6.2: Evolution of Wave-packets

In Section 6.1.1 we looked at the evolution of a general wavefunction under a time-independent Hamiltonian. The solution to the Schrödinger equation was given in terms of a linear superposition of energy eigenfunctions, each acquiring a time-dependent phase factor. The solution was then the superposition of waves each with a different frequency.

Now we want to study the case where the eigenfunctions form a continuous basis, $\{\varphi_k\} \rightarrow \{\varphi(k)\}$. More precisely, we want to describe how a free particle evolves in time. We already found the eigenfunctions of the free particle Hamiltonian ($\mathcal{H} = \hat{p}^2/2m$): they were given by the momentum eigenfunctions e^{ikx} and describe more properly a traveling wave. A particle localized in space instead can be described by wavepacket $\psi(x,0)$ initially well localized in x-space (for example, a Gaussian wavepacket).

How does this wave-function evolve in time? First, following Section 2.2.1, we express the wavefunction in terms of momentum (and energy) eigenfunctions:

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

We saw that this is equivalent to the Fourier transform of $\bar{\psi}(k)$, then $\psi(x,0)$ and $\bar{\psi}(k)$ are a Fourier pair (can be obtained from each other via a Fourier transform).

Thus the function $\bar{\psi}(k)$ is obtained by Fourier transforming the wave-function at t = 0. Notice again that the function $\bar{\psi}(k)$ is the continuous-variable equivalent of the coefficients $c_k(0)$.

The second step is to evolve in time the superposition. From the previous section we know that each energy eigenfunction evolves by acquiring a phase $e^{-i\omega(k)t}$, where $\omega(k) = E_k/\hbar$ is the energy eigenvalue. Then the time evolution of the wavefunction is

$$\psi(x,t) = \int_{-\infty}^{\infty} \bar{\psi}(k) \mathrm{e}^{\mathrm{i}\varphi(k)} dk,$$

where

$$\varphi(k) = kx - \omega(k)t.$$

For the free particle we have $\omega_k = \frac{\hbar k^2}{2m}$. If the particle encounters instead a potential (such as in the potential barrier or potential well problems we already saw) ω_k could have a more complex form. We will thus consider this more general case.

Now, if $\bar{\psi}(k)$ is **strongly peaked** around $k = k_0$, it is a reasonable approximation to Taylor expand $\varphi(k)$ about k_0. We can then approximate $\bar{\psi}(k)$ by

$$\bar{\psi}(k) \approx e^{-\frac{(k-k_0)^2}{4(\Delta k)^2}}$$

and keeping terms up to second-order in $k - k_0$, we obtain

$$\psi(x,t) \propto \int_{-\infty}^{\infty} e^{-\frac{(k-k_0)^2}{4(\Delta k)^2}} \exp\left[-\mathrm{i}kx + \mathrm{i}\left\{\varphi_0 + \varphi_0'(k-k_0) + \frac{1}{2}\varphi_0''(k-k_0)^2\right\}\right],$$

where

$$\begin{aligned}
\varphi_0 &= \varphi(k_0) = k_0 x - \omega_0 t, \\
\varphi_0' &= \frac{d\varphi(k_0)}{dk} = x - v_g t, \\
\varphi_0'' &= \frac{d^2\varphi(k_0)}{dk^2} = -\alpha t, \\
-\mathrm{i}kx + \mathrm{i}&\left\{k_0 x - \omega_0 t + (x - v_g t)(k-k_0) + \frac{1}{2}\varphi_0''(k-k_0)^2\right\}
\end{aligned}$$

with

$$\omega_0 = \omega(k_0), \quad v_g = \frac{d\omega(k_0)}{dk}, \quad \alpha = \frac{d^2\omega(k_0)}{dk^2},$$

As usual, the variance of the initial wavefunction and of its Fourier transform are relates: $\Delta k=1/(2\Delta x)$, where Δx is the initial width of the wave-packet and Δk the spread in the momentum. Changing the variable of integration to $y=(k-k_0)/(2\Delta k)$, we get

$$\psi(x,t)\propto \mathrm{e}^{\mathrm{i}(k_0 x-\omega_0 t)}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\beta_1 y-(1+\mathrm{i}\beta_2)y^2}dy$$

where

$$\begin{aligned}\beta_1 &= 2\Delta k\left(x-x_0-v_g t\right),\\ \beta_2 &= 2\alpha(\Delta k)^2 t,\end{aligned}$$

The above expression can be rearranged to give

$$\psi(x,t)\propto e^{i(k_0 x-\omega_0 t)-(1+i\beta_2)\beta^2/4}\int_{-\infty}^{\infty}e^{-(1+i\beta_2)(y-y_0)^2}dy,$$

where $y_0=\mathrm{i}\beta/2$ and $\beta=\beta_1/\left(1+\mathrm{i}\beta_2\right)$.

Again changing the variable of integration to $z=\left(1+\mathrm{i}\beta_2\right)^{1/2}\left(y-y_0\right)$, we get

$$\psi(x,t)\propto\left(1+\mathrm{i}\beta_2\right)^{-1/2}\mathrm{e}^{\mathrm{i}(k_0 x-\omega_0 t)-(1+\mathrm{i}\beta_2)\beta^2/4}\int_{-\infty}^{\infty}\mathrm{e}^{-z^2}dz.$$

The integral now just reduces to a number. Hence, we obtain

$$\psi(x,t)\propto\frac{e^{i(k_0 x-\omega_0 t)}\,e^{-\frac{(x-x_0-v_g t)^2\left[1-i2\alpha\Delta k^2 t\right]}{4\sigma(t)^2}}}{\sqrt{1+i2\alpha(\Delta k)^2 t}},$$

where

$$\sigma^2(t)=(\Delta x)^2+\frac{\alpha^2 t^2}{4(\Delta x)^2}.$$

Note that even if we made an approximation earlier by Taylor expanding the phase factor $\varphi(k)$ about $k=k_0$, the above wave-function is still identical to our original wave-function at t = 0.

The probability density of our particle as a function of times is written

$$|\psi(x,t)|^2\propto\sigma^{-1}(t)\exp\left[-\frac{\left(x-x_0-v_g t\right)^2}{2\sigma^2(t)}\right].$$

Hence, the probability distribution is a Gaussian, of characteristic width $\sigma(t)$ (increasing in time), which peaks at $x=x_0+v_g t$. Now, the most likely position of our particle obviously coincides with the peak of the distribution function. Thus, the particle's most likely position is given by

$$x=x_0+v_g t.$$

It can be seen that the particle effectively moves at the uniform velocity

$$v_g=\frac{d\omega}{dk},$$

which is known as the **group-velocity**. In other words, a plane-wave travels at the phase-velocity, $v_p=\omega/k$, whereas a wave-packet travels at the group-velocity, $v_g=d\omega/dt v_g=d\omega/dt$. From the dispersion relation for particle waves the group velocity is

$$v_g=\frac{d(\hbar\omega)}{d(\hbar k)}=\frac{dE}{dp}=\frac{p}{m}.$$

which is identical to the classical particle velocity. Hence, the dispersion relation turns out to be consistent with classical physics, after all, as soon as we realize that particles must be identified with **wave-packets** rather than plane-waves.

Note that the width of our wave-packet grows as time progresses: the characteristic time for a wave-packet of original width $\Delta x \Delta x$ to double in spatial extent is

$$t_2 \sim \frac{m(\Delta x)^2}{\hbar}.$$

So, if an electron is originally localized in a region of atomic scale (i.e., $\Delta x \sim 10^{-10}\ \mathrm{m}$) then the doubling time is only about 10^{-16}s. Clearly, particle wave-packets (for freely moving particles) spread very rapidly.

The rate of spreading of a wave-packet is ultimately governed by the second derivative of $\omega(k)$ with respect to k, $\frac{\partial^2 \omega}{\partial k^2}$. This is why the relationship between ω and k is generally known as a **dispersion relation**, because it governs how wave-packets disperse as time progresses.

If we consider light-waves, then ω is a *linear* function of k and the second derivative of ω with respect to k is zero. This implies that there is no dispersion of wave-packets, wave-packets propagate without changing shape. This is of course true for any other wave for which $\omega(k) \propto k$. Another property of linear dispersion relations is that the phase-velocity, $v_p = \omega/k$, and the group-velocity, $v_g = d\omega/dk$ are identical. Thus a light pulse propagates at the same speed of a plane light-wave; both propagate through a vacuum at the characteristic speed $c = 3 \times 10^8\ \mathrm{m/s}$.

Of course, the dispersion relation for particle waves is *not* linear in k (for example for free particles is quadratic). Hence, particle plane-waves and particle wave-packets propagate at different velocities, and particle wave-packets also gradually disperse as time progresses.