

PHY566 - Diffusion Equation

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1 Problem 1

2 Problem 2

2.1 Part A

To calculate $\langle x(t)^2 \rangle$, we can integrate it by part:

$$\begin{aligned}\rho(x, t) &= \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right) \\ \langle x(t)^2 \rangle &= \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right) dx \\ \langle x(t)^2 \rangle &= \int_{-\infty}^{\infty} \sigma(t)^2 x \frac{1}{\sqrt{2\pi\sigma(t)^2}} d\left(\exp \frac{-x^2}{2\sigma(t)^2}\right) \\ \langle x(t)^2 \rangle &= \sigma(t)^2 \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right) dx \\ \langle x(t)^2 \rangle &= \sigma(t)^2\end{aligned}$$

Therefore, the spatial expectation value $\langle x(t)^2 \rangle$ of the 1D Normal Distribution equals $\sigma(t)^2$

2.2 Part B

The diffusion equation is:

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

where $D = 2$ is a diffusion constant. For a linear diffusion equation:

$$\frac{\partial \phi(\vec{r}, t)}{\partial t} = D \frac{d^2 \phi(\vec{r}, t)}{dx^2}$$

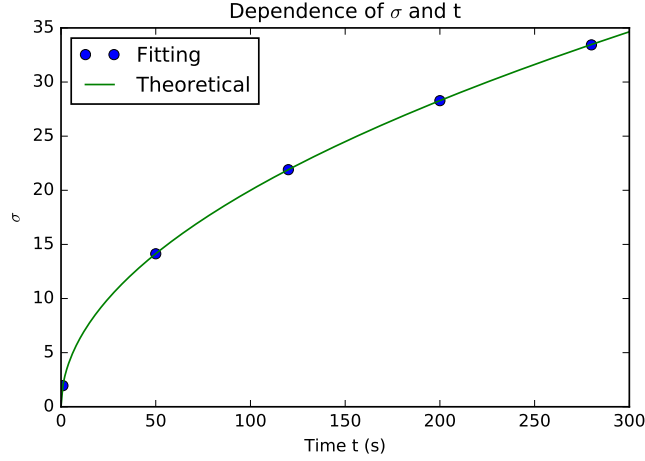
The numerical solution is:

$$\begin{aligned}\frac{y_{j+1,i} - y_{j,i}}{\Delta t} &= D \frac{y_{j,i+1} + y_{j,i-1} - 2y_{j,i}}{\Delta x^2} \\ y_{j+1,i} &= y_{j,i} + \frac{D\Delta t}{\Delta x^2} (y_{j,i+1} + y_{j,i-1} - 2y_{j,i})\end{aligned}$$

After getting y in each x for each time snapshot, we obtained $\sigma(t)$ by fitting it into equation:

$$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right)$$

We choose 5 time snapshots [1,50,120,200,280] ($\Delta t = 0.01$) to get $\sigma(t)$ and plot them in following figure.



The fitting points match the analytical function perfectly.