One-dimensional diffusion on a finite region

Markus Deserno

Department of Chemistry and Biochemistry, UCLA, USA
(Dated: December 10, 2004)

We study the problem of simple diffusion of one particle on a finite line with reflecting boundaries. Probability density and variance are expressed as an expansion in eigenmodes of the Fokker-Planck operator for a particle which starts to diffuse in the middle of the line. We find the well known short-time behavior \( \sigma^2(t) = 2Dt \), but the full solution also yields precise asymptotics for long times.

I. THE DIFFUSION EQUATION

We want to solve the diffusion equation

\[
\frac{\partial}{\partial t} P(x, t) = D \frac{\partial^2}{\partial x^2} P(x, t),
\]

where \( P(x, t) \) is the probability density of finding a particle at position \( x \) at time \( t \) and \( D \) is the diffusion constant. The factorization ansatz

\[
P(x, t) = \varphi(x) e^{-\lambda t}
\]

leads to the eigenvalue equation

\[
\left[ \frac{d^2}{dx^2} + \omega^2 \right] \varphi(x) = 0 \quad \text{with} \quad \omega^2 = \frac{\lambda}{D}.
\]

We want to find a solution of the diffusion problem on the line \([-L/2; L/2]\). The eigenfunctions of the harmonic oscillator type equation (3) are sine and cosine functions. In the present case the eigenfunctions can additionally be classified by the symmetry of the mode:

\[
\varphi_{o,n}(x) = \sin(\omega_{o,n} x), \quad \varphi_{e,n}(x) = \cos(\omega_{e,n} x)
\]

The eigenvalues \( \omega_{o,n} \) and \( \omega_{e,n} \) follow from the boundary conditions. We will assume reflecting boundaries and hence set the probability current at \( \pm L/2 \) to zero [1]:

\[
0 \equiv -D \frac{\partial}{\partial x} P(x, t) \implies \varphi'(\pm L/2) = 0.
\]

This determines the eigenvalues

\[
\omega_{o,n} = \frac{2\pi(n + 1/2)}{L}, \quad \omega_{e,n} = \frac{2\pi n}{L}.
\]

From there we get \( \lambda_n = D\omega_n^2 \) for odd and even modes. We now can write down the spatial part of the solution:

\[
\varphi(x) = \sum_{n=0}^{\infty} \left[ A_{e,n} \cos \frac{2\pi nx}{L} + A_{o,n} \sin \frac{2\pi(n + 1/2)x}{L} \right]
\]

The normalization condition

\[
1 \equiv \int_{-L/2}^{L/2} dx \left[ \frac{2\pi n x}{L} \right] A_{e,n} \cos \frac{2\pi nx}{L} + A_{o,n} \sin \frac{2\pi(n + 1/2)x}{L}
\]

fixes \( A_{e,0} = 1/L \), but leaves all other amplitudes unspecified.

II. START IN THE MIDDLE

A. Probability density

We now want to find the particular solution for the symmetric initial condition \( P(x, 0) = \delta(x) \), i.e., a particle starting to diffuse in the middle of the line. Since \( \delta(x) \) is an even “function”, all \( A_{o,n} \) must vanish. Furthermore, on the interval \([-L/2; L/2]\) the delta function can be represented as

\[
L \delta(x) = 1 + 2 \sum_{n=1}^{\infty} \cos \frac{2\pi n x}{L}.
\]

The right hand side is actually periodic with period \( L \), but this does not matter since we are only interested in its values within \([-L/2; L/2]\). Comparing coefficients with Eqn. (7) shows that \( A_{e,n} = 2/L \) for \( n > 0 \). The full time-dependent solution of the diffusion problem is thus

\[
P(x, t) = \frac{1}{L} + \frac{2}{L} \sum_{n=1}^{\infty} \cos \frac{2\pi n x}{L} \exp \left\{ -\frac{4\pi^2 n^2 D t}{L^2} \right\}.
\]

An illustration of the time evolution of this probability density is given in Fig. 1.

FIG. 1: Time evolution of the probability density \( P(x, t) \) from Eqn. (10) for the time steps \( Dt/L^2 = 0.0001, 0.0002, 0.0005, 0.001, \ldots, 1.0 \).
B. Variance

Using the integral $\int_{-\pi}^{\pi} dy y^2 \cos(y) = 4\pi n(-1)^n$ for $n \in \mathbb{N}_0$, we can compute the time-dependent variance of the distribution function $P(x,t)$ from Eqn. (10):

$$\frac{\sigma^2(t)}{L^2} = \frac{1}{L^2} \int_{-L/2}^{L/2} dx x^2 P(x,t)$$
$$= \frac{1}{12} + \frac{1}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \exp \left\{ -\frac{4\pi^2 n^2 Dt}{L^2} \right\}. \quad (11)$$

This can be viewed as an expansion for large times, but it is valid for all $t$. The lowest nontrivial order is

$$\frac{\sigma^2(t)}{L^2} = \frac{1}{12} - \frac{1}{\pi^2} \exp \left\{ -\frac{4\pi^2 Dt}{L^2} \right\}. \quad (12)$$

To get the asymptotic behavior at small $t$ is a little bit more tricky: A naive expansion of the exponential $\exp\{-4\pi^2 n^2 Dt/L^2\}$ for small $t$ is barred by the fact that $n^2$ will always become large during the course of performing the sum [3]. Instead, we will use the Euler-Maclaurin summation formula [2], which is a controlled way for replacing a sum by an integral. It reads

$$\sum_{k=1}^{n} f(k) = \int_0^n dk \ f(k) - \frac{1}{2} [f(0) + f(n)] + \frac{1}{12} [f'(n) - f'(0)] - \frac{1}{720} [f'''(n) - f'''(0)] \pm \cdots \quad (13)$$

Using this, we can rewrite the sum entering the expression of $P(x,t)$ as

$$\sum_{n=1}^{\infty} \cos \frac{2\pi nx}{L} \exp \left\{ -\frac{4\pi^2 n^2 Dt}{L^2} \right\}$$
$$= \int_0^\infty dn \ \cos \frac{2\pi nx}{L} \exp \left\{ -\frac{4\pi^2 n^2 Dt}{L^2} \right\} - \frac{1}{2}$$
$$= \frac{\exp\{-x^2/4Dt\}}{4\sqrt{\pi Dt/L^2}} - \frac{1}{2}, \quad (14)$$

from which by inserting into Eqn. (10) we get

$$P(x,t) \quad \frac{Dt \leq L^2}{\sqrt{2\pi(2Dt)}} \exp \left\{ -\frac{x^2}{2(2Dt)} \right\}. \quad (15)$$

This is obviously a Gaussian with variance $\sigma^2(t) = 2Dt$.

A plot of the variance $\sigma^2(t)$ and a few of its asymptotics and approximations is shown in Fig. 2.

---

[3] The only exception is $t = 0$, in which case the summation formula $\sum_{n=1}^{\infty} (-1)^n / n^2 = -\pi^2/12$ correctly results in $\sigma^2(0) = 0$. 

---

FIG. 2: Variance $\sigma^2(t)$ from Eqn. (11) and some of its asymptotics and approximations.