THE FREE PARTICLE AS A WAVE PACKET

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 2.4, Problem 2.21.

We've seen that the stationary states of a free particle are:

$$\Psi(x,t) = (Ae^{ikx}+Be^{-ikx})e^{-iEt/\hbar}$$

where

$$k=\frac{\sqrt{2mE}}{\hbar}$$

We've also seen that this wave function cannot be normalized, so the only acceptable solution for a free particle is one consisting of a combination of stationary states that is normalizable. That is

$$\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}e^{-i\hbar k^2t/2m}dk \tag{1}$$

Returning to an individual stationary state, we can see that it has the general form

$$\Psi_k(x,t)=e^{i(kx-\omega t)}$$

where

$$\omega(k)=\frac{\hbar k^2}{2m}$$

Such a function represents a travelling wave. To see this, suppose we want to follow a point where Ψ_k has a particular value, that is where $kx-\omega t=C$ for some constant C. By taking the derivative of this expression with respect to t, we get

$$\frac{dx}{dt}=\frac{\omega}{k}$$

That is, the speed of a point with a fixed value is given by $v = \omega/k$ which is a constant for a given value of k (and thus for a given energy). In the particular case of the free particle, this means that a stationary state with energy E (which translates into a particular value of k as given above) is a travelling wave with speed

$$\begin{aligned} v(E) &= \frac{\hbar k}{2m} \\ &= \sqrt{\frac{E}{2m}} \end{aligned}$$

The problem is that a physical free particle must contain contributions from many (possibly infinite) individual stationary states all combined in the integral above. Since all these states have different wave speeds, what can we say about the speed of the free particle itself?

If the particle consists of contributions from a wide range of energies, then $\phi(k)$ has an appreciable value for a wide range of k, and the 'particle' will tend to spread out with time, so it's difficult to talk of a well-defined speed in this case.

If $\phi(k)$ is peaked around a particular value of k such as k_0, however, the concept of a speed for the particle makes a bit more sense. In this case, we can expand $\omega(k)$ in a Taylor series around $k = k_0$:

$$\omega(k) = \omega(k_0) + \omega'(k_0)(k - k_0) + \ldots$$

In the particular case of the quantum free particle, the series has only 3 terms:

$$\omega(k) = \frac{\hbar k_0^2}{2m} + \frac{\hbar k_0}{m}(k - k_0) + \frac{\hbar}{2m}(k - k_0)^2$$

The idea is to assume that $\phi(k)$ is peaked about k_0 and thus we can ignore the quadratic term at the end. If we do this, we can plug this approximation into 1 to get

$$\Psi(x,t) \approx \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} e^{-i\left[\hbar k_0^2 t/2m + \hbar k_0 (k-k_0) t/m\right]} dk$$

We can now define a variable $\kappa \equiv k - k_0$. We can also pull out of the integral terms that don't depend on k, and we get

$$\Psi(x,t) \approx \frac{1}{\sqrt{2\pi}} e^{-i\hbar k_0^2 t/2m} \int_{-\infty}^{\infty} \phi(\kappa + k_0) e^{i(\kappa + k_0)x} e^{-i\hbar k_0 \kappa t/m} d\kappa$$

Observe that

$$(\kappa+k_0)x-\frac{\hbar k_0\kappa t}{m}=(\kappa+k_0)\left(x-\frac{\hbar k_0 t}{m}\right)+\frac{\hbar k_0^2 t}{m}$$

so we can rewrite the integral as

$$\Psi(x,t)\approx\frac{1}{\sqrt{2\pi}}e^{-i\hbar k_0^2 t/2m}e^{i\hbar k_0^2 t/m}\int_{-\infty}^{\infty}\phi(\kappa+k_0)e^{i(\kappa+k_0)(x-\hbar k_0 t/m)}d\kappa$$

This integral is the superposition of waves of form

$$e^{i(\kappa+k_0)(x-\hbar k_0 t/m)}$$

However, note that *all* these waves have the same speed of $\hbar k_0/m$. In terms of the energy E_0, this comes out to

$$\begin{aligned}v_0&=\frac{\hbar k_0}{m}\\&=\sqrt{\frac{2E_0}{m}}\end{aligned}$$

Comparing this with the speed of individual stationary states above, we see that it's actually twice as fast. In fact, if we compare this to the classical speed of a free particle with energy $E_0=mv_0^2/2$ (all the energy is kinetic since there is no potential energy), we see that the speeds are the same.

The velocity of an individual stationary state is called the *phase velocity*, while the velocity of the wave packet composed of a number of stationary states is the *group velocity*.

We need to treat this result with some caution, since as we noted above, it relies on the assumption that only a narrow range of energies contributes to the free particle, so the result isn't exact.

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