A short introduction to quantum mechanics XI: comparison with de Broglie's matter waves and the time-dependent Schrödinger equation

What would be the wave function of a particle with constant momentum? In other words, what would be the eigenvector of the momentum matrix for a given eigenvalue? To calculate this, recall that the momentum matrix corresponds to $-i\hbar\frac{\partial}{\partial x}$. Then, we get:

$$\hat{p}\psi = -i\hbar\frac{\partial \psi}{\partial x} = p\psi \tag{1}$$

where p is the eigenvalue. Solving this differential equation, we get:

$$\psi = Ce^{ipx/\hbar} \tag{2}$$

where C is a constant that doesn't depend on the position x. Clearly, this is an equation for a wave. If you are not sure, consider Euler's formula. Then, we get:

$$\psi = C(\cos(ipx/\hbar) + i\sin(ipx/\hbar)) \tag{3}$$

Here, ψ indeed looks like a wave, as it is a sum of cosine and sine functions. Given this, let's calculate λ, the wavelength of this wave.

$$\psi(x) = \psi(x+\lambda) = Ce^{ipx/\hbar + ip\lambda/\hbar} = Ce^{ipx/\hbar + 2\pi i} \tag{4}$$

$$p\lambda/\hbar = 2\pi \tag{5}$$

Considering the fact that $\hbar = h/(2\pi)$, we conclude:

$$\lambda = \frac{h}{p} \tag{6}$$

So, we recovered the equation for the wavelength of de Broglie's matter wave! (If you are unfamiliar with de Broglie's matter wave, please read my article on it listed in "Historical introduction to quantum mechanics.")

To go one step further, notice that a wave function for a travelling wave should have dependence on the time coordinate as well. From elementary physics, we know that a wave travelling in the positive x-direction with constant velocity can be expressed as follows:

$$\psi(x,t) = Ae^{i(kx-\omega t)} \tag{7}$$

In our case we had $k = p/\hbar$. Now, what would be the frequency of this wave? Let's find T, the period, first.

$$\psi(x,t) = \psi(x,t+T) = Ae^{i(kx-\omega(t+T))} = Ae^{i(kx-\omega t-2\pi)} \tag{8}$$

$$\omega T = 2\pi \tag{9}$$

$$T = \frac{2\pi}{\omega} \tag{10}$$

Since f, the frequency, is given by $f = \frac{1}{T}$, we conclude that $f = \frac{\omega}{2\pi}$. Given this, what would be the energy of the particle described by the wave function (7)? Now we can use Planck's relation:

$$E = hf = h\frac{\omega}{2\pi} = \hbar\omega \tag{11}$$

(If you don't know what Planck's relation is, please read my article listed in "Historical introduction to quantum mechanics.") Therefore, the wave function for a travelling wave with constant velocity energy E, and momentum p can be written as (i.e. (7)):

$$\psi(x,t) = Ae^{i(px-Et)/\hbar} \tag{12}$$

This wave function satisfies the following equation:

$$i\hbar\frac{\partial\psi}{\partial t} = E\psi \tag{13}$$

Actually, this equation is satisfied not just for plane waves (i.e. waves such as (12) which have a definite frequency, wavelength and a definite direction), but also for any waves. Given this, recall our earlier Schrödinger equation:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y,z)}{\partial x^2} + \frac{\partial^2\psi(x,y,z)}{\partial y^2} + \frac{\partial^2\psi(x,y,z)}{\partial z^2}\right) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z) \tag{14}$$

Precisely speaking, this version of Schrödinger equation is called "time-independent Schrödinger equation." Then, plugging this equation to (13), we get the following equation called "time-dependent Schrödinger equation":

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + V(x,y,z)\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{15}$$

where ψ is now a function of x, y, z and t. (i.e., $\psi = \psi(x,y,z,t)$) Of course, we can solve the above time-dependent Schrödinger equation by using the separation of variable method which will lead back to the time-independent Schrödinger equation and (13). Now, it is also easy to check that the solution to (13) is given by

$$\psi(x, y, z, t) = e^{-iEt/\hbar}\psi(x, y, z, t = 0) \tag{16}$$

where $\psi(x, y, z, t = 0)$ is a solution to time-independent Schrödinger equation.

In quantum mechanics, the energy operator is often denoted by H, called the "Hamiltonian operator." In other words,

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z) \tag{17}$$

Then, time-independent Schrödinger equation can be re-written as

$$H\psi = E\psi \tag{18}$$

Written in this form, it is apparent that Schrödinger equation is an eigenvalue problem. Also, time-dependent Schrödinger equation can be re-written as

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{19}$$

Now it is easy to see that the solution to the above differential equation is given by following:

$$\psi(x, y, z, t) = e^{-iHt/\hbar}\psi(x, y, z, t = 0) \tag{20}$$

If you remember the time evolution operator from our seventh article on quantum mechanics, you immediately see that $U(t) = e^{-iHt/\hbar}$. Furthermore, its unitary implies that H is necessarily Hermitian. To this end, consider

$$U^\dagger U = e^{iH^\dagger t/\hbar}e^{-iHt/\hbar} = 1 \tag{21}$$

whose last equality would be violated if $H^\dagger \neq H$.

Final comment. In our earlier article "traveling wave," we have seen that the velocity of wave is given by $v = \omega/k = \lambda/T = \lambda f$. Plugging (6) and (11) into this equation (or equivalently using (12)), we get:

$$v = \frac{E}{p} = \frac{\frac{1}{2}mv^2}{mv} = \frac{v}{2} \tag{22}$$

So, we get a contradiction. The propagating speed of the wave function seems to be half of the speed of the object that the wave function describes. Nevertheless, we will resolve this contradiction in our later article "Group velocity and phase velocity."

Problem 1. Let's say that A is an observable and $|a\rangle$ is an eigenvector of Hamiltonian with eigenvalue E_a. Let's say that a state is initially (i.e.

$t = 0$) given by $|a\rangle$. Calculate its expectation value of A at time t if its initial expectation value is given by $\langle A(t=0)\rangle = \langle a|A|a\rangle$.

Problem 2. Let's say that $|a\rangle$s are eigenvectors of Hamiltonian with eigenvalues E_a, respectively. Convince yourself or prove the followings (Hint[1]):

$$e^{-iHt/\hbar}\left(\sum_a c_a|a\rangle\right) = \sum_a \left(c_a e^{-iE_at/\hbar}|a\rangle\right) \tag{23}$$

$$e^{-iHt/\hbar} = \sum_a |a\rangle e^{-iE_at/\hbar}\langle a| \tag{24}$$

Summary

- A wave travelling in the positive x-direction with wave number k, angular frequency ω, momentum p, and energy E, can be written as

$$\psi(x,t) = Ae^{i(kx-\omega t)} = Ae^{i(px-Et)/\hbar}$$

- Schrödinger equation can be written as

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi$$

where

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x,y,z)$$

[1] For the second one, sse the completeness relation $I = \sum_a |a\rangle\langle a|$