Physics 342 Lecture 19

Welcome back for more quantum mechanics! Last week, we had discussed the quantum properties of the harmonic oscillator, and this week we will discuss the free particle, for which the potential is simply 0. That is, the Hamiltonian is just the kinetic energy:

$\hat{H} = \frac{\hat{p}^2}{2m}$, and thus energy eigenstates are also momentum eigenstates. That is, for some momentum eigenstate with eigenvalue p, the energy of such a state is:

$$\hat{H}|p\rangle = \frac{\hat{p}^2}{2m}|p\rangle = \frac{p^2}{2m}|p\rangle = E_p|p\rangle$$, where we have denoted

the momentum eigenstate with momentum p as $|p\rangle$. So, in position space, we can express the momentum eigenstate as a wavefunction $\psi_p(x,t)$ as:

$$\psi_p(x,t) = e^{-i\frac{E_p t}{\hbar}} e^{i\frac{px}{\hbar}} = e^{-\frac{i}{\hbar}(E_p t - px)} = e^{-\frac{i}{\hbar}\left(\frac{p^2}{2m}t - px\right)}.$$

To write this, all we have done is take a product of the energy eigenstate $\left(e^{-i\frac{E_p t}{\hbar}}\right)$ and momentum eigenstate $\left(e^{i\frac{px}{\hbar}}\right)$, which energy E_p for some momentum p.

This momentum eigenstate has some weird and disturbing properties. First, we have said that the potential is 0 for all $x \in [-\infty, \infty)$, so this momentum eigenstate is allowed to be anywhere on the real, position axis. This wavefunction oscillates everywhere, at every possible position, which is problematic for normalization of this wavefunction. Recall that a wavefunction or quantum state is only in the Hilbert space (i.e., the space of physical states of a system) if it is normalizable. So, let's see if this state is normalizable. We need to evaluate:

$$\int_{-\infty}^{\infty} dx\, \psi_p^*(x,t)\,\psi_p(x,t) = \int_{-\infty}^{\infty} dx \left(e^{\frac{i}{\hbar}(E_p t - px)}\right)\left(e^{-\frac{i}{\hbar}(E_p t - px)}\right)$$

$$= \int_{-\infty}^{\infty} dx\, 1 = \infty\ !?!$$

Note that the magnitude of the momentum eigenstate wavefunction is unity for all x, so we just integrate 1 over all real numbers. What is the result? Infinite? If so, there's no way for this momentum eigenstate to be normalizable, and thus such a state does not live in the Hilbert space. This is fascinating: it means that a momentum eigenstate of a free particle is not a possible physical state for a particle to exist in.

There's another strange feature of the momentum eigenstate wavefunction. Let's write the wavefunction using Euler's formula, to express it as a sum of sinusoidal functions:

$$\psi_p(x,t) = e^{-\frac{i}{\hbar}(E_p t - px)} = \cos\frac{E_p t - px}{\hbar} - i \sin\frac{E_p t - px}{\hbar}$$

Now, from your study of waves in introductory physics, you know that the arguement of a sinusoidal function describing the wave can also be expressed as:

wave $\sim \cos(\omega t - kx)$, where ω is the angular frequency and k is the wave number of the wave. With this analogy, note that the angular frequency ω of the momentum eigenstate is: $\omega = \frac{E_p}{\hbar} = \frac{2\pi}{T} = 2\pi f$, where ~~T~~ T is

the period of the wave and f is its frequency. Further, the wavenumber k would be:

$$k = \frac{p}{\hbar} = \frac{2\pi}{\lambda},$$ where λ is the wavelength. Note that

these identifications demonstrate that the energy can be written as: $E_p = \hbar\omega = hf$ and the momentum can be written as: $p = 2\pi\hbar/\lambda = h/\lambda$. You might recognize these expressions from your course on modern physics; in particular, $p = h/\lambda$ or $\lambda = h/p$ is called the <u>de Broglie wavelength</u>.

Now, given an angular frequency ω and wave number k, we can determine the velocity of the wave by taking their ratio:

$$v = \lambda f = \frac{\omega}{k} = \frac{E_p}{\hbar}\frac{\hbar}{p} = \frac{E_p}{p} = \frac{\frac{p^2}{2m}}{p} = \frac{p}{2m},$$

where on the right we have plugged in the expression of E_p in terms of momentum eigenvalue p. This resulting velocity is a bit strange: if this were just a particle of mass m, its momentum would be: $p = mv$, or its velocity v would be:

$$v = \frac{p}{m}.$$

However, somehow, the velocity of this single wave specified by momentum p is <u>half</u> of that. Huh? The velocity ~~the~~ of a wave just found from the ratio of angular frequency to the wave number is called the <u>phase velocity</u>, as it's the velocity of a single wave with a unique phase (i.e., argument of the sinusoidal function).

So, let's see if we can fix up this behavior of both non-normalizability and the strange half-velocity expression. If a momentum eigenstate has these problems, let's now consider a linear combination of momentum eigenstates, a wavefunction denoted by $\psi(x,t)$. We can write this as:

$$\psi(x,t) = \int_{-\infty}^{\infty} dp\, g(p)\, e^{-\frac{i}{\hbar}(E_p t - px)}\ ,$$ for some function of momentum $g(p)$.

In going forward, we'll just study properties of this wave function at $t=0$, so we have

$$\psi(x,t=0) \equiv \psi(x) = \int_{-\infty}^{\infty} dp\, g(p)\, e^{\frac{ipx}{\hbar}}\ .$$

We'll add back the time dependence when we study its velocity later. If such a wavefunction is to be in the Hilbert space, it <u>must</u> be normalizable; in particular, it must be L^2-normalized. Let's see what constraints this imposes on the function $g(p)$. We require:

$$\int_{-\infty}^{\infty} dx\, \psi^*(x)\psi(x) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp\, g^*(p)\, e^{-\frac{ipx}{\hbar}} \int_{-\infty}^{\infty} dk\, g(k)\, e^{\frac{ikx}{\hbar}} = 1$$

$$= \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx\, g^*(p)\, g(k)\, e^{\frac{i(k-p)x}{\hbar}}$$

$$= 2\pi\hbar \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dk\, g^*(p)\, g(k)\, \delta(p-k)$$

$$= 2\pi\hbar \int_{-\infty}^{\infty} dp\, g^*(p)\, g(p).$$

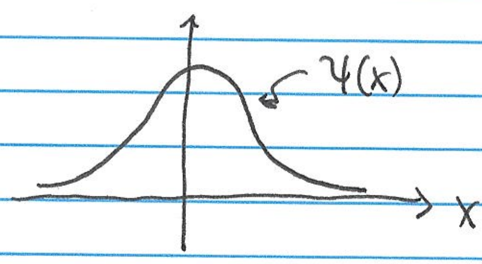
To do these integrals, we have used the definition of the δ-function:

$$\int_{-\infty}^{\infty} dx\, e^{\frac{i(k-p)x}{\hbar}} = 2\pi\, \delta\left(\frac{p-k}{\hbar}\right) = 2\pi\hbar\, \delta(p-k).$$

Compactly, then, we have showed that if a linear combination of momentum eigenstates $\Psi(x)$ is in the Hilbert space $\mathcal{H}$, then

$$\int_{-\infty}^{\infty} dx\, |\Psi(x)|^2 = 2\pi\hbar \int_{-\infty}^{\infty} dp\, |g(p)|^2 = 1,$$

where $g(p)$ is the Fourier conjugate of $\Psi(x)$. This result is called Plancherel's theorem and states that both the wavefunction and its Fourier transform must be L^2-normalizable. In particular, the wavefunction (or $g(x)$) must have compact support for this normalization to be possible. Compact support means that $\Psi(x)$ only has non-zero values (or not excessively small values) over a finite range in x. That is, the wavefunction must look something like:



, or possibly translated, or possibly double humped, etc., but all of the interesting part of $\Psi(x)$ is contained in a finite domain.

This is clearly not a wave, as is is a localized disturbance/bump in probability amplitude. We therefore refer to such a wavefunction as a wave packet, as it is a linear combination of many waves (i.e., a collection of waves in a packet).

Okay, normalization of the free particle has been corrected; what about the velocity of the wave packet? A useful way to think about the wave packet is in analogy to a collection of point particles:

With a collection of such particles, what would we call its "velocity"? well, there is a preferred, single position that describes the global/total motion of the collection of particles: its center of mass, x_{cm}. Recall that the center of mass is:

$$x_{cm} = \frac{\sum_i x_i m_i}{\sum_i m_i},$$

where x_i is the position of the i^{th} particle and m_i is its mass.

One way to think of the mass of a particle is as a relative probability: a particle with large mass has more effect/control over the location of the center-of-mass than does a light particle. So, when thinking about the wave function $\Psi(x,t)$, locations x with large value of $|\Psi|^2$ affect the location of the mean or expected value of position more than places with low probability density. Thus, this suggests that, for a wave function, the expectation value of position, $\langle \hat{x} \rangle$, is analogous to the center-of-mass of some classical system.

So, we can define the velocity of the wavepacket to be the velocity of the expectation value of position, $\langle \hat{x} \rangle$. This velocity is just the time derivative:

$$V_{cm} \equiv \frac{d\langle \hat{x} \rangle}{dt} = \frac{i}{\hbar}\langle [\hat{H}, \hat{x}] \rangle,$$

where, on the right, we have used the expression we derived for time dependence of expectation values a couple weeks ago. Note that also the position operator

$\hat{x}$ has no explicit time dependence, so no partial derivative with respect to time appears.

Let's now evaluate the commutation relation of the Hamiltonian $\hat{H}$ and position $\hat{x}$. We first note that the Hamiltonian, in general, is a function of the momentum operator: $\hat{H} \equiv \hat{H}(\hat{p})$. We'll leave the explicit functional form unevaluated until the end.

Next, let's swith the order of $\hat{x}$ and $\hat{H}$ in the commutator:

$$[\hat{H}, \hat{x}] = -[\hat{x}, \hat{H}].$$

Recall the canonical commutation relation: $[\hat{x}, \hat{p}] = i\hbar$. From this, I leave it to you to show by induction that the commutator of $\hat{x}$ and $\hat{p}$ to the n^{th} power is:

$$[\hat{x}, \hat{p}^n] = i\hbar n\hat{p}^{n-1} = i\hbar \frac{\partial \hat{p}^n}{\partial \hat{p}}.$$

Because we can, generically, express the Hamiltonian as a Taylor series in $\hat{p}$, this suggests that its commutator with $\hat{x}$ is:

$$[\hat{x}, \hat{H}] = [\hat{x}, \hat{H}(\hat{p})] = i\hbar \frac{\partial \hat{H}}{\partial \hat{p}}.$$

Using this result in the expression for the velocity of the center-of-mass of the wave packet, we find:

$$V_{cm} = \frac{d\langle\hat{x}\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H}, \hat{x}]\rangle = \frac{i}{\hbar}\left(-i\hbar\left\langle\frac{\partial \hat{H}}{\partial \hat{p}}\right\rangle\right) = \left\langle\frac{\partial \hat{H}}{\partial \hat{p}}\right\rangle.$$

Now this expression is particularly interesting. Recall that the Hamiltonian is just the total energy, so, in terms of energy and momentum eigenvalues E_p and p, this velocity is:

$$V_{cm} = \frac{\partial E_p}{\partial p} = \frac{\partial(\hbar\omega)}{\partial(\hbar k)} = \frac{\partial \omega}{\partial k},$$ the <u>derivative</u> of the angular velocity ω with respect to wave number k.

This is velocity is called the <u>group</u> <u>velocity</u>, because it is the velocity of an honest normalizable, physical state that is necessarily a "group" of momentum eigenstates.

Now, if we use the fact that the energy of a momentum eigenstate is:

$E_p = \frac{p^2}{2m}$, we find the group velocity of our wave packet to be:

$$V_{group} = \frac{\partial E_p}{\partial p} = \frac{1}{2m}\frac{\partial p^2}{\partial p} = \frac{p}{m},$$ which is indeed the velocity that we know and love.

Now that we've established familiarity with the free particle, next lecture we'll attempt to understand some more of its physical properties.