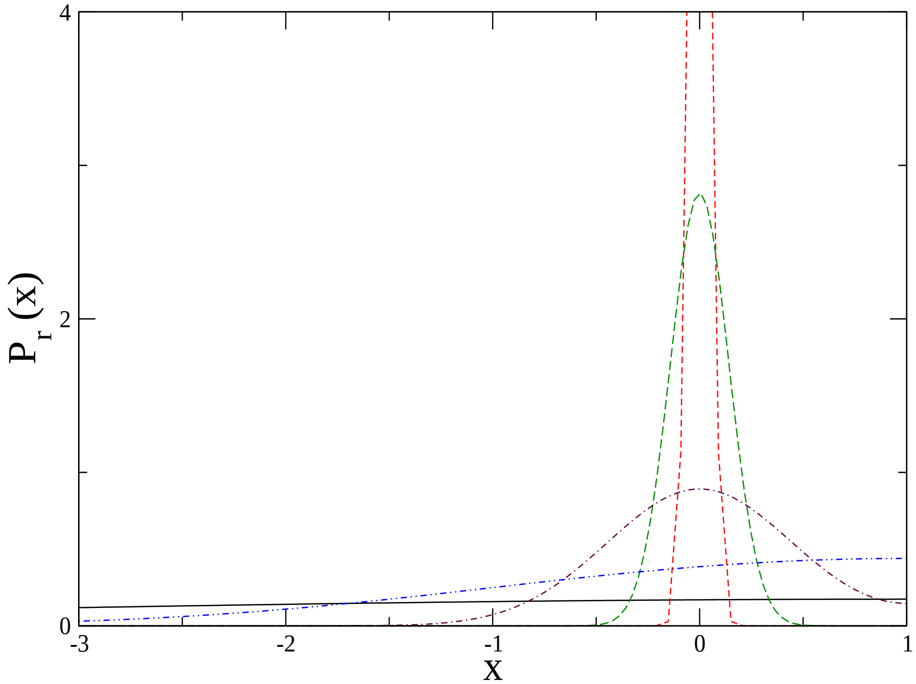
The solution for this boundary condition and the initial condition $P_r(x, t = 0) = \delta(x)$ can be obtained in the same way as for the absorbing boundary (expanding in a basis satisfying the new boundary conditions, etc.). The final solution is simple and is given by:

$$P_r(x,t) = P(x,t) + P(2x_r - x, t) \tag{13}$$

It is easily verified that this is a solution of the diffusion equation and also satisfies the correct boundary and initial conditions. In this case we can also verify, as expected, that $\int_{-\infty}^{x_r} dx P_r(x) = 1$.

The plots below show the time evolution of the probability densities of a random walker with absorbing and reflecting boundaries (at $x = 1$).





Problems:

(1) We have obtained a solution of the first passage problem by working directly in the continuum limit. This problem can also be solved by studying the discrete random walk. Understand this solution for the absorbing and reflecting barriers given in Refns. (1) and (2).

(2) Solve the diffusion equation with the following boundary conditions:

(i) One reflecting and one absorbing wall.

(ii) Two absorbing walls. In this case solve the problem by inspection using the method of images. Also solve it directly using expansion in with an appropriate basis. Compare the two solutions and prove that they are equal. You may need to use the following

$$\textit{Poisson summation formula:} \quad \sum_{-\infty}^{\infty} f(n) = \sum_{-\infty}^{\infty} \tilde{f}(2\pi p) \tag{14}$$

where $f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \tilde{f}(k)$.

REFERENCES:

(1) S. Chandrashekhar, Rev. Mod. Phys. **15**, 1 (1943).

(2) W. Feller, An Introduction to probababilty theory and its applications.

(3) S. Redner, A guide to first-passage processes.

(4) Itzykson and Drouffe, Statistical Field Theory (Chapter 1).