Chapter 2

Informal Introduction to QM: Free Particle

Remember that in case of light, the probability of finding a photon at a location is given by the square of the square of electric field at that point. And if there are no sources present in the region, the components of the electric field are governed by the wave equation (1D case only)

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = 0 \tag{2.1}$$

Note the features of the solutions of this differential equation:

1. The simplest solutions are harmonic, that is

$$u \sim \exp\left[i\left(kx - \omega t\right)\right]$$

   where $\omega = c\left|k\right|$. This function represents the *probability amplitude* of photons with energy $\hbar\omega$ and momentum $\hbar k$.

2. Superposition principle holds, that is if $u_1 = \exp\left[i\left(k_1 x - \omega_1 t\right)\right]$ and $u_2 = \exp\left[i\left(k_2 x - \omega_2 t\right)\right]$ are two solutions of equation 2.1 then $c_1 u_1 + c_2 u_2$ is also a solution of the equation 2.1.

3. A general solution of the equation 2.1 is given by

$$u = \int_{-\infty}^{\infty} A(k) \exp\left[i\left(kx - \omega t\right)\right] dk.$$

Now, by analogy, the rules for matter particles may be found. The functions representing matter waves will be called *wave functions*.

▷ First, the wave function

$$\psi(x,t) = A \exp\left[i(px - Et)/\hbar\right]$$

represents a particle with momentum p and energy $E = p^2/2m$. Then, the probability density function $P(x,t)$ for finding the particle at x at time t is given by

$$\begin{aligned} P(x,t) &= |\psi(x,t)|^2 \\ &= |A|^2 . \end{aligned}$$

Note that the probability distribution function is independent of both x and t.

▷ Assume that superposition of the waves hold. Then the wave function

$$\psi(x,t) = A \exp\left[i(p_1 x - E_1 t)/\hbar\right] + B \exp\left[i(p_2 x - E_2 t)/\hbar\right]$$

represents a particle with momentum either p_1 or p_2 with propabilities $|A|^2$ and $|B|^2$ respectively. Extending this to the wave function

$$\psi(x,t) = \sum_{n=1}^{N} A_n \exp\left[i(p_i x - E_i t)/\hbar\right]$$

represents a particle with momentum p_i with probability $|A_i|^2$.

▷ In general, since p is a continuous variable,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A(p) \exp\left[i(px - Et)/\hbar\right] dp$$

represents a particle with momentum p with probability density function $|A(p)|^2$.

Example 1. Let

$$\psi(x,t) = \frac{1}{\sqrt{2}} \exp\left[i(px - Et)/\hbar\right] + \frac{1}{\sqrt{2}} \exp\left[i(-px - Et)/\hbar\right].$$

The pdf for finding particle at x at time t is

$$\begin{aligned} P(x,t) &= \psi^*(x,t)\psi(x,t) \\ &= 1 + \cos\left(\frac{2px}{\hbar}\right). \end{aligned}$$

Now this pdf is not what one expects in classical mechanics. There are some points, in the vicinity of which, the probability of finding particle is 0!

Now the wavefunction of a particle with definite momentum presents a problem. The probability density function $P(x,t)$ is not integrable. Thus the net probability of finding a particle somewhere is infinite. One way to look at this is to say that $P(x,t)$ represents the relative probability and not the absolute.

Really speaking, one does not find harmonic waves in nature. What one encounters are wave trains or wave pulses. Think of water ripples when a stone is dropped in it. Think of particles which make tracks in bubble chambers. It is always known that particles is in some region of space. This can be put in mathematical terms as

$$\int_{-\infty}^{\infty} P(x,t)dx < \infty$$

or

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2\, dx < \infty$$

Here are the rules for the wave function of a free particle.

1. A free particle will be described by a *square integrable function* called as *wave function* or *probability amplitude.* The absolute square of the wave function is proportional to the probability of finding the particle at a location at an instant.

2. The wave function

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A(p) \exp\left[i(px - E(p)t)/\hbar\right] dp$$

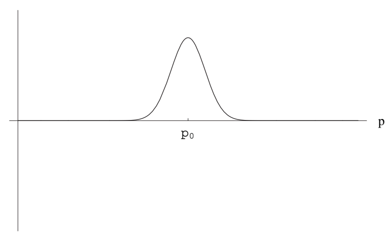
where $A(p)$ is a square integrable function, represents a free particle with momentum p with probability density function $|A(p)|^2$and energy $E(p) = p^2/2m$.

Wave Packets

Thus, the particles with reasonably sharply defined momentum may be described by a pulse like wave functions. Consider a particle with momentum p_0 with uncertainty of $\Delta p_0\,(\ll p_0)$. If the wave function of the particle is

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A(p) \exp\left[i(px - E(p)t)/\hbar\right] dp$$

then the form of $A(p)$ must be a sharply peaked function about p_0 (see figure). (For present argument, assume that $A(p)$ is real.)



Claim 2. If $A(p)$ is a sharply peaked function about p_0 with uncertainty Δp_0, then the wave function ψ is also localized. (such wave functions will be called *wave packets*).

To justify the claim, first, let $t = 0$. It is the behaviour of $\exp(ipx/\hbar)$ that must be investigated as a function of p near p_0. Now period of $\exp(ipx/\hbar)$ is $h/|x|$.

- ▷ Case 1: When $|x| \gg \frac{h}{\Delta p_0}$, then $\Delta p_0 \gg h/|x|$. That is Δp_0 is very large compared to the period of $\exp(ipx/\hbar)$. Thus this function has highly oscillatory behaviour near p_0 and hence
$$\psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A(p) \exp[i(px)/\hbar]\, dp \approx 0$$

- ▷ Case 2: When $|x| \ll \frac{h}{\Delta p_0}$, then $\Delta p_0 \ll h/|x|$. That is Δp_0 is very small compared to the period of $\exp(ipx/\hbar)$. Thus this function is nearly constant near p_0 and hence
$$\begin{aligned}\psi(x,0) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A(p) \exp[i(px)/\hbar]\, dp \\ &= \frac{1}{\sqrt{2\pi\hbar}} \exp[i(p_0 x)/\hbar] \int_{-\infty}^{\infty} A(p) dp\end{aligned}$$

Thus ψ is significantly nonzero only for $|x| < h/\Delta p_0$. Thus $\Delta x \Delta p_0 \sim h/2$.

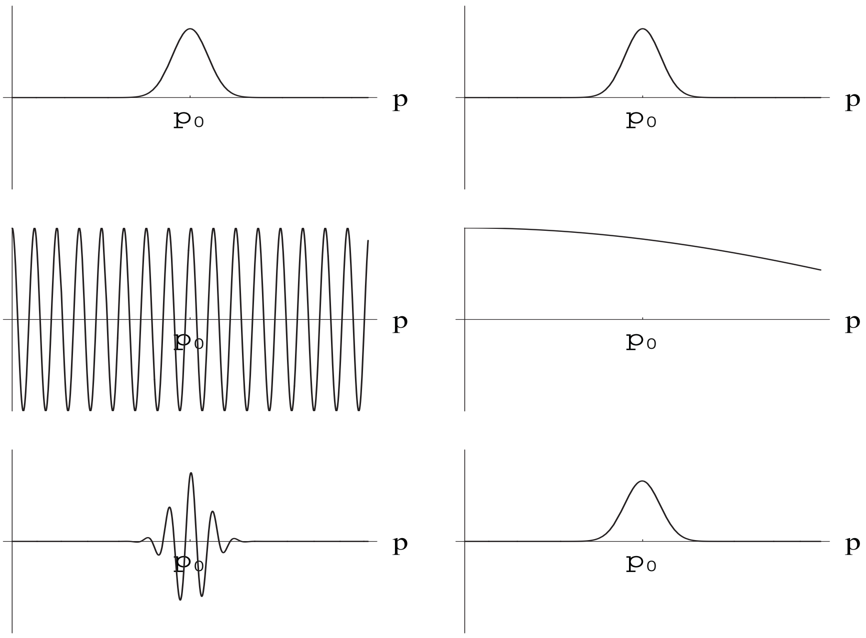
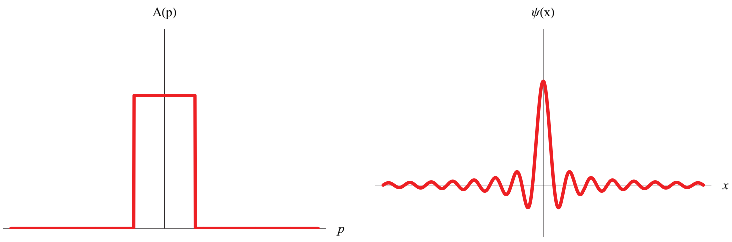


Figure 2.1: The three graphs in the first column are that of $A(p)$, $\cos(px/\hbar)$ and the product of the two when $x \gg h/\Delta p_0$. The second column contains the same graphs, but for $x \ll h/\Delta p_0$.

Example 3. Let $A(p) = 1/\sqrt{\Delta_p}$ if $|p - p_0| < \Delta_p/2$. Then the wave functin is given by

$$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} A(p)\exp\left[i(px)/\hbar\right] dp \\ &= \frac{2\sqrt{\Delta_p}}{\sqrt{2\pi\hbar}}\frac{\sin\left(\Delta_p x/\hbar\right)}{\Delta_p x/\hbar}\end{aligned}$$

The plots are shown in the figure.



To analyze the wavefunction $\psi(x,t)$, when $t \neq 0$, remember E is a function of p. Let $\beta = (px - Et)/\hbar$ be the phase of the exponential function. If β changes rapidly, then exponential function is oscillatory. Alternatively if β is stationary, exponential function is nearly constant. Thus, the peak of the wave packet ψ is at x_0 if

$$\begin{aligned}\frac{\partial\beta}{\partial p}(p_0) &= 0 \\ \text{when} \quad x_0 - \frac{\partial E}{\partial p}(p_0)\,t &= 0\end{aligned}$$

This means that the peak of the wave packet is moving with speed

$$v_g = \frac{\partial E}{\partial p}(p_0)\,.$$

This is called as *group velocity* as against the phase velocity of the wave which is defined as E/p_0. In macroscopic limit, the velocity of the particle is p_0/m, this suggests that $E(p) = p^2/2m$. This fits nicely. Now,

$$E(p) = E(p_0) + v_g(p - p_0) + \cdots$$

Thus if t is sufficiently small, then

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}e^{i(p_0 x - E(p_0)t)/\hbar}\int_{-\infty}^{\infty} A(p)\exp\left[i(p - p_0)(x - v_g t)/\hbar\right] dp$$

And compare this with

$$\psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}}e^{i(p_0 x/\hbar)}\int_{-\infty}^{\infty} A(p)\exp\left[i(p - p_0)x/\hbar\right] dp$$

the wave packet just moves without changing shape with speed v_g.

Gaussian Wave Packets

Now let

$$A(p) = \left(\frac{1}{\sqrt{\pi}\Delta_p}\right)^{\frac{1}{2}} \exp\left[-\frac{(p-p_0)^2}{2\Delta_p^2}\right].$$

Note that this function is normalized to 1, that is,

$$\int_{-\infty}^{\infty} |A(p)|^2 dp = 1.$$

The wave packet is

$$\begin{aligned}\psi(x,0) &= \frac{1}{\sqrt{2\pi\hbar}}\left(\frac{1}{\sqrt{\pi}\Delta_p}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left[-\frac{(p-p_0)^2}{2\Delta_p^2} + i\frac{px}{\hbar}\right] dp \\ &= \left(\frac{\Delta_p}{\sqrt{\pi}\hbar}\right)^{\frac{1}{2}} \exp\left[i\frac{p_0 x}{\hbar}\right] \exp\left[-\frac{\Delta_p x^2}{2\hbar^2}\right]\end{aligned}$$

(See footnote[1]) The following figures show the plot of Gaussian wavepacket.

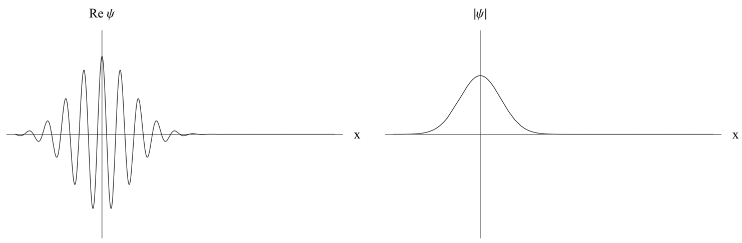


Figure 2.2: The left figure shows Reψ and right hand figure shows $|\psi|^2$.

Differential Equation (Schrödinger Equation)

If the wave function at time $t = 0$ is known, that is $\psi(x,0)$ is known for all x, how does one find $\psi(x,t)$? Remeber that em waves are governed by a differential equation called as wave equation. What is the differential equation for matter waves? Here one borrows the classical energy expression $E = p^2/2m$. The wave function $\psi(x,t)$ of a free particle is

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A(p) \exp\left[i(px - E(p)t)/\hbar\right] dp.$$

Then

$$\left(i\hbar\frac{\partial}{\partial t}\right)\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} E A(p) \exp\left[i(px - E(p)t)/\hbar\right] dp$$

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[1]

$$\int_{-\infty}^{\infty} e^{-\alpha u^2} e^{-\beta u} du = \left(\frac{\pi}{\alpha}\right)^{1/2} e^{\beta^2/4\alpha}$$

and

$$\begin{aligned}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi(x,t) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(\frac{p^2}{2m}\right)A(p)\exp\left[i(px-E(p)t)/\hbar\right]dp \\ &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}EA(p)\exp\left[i(px-E(p)t)/\hbar\right]dp\end{aligned}$$

since $p^2/2m = E$. Thus,

$$\left(i\hbar\frac{\partial}{\partial t}\right)\psi(x,t) = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2\psi(x,t).$$

This is called Schrödinger equation. Note this first ordered differential equation in t. Thus knowledge of $\psi(x,0)$ is enough obtain $\psi(x,t)$.[2]

It was implicitly assumed that $A(p)$ is time-independent. In classical case, momentum of a free particle does not change in time. Simillary, in QM, the pdf of momentum does not change in time and so does $A(p)$. Then there is another way to find $\psi(x,t)$ from $\psi(x,0)$:

1. Given $\psi(x,0)$, compute momentum space wave function:
$$A(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x,0)\exp\left[-i(px)/\hbar\right]dx$$
2. Then
$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}A(p)\exp\left[i(px-Et)/\hbar\right]dp$$

Example 4. A wave function of a free particle at $t = 0$, is

$$\psi(x,0) = \begin{cases} B & |x| < a \\ 0 & \text{otherwise.}\end{cases}$$

B is a real constant. Find $\psi(x,t)$.

First normalize the wave function.

$$\int_{-a}^{a}|\psi(x,0)|^2\,dx = 1$$

This implies that $B = 1/\sqrt{2a}$. Now the momemtum space wave function is

$$\begin{aligned}A(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x,t)\exp\left[-i(px)/\hbar\right]dx \\ &= \sqrt{\frac{a}{\pi\hbar}}\,\text{sinc}\left(\frac{pa}{\hbar}\right).\end{aligned}$$

[2] Of course, one also must know $\psi(\pm\infty,t)$, since its a second ordered differential equation in x. For free particle, the square integrability requires that $\psi(\pm\infty,t) = 0$.

Now

$$\psi(x,t) = \psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\sqrt{\frac{a}{\pi\hbar}}\int_{-\infty}^{\infty} \text{sinc}\left(\frac{pa}{\hbar}\right)\exp\left[i\left(px - \frac{p^2}{2m}t\right)/\hbar\right] dp$$

But this integral is not easy to evaluate in terms of simple functions. But it can be numerically evaluated and plotted. Clearly the average momentum is zero, thus the peak of the wavefunction remains at $x = 0$.|

Expectation Values

Thus, if the wave packet (or wave function) of a particle is known then all other information can be obtained. Let $\psi(x,t)$ is the wave function of a particle.

- ▷ Probability density function for finding the particle at x is

$$P(x,t) = |\psi(x,t)|^2$$

- ▷ The average position of the particle or expectation value of x is

$$\begin{aligned}\langle x(t)\rangle &= \int_{-\infty}^{\infty} xP(x,t)dx \\ &= \int_{-\infty}^{\infty} \psi*(x,t)\left[x\psi(x,t)\right]dx\end{aligned}$$

- ▷ Let

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x,t)\exp\left[-i(px - E(p)t)/\hbar\right]dx.$$

  Then probability density function for finding the particle with momentum p is given by

$$P(p) = |\phi(p)|^2$$

- ▷ The expectation value of p is

$$\begin{aligned}\langle p\rangle &= \int_{\infty}^{\infty} p\,|\phi(p)|^2\,dp \\ &= \int_{\infty}^{\infty}\phi^*(p)\left[p\phi(p)\right]dp\end{aligned}$$

  Now, notice that

$$-i\hbar\frac{\partial}{\partial x}\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left[p\phi(p)\right]\exp\left[i(px - E(p)t)/\hbar\right]dp$$

Then

$$\begin{aligned}
\langle p \rangle &= \frac{1}{2\pi\hbar} \int dx \int dx' \psi^*(x',t) \left[-i\hbar \frac{\partial}{\partial x} \psi(x,t) \right] \int dp \exp[i \left(p(x-x')/\hbar \right) \\
&= \frac{1}{2\pi\hbar} \int dx \int dx' \psi^*(x',t) \left[-i\hbar \frac{\partial}{\partial x} \psi(x,t) \right] \left(2\pi\hbar\delta(x-x') \right) \\
&= \int_{-\infty}^{\infty} \psi(x,t) \left[\left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x,t) \right] dx
\end{aligned}$$

Exercise 5. Show that

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi(x,t) \left[\left(i\hbar \frac{\partial}{\partial t} \right) \psi(x,t) \right] dx.$$