Computational Physics Group Assignment 1

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1 2D Random Walk

2 Diffusion Equation

a) Consider the 1D Normal Distribution

$$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} e^{-\frac{x^2}{2\sigma^2(t)}} \tag{1}$$

The spatial expectation value $< x^2(t) >$ can be computed by

$$\begin{aligned}
< x^2(t) > &= \int_{-\infty}^{\infty} x^2 \rho(x,t) dt \\
&= \frac{1}{\sqrt{2\pi\sigma^2(t)}} \int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{2\sigma^2(t)}} dx \\
&= \frac{1}{\sqrt{2\pi\sigma^2(t)}} \frac{1}{2} (\sqrt{2}\sigma(t))^3 \sqrt{\pi} \\
&= \sigma^2(t)
\end{aligned}$$

Here $\int_{-\infty}^{\infty} x^{2k} e^{-\frac{x^2}{a^2}} dx = \frac{(2k+1)!!}{(2k+1)2^k} a^{2k+1} \sqrt{\pi}$ $(k = 0, 1, 2, ...)$ is used.

b) The diffusion equation with a constant diffusion coefficient has the following form:

$$\frac{\partial u(r,t)}{\partial t} = D \nabla^2 u(r,t) \tag{2}$$

In one-dimensional case, equation (2) becomes

$$\frac{\partial u(r,t)}{\partial t} = D \frac{\partial^2 u(x,t)}{\partial x^2} \tag{3}$$

The first derivative in time and second derivative in space can be approximated by the finite difference:

$$\begin{aligned}
\frac{\partial u(r,t)}{\partial t} &= \frac{u(x, t+\Delta t) - u(x,t)}{\Delta t} \\
\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{u(x+\Delta x, t) + u(x-\Delta x, t) - 2u(x,t)}{(\Delta x)^2}
\end{aligned}$$

Then equation (3) can be rewritten as

$$\frac{u(x, t+\Delta t) - u(x,t)}{\Delta t} = D \cdot \frac{u(x+\Delta x, t) + u(x-\Delta x, t) - 2u(x,t)}{(\Delta x)^2}$$

or equivalently,

$$u(x, t+\Delta t) = u(x,t) + D \cdot \Delta t \cdot \frac{u(x+\Delta x, t) + u(x-\Delta x, t) - 2u(x,t)}{(\Delta x)^2} \tag{4}$$

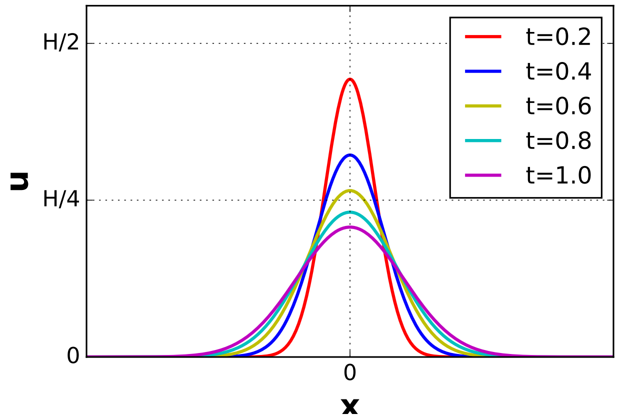

Figure 1: Solution of 1D diffusion equation at time 0, 0.2, 0.4, 0.6, 0.8, 1.0.

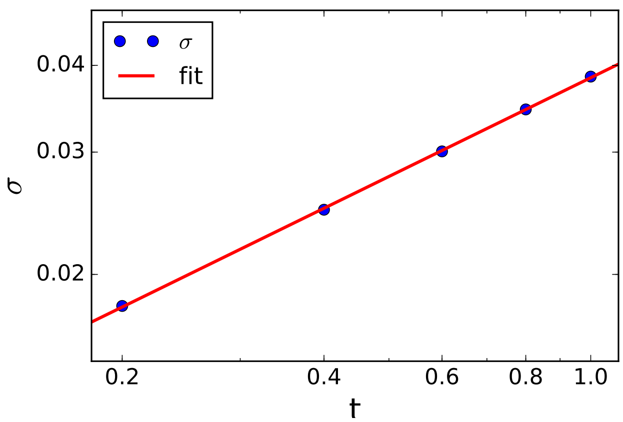

Figure 2: σ versus t (log plot).

Starting from an initial box density profile, the 1D diffusion equation (3) is numerically solved based on equation (4). The density profile at later times is plotted in figure 1. The density are normally distributed, with different standard deviation σ. The value of σ at time t can be extracted from the maximum value of density u_{max} at $x = 0$.

$$u_{max}(t) = \rho(0, t) = \frac{1}{\sqrt{2\pi\sigma^2(t)}}$$
$$\Rightarrow \sigma(t) = \frac{1}{\sqrt{2\pi u_{max}^2(t)}}$$

The maximum values u_{max} and derived *sigma* at time 0.2, 0.4, 0.6, 0.8, 1.0 are listed in table **??**. The $\sigma(t)$ versus time t is plotted (log scale) in figure 2 with a linear fit line, which has a scope of 0.478. This indicates that $\sigma(t) \propto \sqrt{t}$.

Table 1: u_{max} at time 0.2, 0.4, 0.6, 0.8, 1.0.

t	0.2	0.4	0.6	0.8	1.0
u_{max}	22.1449	16.0971	13.2666	11.5433	10.3539
σ [$\times 10^{-2}$]	1.8015	2.4783	3.0071	3.4560	3.8531

3 Mixing of two Gases