APM346 Tutorial 3

Partial Differential Equations

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The focus of this tutorial is the *Schrödinger equation* $i\hbar\Psi_t = \frac{-\hbar^2}{2m}\Psi_{xx} + V\Psi$. As in the class notes ([1]), we work with the following simple form of the potential ("particle in a box"):

$$V(x) = \begin{cases} 0, \ 0 < x < l \\ \infty, \ \text{else} \end{cases}$$

So, we are dealing with the PDE

$$\begin{cases} i\hbar\Psi_t = \frac{-\hbar^2}{2m}\Psi_{xx} \ (0 < x < l, \ t > 0) \\ \Psi(x,0) = \phi(x) \\ \Psi(0,t) = \Psi(l,t) = 0 \end{cases} \tag{1}$$

where we require the normalization $\int_0^l |\Psi(x,t)|^2 dx = 1$.

Remark. Since $\int_0^l |\Psi(x,t)|^2 dx = 1$, taking $t = 0$ we must have that $\int_0^l |\phi(x)|^2 dx = 1$

From the class notes ([1]), via separation of variables we have the following general solution:

$$\Psi(x,t) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{l}\right) e^{-iE_n t/\hbar}$$

where the constants (now possibly complex) are given by $A_n = \frac{2}{l}\int_0^l \phi(x)\sin\left(\frac{n\pi x}{l}\right)dx$. Here $E_n = \frac{n^2\pi^2\hbar^2}{2ml^2}$ is the energy of the n-th stationary state.

Example 1

Find the solution $\Psi(x,t)$ to the Schrödinger equation (1) (including the normalization constant N) given initial condition

$$\Psi(x,0) = \phi(x) = N\left(2\sin\left(\frac{3\pi x}{l}\right) + e^{i\pi/3}\sin\left(\frac{4\pi x}{l}\right)\right)$$

We have:

$$\begin{aligned} 1 &= \int_0^l |\phi(x)|^2 dx \\ &= N^2 \int_0^l \left(2\sin\left(\frac{3\pi x}{l}\right) + e^{-i\pi/3}\sin\left(\frac{4\pi x}{l}\right)\right)\left(2\sin\left(\frac{3\pi x}{l}\right) + e^{i\pi/3}\sin\left(\frac{4\pi x}{l}\right)\right) dx \\ &= N^2 \int_0^l \left[4\sin^2(\frac{3\pi x}{l}) + 2e^{i\pi/3}\sin\left(\frac{3\pi x}{l}\right)\sin\left(\frac{4\pi x}{l}\right) + 2e^{-i\pi/3}\sin\left(\frac{3\pi x}{l}\right)\sin\left(\frac{4\pi x}{l}\right)\right. \\ &\quad \left. + e^{-i\pi/3}e^{i\pi/3}\sin^2(\frac{4\pi x}{l})\right] dx \\ &= N^2\left(4\frac{l}{2} + 0 + 0 + \frac{l}{2}\right) \\ &= N^2\frac{5l}{2} \end{aligned}$$

where we used the orthogonality relations. Hence, $N = \sqrt{\frac{2}{5l}}$ and we conclude that

$$\Psi(x,t) = \sqrt{\frac{2}{5l}}\left(2\sin\left(\frac{3\pi x}{l}\right)e^{-iE_3t/\hbar} + e^{i\pi/3}\sin\left(\frac{4\pi x}{l}\right)e^{-iE_4t/\hbar}\right)$$

Example 2

Noting that $|\Psi(x,t)|^2$ is the probability density for the position of the particle, we define the expected value at time t to be

$$< x >= \int_0^l x|\Psi(x,t)|^2 dx$$

Consider the following normalized solution

$$\Psi(x,t) = \sqrt{\frac{2}{5l}}\left(2\sin\left(\frac{\pi x}{l}\right)e^{-iE_1t/\hbar} + \sin\left(\frac{3\pi x}{l}\right)e^{-iE_3t/\hbar}\right)$$

Find $|\Psi(x,t)|^2$ and $< x >$ for all time. Does $< x >$ oscillate in time? If so, at what frequency?

We have that:

$$|\Psi(x,t)|^2 = \frac{2}{5l}\left(2\sin\left(\frac{\pi x}{l}\right)e^{iE_1t/\hbar} + \sin\left(\frac{3\pi x}{l}\right)e^{iE_3t/\hbar}\right)\left(2\sin\left(\frac{\pi x}{l}\right)e^{-iE_1t/\hbar} + \sin\left(\frac{3\pi x}{l}\right)e^{-iE_3t/\hbar}\right)$$
$$= \frac{2}{5l}\left(4\sin^2(\frac{\pi x}{l}) + \sin^2(\frac{3\pi x}{l}) + 2\sin\left(\frac{\pi x}{l}\right)\sin\left(\frac{3\pi x}{l}\right)e^{\frac{iE_1t}{\hbar}}e^{\frac{-iE_3t}{\hbar}} + 2\sin\left(\frac{\pi x}{l}\right)\sin\left(\frac{3\pi x}{l}\right)e^{\frac{-iE_1t}{\hbar}}e^{\frac{iE_3t}{\hbar}}\right)$$
$$= \frac{2}{5l}\left[4\sin^2(\frac{\pi x}{l}) + \sin^2(\frac{3\pi x}{l}) + 2\sin\left(\frac{\pi x}{l}\right)\sin\left(\frac{3\pi x}{l}\right)\left(e^{i(E_1-E_3)t/\hbar} + e^{-i(E_1-E_3)t/\hbar}\right)\right]$$
$$= \frac{2}{5l}\left[4\sin^2(\frac{\pi x}{l}) + \sin^2(\frac{3\pi x}{l}) + 2\sin\left(\frac{\pi x}{l}\right)\sin\left(\frac{3\pi x}{l}\right)2\cos\left(\frac{(E_1-E_3)t}{\hbar}\right)\right]$$

where we have used that $\cos(\theta) = \frac{e^{i\theta}+e^{-i\theta}}{2}$. Now,

$$< x >= \int_0^l x\frac{2}{5l}\left[4\sin^2(\frac{\pi x}{l}) + \sin^2(\frac{3\pi x}{l}) + 2\sin\left(\frac{\pi x}{l}\right)\sin\left(\frac{3\pi x}{l}\right)2\cos\left(\frac{(E_1-E_3)t}{\hbar}\right)\right]dx$$
$$= \frac{2}{5l}\left(4\frac{l^2}{4} + \frac{l^2}{4} + 4\cos\left(\frac{(E_1-E_3)t}{\hbar}\right)\int_0^l x\frac{1}{2}\left[\cos\left(\frac{2\pi x}{l}\right) - \cos\left(\frac{4\pi x}{l}\right)\right]dx\right)$$
$$= \frac{l}{2} + \frac{4}{5l}\cos\left(\frac{(E_1-E_3)t}{\hbar}\right)[0-0]$$
$$= \frac{l}{2}$$

In the above we have used the trigonometric identity $\sin(A)\sin(B) = \frac{1}{2}(\cos(A-B) - \cos(A+B))$ as well as the formulas:

$$\int_0^l x\sin^2(\frac{n\pi x}{l})dx = \frac{l^2}{4}, \qquad \int_0^l x\cos\left(\frac{n\pi x}{l}\right)dx = \frac{l^2(\cos(n\pi)-1)}{n^2\pi^2}$$

We conclude that $< x >$ does not oscillate with time.

Example 3

Find the solution $\Psi(x,t)$ to the Schrödinger equation (1) (including the normalization constant N) given initial condition

$$\Psi(x,0) = \phi(x) = N\left(\sin\Big(\frac{\pi x}{l}\Big) + \sin\Big(\frac{3\pi x}{l}\Big)\right)$$

We have:

$$\begin{aligned} 1 &= \int_0^l |\phi(x)|^2 dx \\ &= N^2 \int_0^l \left[\sin^2(\frac{\pi x}{l}) + 2\sin\Big(\frac{\pi x}{l}\Big)\sin\Big(\frac{3\pi x}{l}\Big) + \sin^2(\frac{3\pi x}{l})\right] dx \\ &= N^2\left(\frac{l}{2} + \frac{l}{2}\right) \\ &= N^2 l \end{aligned}$$

where we used the orthogonality relations. Hence $N = \sqrt{\frac{1}{l}}$ and we conclude that

$$\Psi(x,t) = \sqrt{\frac{1}{l}}\left(\sin\Big(\frac{\pi x}{l}\Big)e^{-iE_1 t/\hbar} + \sin\Big(\frac{3\pi x}{l}\Big)e^{-iE_3 t/\hbar}\right)$$

Important formulas

Here I just want to recall some new formulas we used that are useful to remember.

- $i^2 = -1$
- $|z|^2 = \bar{z} \cdot z$
- Normalization $\int_0^l |\Psi(x,t)|^2 dx = 1 \quad \xrightarrow[t=0]{} \quad \int_0^l |\phi(x)|^2 dx = 1$
- Euler's formula $e^{i\theta} = \cos(\theta) + i\sin(\theta)$
- $< x >= \int_0^l x|\Psi(x,t)|^2 dx$
- $\cos(\theta) = \frac{e^{i\theta}+e^{-i\theta}}{2}$
- $\sin(\theta) = \frac{e^{i\theta}-e^{-i\theta}}{2i}$

Bibliography

[1] Xiao Jie, Instructor's course notes (Quercus)

[2] W. Strauss, *Partial Differential Equations: An Introduction*, 2nd edition, Wiley