# Lecture 5 - Schrödinger equation for a free particle

*What's important*:
- Schrödinger equation for a free particle

*Text* Gasiorowicz, Chap. 3

In the previous lecture, we proposed a candidate function that had many of the attributes that we desire for a wave packet. Starting with the momentum distribution,

$$g(k) = \exp(-\alpha[k-k_o]^2) \qquad \text{(not normalized)}$$

we use the transformation for stationary packets

$$f(x) = \int_{-\infty}^{+\infty} g(k) \exp(ikx)\, dk = \int_{-\infty}^{+\infty} \exp(-\alpha[k-k_o]^2) \exp(ikx)\, dk$$

to obtain

$$f(x) = \exp(-x^2/4\alpha) \bullet \exp(+ik_o x)\, (\pi/\alpha)^{1/2}. \qquad \text{(not normalized, stationary)}$$

For moving wavepackets, we started with

$$f(x,t) = \int_{-\infty}^{+\infty} g(k) \exp(ikx - i\omega t)\, dk, \qquad (1)$$

and then removed $\omega$ in favour of $k$ through the relation

$$\omega = E/\hbar = (\hbar / 2m)\, k^2, \qquad (2)$$

which we found from

$$E = \omega\hbar \qquad (3)$$

and the de Broglie hypothesis

$$p = \hbar k = h / 2\lambda. \qquad (4)$$

Our interpretation of $f(x)$ and $g(k)$ requires that the probabilities $P(x)$ and $P(p)$ are proportional to $|f(x)|^2$ and $|g(x)|^2$, respectively.

We performed these manipulations without much regard to normalization, which we now restore. Transformation (1) becomes

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, \phi(p) e^{i(px-Et)/\hbar} \qquad (5)$$

The relationship can also be written as a partial differential equation. Start by taking the time derivative (multiplying by $i\hbar$ in anticipation of its effect):

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, \phi(p) i\hbar \frac{\partial}{\partial t} e^{i(px-Et)/\hbar}$$
$$= \frac{1}{\sqrt{2\pi\hbar}} \int dp\, \phi(p) E e^{i(px-Et)/\hbar} \qquad (6)$$

Then, replace *E* by $p^2/2m$, and recognize that *p* can be obtained from the exponential by taking its derivative *via*

$$p \to -i\hbar\,(\partial/\partial x) \tag{7}$$

(the minus sign is required because of the form exp(+*ipx*...) in the exponent. The steps from Eq. (6) are

$$\begin{aligned} i\hbar \frac{\partial}{\partial t}\psi(x,t) &= \frac{1}{\sqrt{2\pi\hbar}}\int dp\,\phi(p)\frac{p^2}{2m}e^{i(px-Et)/\hbar} \\ &= \frac{1}{\sqrt{2\pi\hbar}}\int dp\,\phi(p)\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 e^{i(px-Et)/\hbar} \\ &= -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\right)^2\frac{1}{\sqrt{2\pi\hbar}}\int dp\,\phi(p)e^{i(px-Et)/\hbar} \end{aligned} \tag{8}$$

Now, the integral is just the wavefunction $\psi(x,t)$, so the differential equation is

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}\ . \tag{9}$$

This is the Schrödinger equation for a free particle - there is no interaction potential yet. We did not **derive** this equation. Rather, we discussed the behaviour that we wanted for wavepackets to satisfy the uncertainty principle, then we made the identifications

$p = \hbar k$
$E = \hbar\omega$.

The form of the wavepackets satisfies the uncertainty relation

$\Delta p\ \Delta x \sim \hbar$

as well as, from the form of travelling waves

$\Delta E\ \Delta t \sim \hbar$.

Mathematically, it is interesting to note that the LHS of Eq. (9) is *linear* in time. This means that once an initial form of $\phi(p)$ is known, the form of $\psi(x,t)$ at all subsequent times can be determined by integration. This is not the same as the *second* order wave equation obtained for classical waves in PHYS 211:

$$\frac{\partial^2 u(x,t)}{\partial t^2} = c^2\,\frac{\partial^2 u(x,t)}{\partial x^2}\,. \tag{10}$$

Eq. (9) involves complex numbers, and gives rise to a complex function $\psi(x,t)$. The **complex** square of the wavefunction gives the **real** probability density in position:

$$P(x,t) = |\psi(x,t)|^2, \tag{11}$$

so that

$$[\textit{probability of particle to be between } \mathrm{x} \textit{ and } \mathrm{x + dx}] = |\psi(x,t)|^2\,dx. \tag{12}$$

The interpretation of $|\psi(x,t)|^2$ as a probability imposes a mathematical condition on $\psi(x,t)$ itself, namely the function must be *square integrable*. This is because the probability of the particle being somewhere in space must be unity:

$$\int P(x,t)\, dx = \int |\psi(x,t)|^2\, dx = 1. \tag{13}$$

Lastly, note that even though any overall phase $\exp(i\phi)$ will be removed by Eq. (11), one should not conclude that phases are unimportant. Just as classical waves interfere in different ways, depending on their phase, the same will be true here: an operation like

$$|\psi_1(x,t) + \psi_2(x,t)|^2$$

can measure the phase difference between $\psi_1(x,t)$ and $\psi_2(x,t)$, just as it can for classical waves.