Probability current

Let P_{ab} be the probability of finding a particle in the range $a \le x \le b$. Let us find $\frac{dP_{ab}}{dt}$:

$$\frac{dP_{ab}}{dt} = \frac{d}{dt}\int_a^b \psi^* \psi \, dx = \int_a^b \left[\frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t}\right] dx$$

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{d^2\psi}{dx^2} - \frac{i}{\hbar} V\psi \qquad \frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{d^2\psi^*}{dx^2} + \frac{i}{\hbar} V\psi$$

$$\frac{dP_{ab}}{dt} = \frac{i\hbar}{2m}\int_a^b \left[-\frac{d^2\psi^*}{dx^2}\psi + \psi^*\frac{d^2\psi}{dx^2}\right] dx = \frac{i\hbar}{2m}\int_a^b \frac{d}{dx}\left[\psi^*\frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right] dx$$

$$= \frac{i\hbar}{2m}\left[\psi^*\frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right]\Bigg|_a^b = -J(b,t) + J(a,t)$$

where $J(x,t) \equiv \frac{i\hbar}{2m}\left(\psi\frac{d\psi^*}{dx} - \psi^*\frac{d\psi}{dx}\right)$ ← probability current

Recall E&M:

$$\frac{dq}{dt} \equiv I$$

In our case we associate current with particle flow, not with the charge flow

Free particle

If $V(x)$ is zero everywhere we have a free particle. The SE equation reads:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \text{or} \quad \frac{d^2\psi}{dx^2} = -k^2\psi \, , \quad k = \frac{\sqrt{2mE}}{\hbar}$$

The general solution is:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

Since there are no boundary conditions, values of k are unrestricted.

If we include the time dependence the solution looks as follows

$$\psi(x,t) = Ae^{ikx - iEt} + Be^{-ikx - iEt} =$$

$$= Ae^{ik(x - \frac{\hbar k}{2m}t)} + Be^{-ik(x + \frac{\hbar k}{2m}t)}$$

This is a solution that depends on the combination $x \pm vt$ – a wave that travels with velocity $\pm v$. Since at every point v is the same, the shape does not change as the wave propagates.

Since k in the two terms above differs by the sign only, we can write the solution as

$$\psi_k(x,t) = Ae^{i(kx - \frac{\hbar k^2}{2m}t)}$$

and let k run from negative to positive.

The stationary states of the free particle are propagating waves with wavelength $\lambda = \frac{2\pi}{|k|}$ and they carry momentum $p = \hbar k$

The speed of the waves is $v_{quant} = \frac{\hbar |k|}{2m} = \sqrt{\frac{E}{2m}}$

This is different from $v_{classical} = \sqrt{\frac{2E}{m}} = 2 v_{quant}$

(we used $E = \frac{m v_{classical}^2}{2}$)

Note that the free particle wave function is not normalizable, becase

$$\int_{-\infty}^{+\infty} |\psi_k|^2 dx = |A|^2 \int_{-\infty}^{+\infty} dx = \infty$$

we can only choose constan A is such a way that a certain number of particles (say 1) is in a certain "volume" (say L).

The general solution of the time-dependent SE can be written as a linear combination of partial solutions corresponding to all possible k values

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk$$ ← this is called a wave packet

Factor $\frac{1}{\sqrt{2\pi}}$ is chosen for convenience, but in principle it is arbitrary since any constant can be absorbed into $\phi(k)$

$\phi(k)$ can be determined from the initial conditions:

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} dk \Rightarrow \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x,0) e^{-ikx} dx$$

We see that $\phi(k)$ is the Fourier transform of $\psi(x,0)$

Fourier transform (aka Fourier integral transform)

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk \iff F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx$$

There exist different conventions regarding the factors ($\frac{1}{\sqrt{2\pi}}$) and the exponent. The one we adopted here is convenient because it is symmetric ($\frac{1}{\sqrt{2\pi}}$ is the same in both expressions) and the normalization of $F(k)$ in k-space is preserved.

Now let us return to the paradox with the "velocity" of the free particle

What corresponds to the particle velocity is not the phase velocity (i.e. the velocity of individual ripples) but the speed of the envelope (i.e. the "speed" of the whole thing as it moves)

We can show that the group velocity is twice the phase velocity of the free particle

The general form of a wave packet is:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx-\omega t)} dk$$

In our case $\omega = \frac{\hbar k^2}{2m}$, but our conclusion will be valid even if $\omega(k)$ has a different functional form. Let us assume that $\phi(k)$ is narrowly peaked about some k_0

Since the most of the integral value comes from the region around k_0 we can just Taylor expand $\omega(k)$: $\omega(k) = \omega_0 + \omega_0'(k-k_0) + \dots$

Making a substitution $s = k - k_0$ yiels:

$$\Psi(x,t) \approx \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i[(k_0+s)x - (\omega_0+\omega_0' s)t]} ds$$

at $t=0$

$$\Psi(x,0) \approx \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i(k_0+s)x} ds$$

and at later times

$$\Psi(x,t) \approx \frac{1}{\sqrt{2\pi}} e^{i(-\omega_0 t + k_0\omega_0' t)} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i(k_0+s)(x-\omega_0' t)} ds$$

Notice that

$$\Psi(x,t) \approx e^{-i(\omega_0 - k_0\omega_0')t}\, \Psi(x-\omega_0' t, 0)$$

Apart from the phase factor (which does not affect $|\Psi|^2$) the wave packet moves along at a speed ω_0':

$$v_{group} = \left.\frac{d\omega}{dk}\right|_{k=k_0}$$

which is to be contrasted with $v_{phase} = \frac{\omega}{k}$

$\frac{d\omega}{dk} = \frac{\hbar k}{m}$ on the other hand $\omega = \frac{\hbar k^2}{2m}$

$$\frac{\omega}{k} = \frac{\hbar k}{2m}$$

so $v_{group} = 2 v_{phase} = v_{classical}$