One-dimensional diffusion on a finite region

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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

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

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

$$P(x,t) \;=\; \varphi(x)\,\mathrm{e}^{-\lambda t} \tag{2}$$

leads to the eigenvalue equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \omega^2\right]\varphi(x) \;=\; 0 \qquad \text{with} \qquad \omega^2 = \frac{\lambda}{D}. \tag{3}$$

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:

$$\varphi_{\mathrm{o},n}(x) = \sin(\omega_{\mathrm{o},n}x) \quad , \quad \varphi_{\mathrm{e},n}(x) = \cos(\omega_{\mathrm{e},n}x) \tag{4}$$

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

$$0 \;\stackrel{!}{=}\; -D\frac{\partial}{\partial x}P(x,t) \quad \Rightarrow \quad \varphi'(\pm L/2) = 0. \tag{5}$$

This determines the eigenvalues

$$\omega_{\mathrm{o},n} \;=\; \frac{2\pi(n+1/2)}{L} \quad , \quad \omega_{\mathrm{e},n} \;=\; \frac{2\pi n}{L}. \tag{6}$$

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:

$$\varphi(x) = \sum_{n=0}^{\infty}\left[A_{\mathrm{e},n}\cos\frac{2\pi nx}{L} + A_{\mathrm{o},n}\sin\frac{2\pi(n+1/2)x}{L}\right]. \tag{7}$$

The normalization condition

$$\begin{aligned} 1 \;&\stackrel{!}{=}\; \int_{-L/2}^{L/2}\mathrm{d}x\;\left[A_{\mathrm{e},n}\cos\frac{2\pi nx}{L} + A_{\mathrm{o},n}\sin\frac{2\pi(n+1/2)x}{L}\right] \\ &=\; A_{\mathrm{e},0}L \end{aligned} \tag{8}$$

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

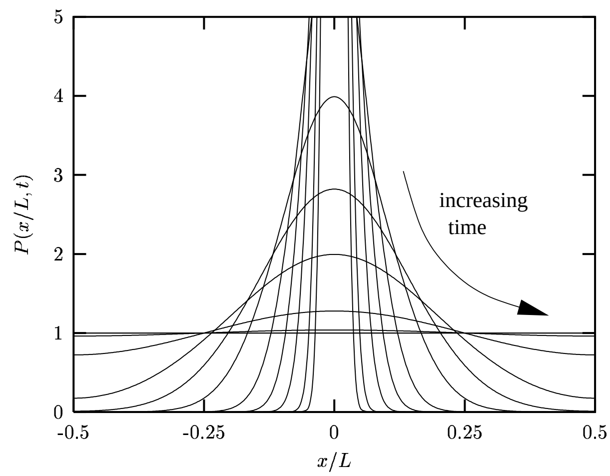

FIG. 1: Time evolution of the probability density $P(x,t)$ from Eqn. (10) for the time steps $Dt/L^2 = 0.0001, 0.0002, 0.0005, 0.001, \ldots, 1.0$.

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 $A_{\mathrm{o},n}$ must vanish. Furthermore, on the interval $[-L/2; L/2]$ the delta function can be represented as

$$L\,\delta(x) \;=\; 1 + 2\sum_{n=1}^{\infty}\cos\frac{2\pi nx}{L}. \tag{9}$$

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 $A_{\mathrm{e},n} = 2/L$ for $n > 0$. The full time-dependent solution of the diffusion problem is thus

$$P(x,t) = \frac{1}{L} + \frac{2}{L}\sum_{n=1}^{\infty}\cos\frac{2\pi nx}{L}\exp\left\{-\frac{4\pi^2n^2Dt}{L^2}\right\}. \tag{10}$$

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

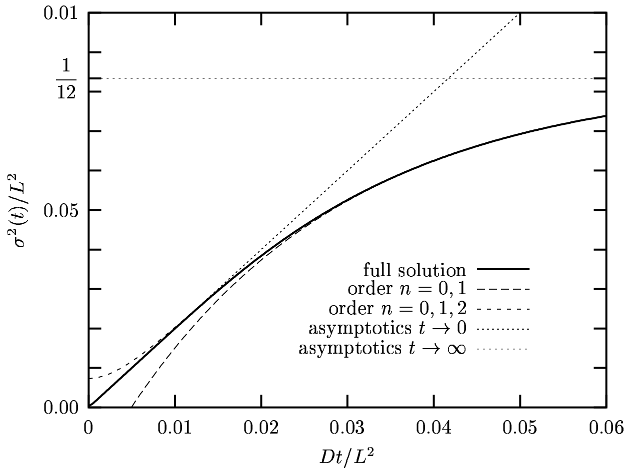

FIG. 2: Variance $\sigma^2(t)$ from Eqn. (11) and some of its asymptotics and approximations.

B. Variance

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

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

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

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

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

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

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

$$P(x,t) \overset{Dt \ll L^2}{=} \frac{1}{\sqrt{2\pi(2Dt)}} \exp\left\{-\frac{x^2}{2(2Dt)}\right\}. \quad (15)$$

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.

[1] H. Risken, "*The Fokker-Planck-Equation*", 2nd ed., Springer, Berlin (1996).

[2] M. Abramowitz and I. A. Stegun (ed.), *Handbook of mathematical functions*, 9th printing, Dover, New York (1970).

[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 $\sigma^2(0) = 0$.