Quantum Mechanics
Day 18

Today

I. Last Time
II. Wave Packets & Group Velocity
III. Henry's Guest Lecture on Gaussian Wave Packets

I. Last Time

- We studied the free ($V = 0$) particle and found that we could parametrize a basis of functions using the wave number k, these are
$$\Psi_k(x,t) = Ae^{ik\left(x - \frac{\hbar k}{2m}t\right)}, \qquad \text{with} \qquad k = \pm\frac{\sqrt{2mE}}{\hbar}.$$
These are energy eigenstates with definite energy, momentum, and wavelength
$$E = \frac{(\hbar k)^2}{2m}, \quad p = \hbar k, \quad \text{and} \quad \lambda = \frac{2\pi}{|k|}.$$
- We found that these waves travel with a surprising phase velocity
$$v_{\text{quantum}} = 2v_{\text{classical}} = \frac{\hbar k}{2m} = \pm\sqrt{\frac{E}{2m}}.$$
We also found that these solutions were not normalizable and that their amplitudes never go to zero.
- Despite these surprising results, these solutions can be used to span the space of solutions. We found that we could form <u>wave packets</u> out of them:
$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{ikx}dx.$$
Using Plancherel's theorem we are able to find the right combination of wave numbers k to do this, namely the function $\phi(k)$,
$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x,0)e^{-ikx}dk.$$
With the 'shape' $\phi(k)$ of the wave packet in hand, we can then compute the full time-dependent wave function
$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{ik\left(x - \frac{\hbar k}{2m}t\right)}dx.$$

II. Wave Packets & Group Velocity

A typical structure for a wave packet is shown at right. The ripples travel at the <u>phase velocity</u>

$$\boxed{v_{\text{phase}} = \frac{\omega}{k}.}$$

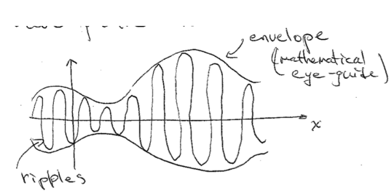

Figure 1: The structure of a wave packet. The packet is made up of the internal ripples, but interference effects cause its amplitude to vary in space and contain the wave packet. The envelope curve is not part of the wave, but just a way to guide the eye through the changes in amplitude. The envelope can be derived mathematically.

[Aside: In the present context

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

but both the phase velocity above and the the argument we are about to make will work for all dispersion relations $\omega = \omega(k)$.]

But, what about the envelope? It moves as well, and travels at the group velocity. Start with

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

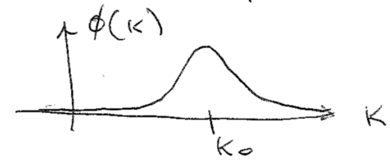

Figure 2: A wave packet's shape function that happens to be peaked around $k = k_0$.

and suppose that the shape function $\phi(k)$ is peaked near k_0, as in the figure at right. If it is peaked enough, it makes sense to expand the dispersion relation around this point

$$\omega(k) = \omega_0 + \omega_0'(k - k_0) + \cdots,$$

where $\omega_0 \equiv \omega(k_0)$ and $\omega_0' \equiv d\omega/dk|_{k_0}$. With these definitions we can change variables in the integral to $s \equiv k - k_0$ to center ourselves around k_0 and get $k = k_0 + s$, $dk = ds$, and

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

where the approximation is because we have dropped the higher order terms in our Taylor expansion of the dispersion relation.

Evaluating our wave function at $t = 0$ gives

$$\Psi(x,0) = \Psi(x,t)\Big|_{t=0} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k_0 + s) e^{i(k_0+s)x} ds.$$

At later times, we can take our time-dependent expression and rewrite it in a clever way. We add and subtract to get

$$e^{i\left[-(\omega_0+\omega_0' s)t\right]} = e^{i\left[-\omega_0 t + k_0\omega_0' t - k_0\omega_0' t - \omega_0' s t\right]} = e^{i\left[-\omega_0 t + k_0\omega_0' t\right]} e^{i\left[-(k_0+s)\omega_0' t\right]}.$$

Notice that the first term doesn't depend on s and so we can pull it out of the integral to finally find

$$\begin{aligned}\Psi(x,t) &\approx \frac{1}{\sqrt{2\pi}} e^{i\left[-\omega_0 t + k_0\omega_0' t\right]} \int_{-\infty}^{\infty} \phi(k_0+s) e^{i\left[(k_0+s)x - (k_0+s)\omega_0' t\right]} ds \\ &= \frac{1}{\sqrt{2\pi}} e^{i\left[-\omega_0 t + k_0\omega_0' t\right]} \int_{-\infty}^{\infty} \phi(k_0+s) e^{i(k_0+s)\left(x - \omega_0' t\right)} ds.\end{aligned}$$

But, then

$$\Psi(x,t) \approx e^{i\left[-\omega_0 t + k_0\omega_0' t\right]} \Psi(x - \omega_0' t, 0)!$$

Hence, up to an overall phase, the whole wave function travels as a group, and moves at velocity

$$v_{\text{group}} = \omega_0' \equiv \left.\frac{d\omega}{dk}\right|_{k_0}.$$

For our particular case
$$\omega = \frac{\hbar k^2}{2m}$$
and so
$$\frac{d\omega}{dk} = \frac{\hbar k}{m}.$$
This is twice the phase velocity v_{phase} we found earlier:
$$v_{\text{group}} = v_{\text{classical}} = 2v_{\text{phase}}.$$

This is an exciting mathematical indication that a quantum wave packet <u>can</u> be the underlying structure for the classical particles so familiar to everyday discussion. To confirm this hypothesis we turn to experiment, of course. There is compelling evidence to support it from the interference properties of buckyballs (C_{60}) to measurements of the internal wave packet structure of neutrons.

III. Henry's Guest Lecture on Gaussian Wave Packets

I will add a scan of Henry's guest lecture when I get a chance.