A short introduction to quantum mechanics VIII: the time-dependent Schrödinger equation

In earlier articles, I explained Schrödinger equation. The wave function with a definite energy was a solution to the Schrödinger equation. The wave function so obtained was a function of x. It was a function of position only, independent of time.

However, this is unsatisfactory. We explained that a particle is described by its wave function. If the wave function doesn't evolve over time, nothing about its particle will change; its position won't change, its momentum won't change, as their expectation values won't have any time-dependence. However, we do know that particles in our Universe change their position and momentum. Thus, we come to the conclusion that a wave function must change over time.

Such a wave function must obey a new Schrödinger equation that dictates how it must evolve over time. Such a Schrödinger equation is called "the time-dependent Schrödinger equation." Our earlier Schrödinger equation that doesn't depend on time is called "the time-independent Schrödinger equation." In this article, we will motivate and introduce the time-dependent Schrödinger equation.

To this end, consider the following plane wave with the wave number k and the angular frequency ω:

$$\psi(x,t) = A\exp(i(kx-\omega t)) \tag{1}$$

where

$$k = \frac{2\pi}{\lambda}, \qquad \omega = \frac{2\pi}{T} = 2\pi f \tag{2}$$

Then, it is easy to see that this plane wave is an eigenvector of momentum operator. If we apply the momentum operator to (1), we get

$$-i\hbar\frac{\partial\psi(x,t)}{\partial x} = \hbar k\psi(x,t) \tag{3}$$

Thus, its momentum eigenvalue is $\hbar k$. Now, notice

$$p = \hbar k = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \frac{h}{\lambda} \tag{4}$$

Thus, we obtain de Broglie's relation. In other words, we obtained that a wave function with a wavelength λ has the momentum h/λ. Put it slightly differently, the wave function of a particle with the momentum p has the wavelength h/p.

Can we also get the following Planck's relation from (1)?

$$E = hf = h\frac{\omega}{2\pi} = \hbar\omega \tag{5}$$

Recall what we did with the momentum operator and de Broglie's relation. We pulled out the factor ik from (1) by taking a partial derivative with respect to x. Then, by multiplying it by $-i\hbar$, we obtained $p = \hbar k$, which is de Broglie's relation.

Thus, we see that we can get the factor $-i\omega$ from (1) by taking a partial derivative with respect to t and by multiplying it by $i\hbar$, we can obtain $E = \hbar\omega$. That is,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hbar\omega\psi(x,t) \tag{6}$$

As much as the momentum operator is $-i\hbar\frac{\partial}{\partial x}$, we can say the energy operator is given by $i\hbar\frac{\partial}{\partial t}$. In other words, a wave function with a definite energy E satisfies

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = E\psi(x,t) \tag{7}$$

Actually, this equation is satisfied not just for plane waves (i.e. waves such as (1) which have a definite frequency, wavelength and a definite direction), but also for any waves; as much as the momentum operator is given by $-i\hbar\frac{\partial}{\partial x}$ regardless of whether the wave function concerned is a plane wave, the energy operator is given by $i\hbar\frac{\partial}{\partial t}$, and (7) is just the eigenvalue problem of the energy operator.

Problem 1. Using Planck's relation and de Broglie's relation, show that (1) can be re-expressed as

$$\psi(x,t) = A\exp(i(px - Et)/\hbar) \tag{8}$$

Finally, we can state the time-dependent Schrödinger equation. Recall the following time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x) \tag{9}$$

As there is no partial derivative with respect to t, we can as well say the above equation as

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = E\psi(x,t) \tag{10}$$

Then, by connecting it with (7), the time-dependent Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V(x)\psi(x,t)=i\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{11}$$

Now, let's obtain the solution to the time-dependent Schrödinger equation.

Problem 2. Show that $\psi(x,t) = \psi(x)e^{-iEt/\hbar}$ satisfies (11) provided that $\psi(x)$ satisfies (9).

Problem 3. Check that the linear combination of the solution to the time-dependent Schrödinger equation is also a solution to the time-dependent Schrödinger equation. In other words, for constant c_ns,

$$\psi(x,t)=\sum_n c_n\psi_n(x,t) \tag{12}$$

satisfies (11) if $\psi_n(x,t)$ satisfies (11).

More concretely, if $\psi_n(x,t)$ is a solution to the time-dependent Schrödinger equation with energy E_n, we can write $\psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar}$, where $\psi_n(x)$ is a normalized solution to the time-independent Schrödinger equation, i.e.,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n(x)}{\partial x^2}+V(x)\psi_n(x)=E_n\psi_n(x) \tag{13}$$

Then, (12) can be re-expressed as

$$\psi(x,t)=\sum_n c_n\psi_n(x)e^{-iE_nt/\hbar} \tag{14}$$

Here, we see that the wave function with arbitrary t is completely determined once we know c_n.

Given the form of the wave function that evolves over time, let's ask a question about such wave functions. In our earlier articles, we emphasized the importance of the normalization. Unless a particle is created or destroyed, its wave function must remain normalized once it is normalized.

Let's check this. First, let's express (14) slightly differently as follows:

$$|\psi(t)\rangle=\sum_n c_n|\psi_n\rangle e^{-iE_nt/\hbar} \tag{15}$$

When $t = 0$, we have

$$|\psi(0)\rangle=\sum_n c_n|\psi_n\rangle \tag{16}$$

As mentioned before, $|\psi_n\rangle$ is the normalized eigenvector of the Hamiltonian operator with eigenvalue E_n, i.e.,

$$H|\psi_n\rangle=E|\psi_n\rangle \tag{17}$$

As H is Hermitian and $|\psi_n\rangle$s are normalized, we have

$$\langle\psi_n|\psi_m\rangle = \delta_{nm} \tag{18}$$

Then, the condition that (16) is normalized means

$$1 = \sum_n |c_n|^2 \tag{19}$$

Given this, let's check (15) is normalized.

$$\begin{aligned}
\langle\psi(t)|\psi(t)\rangle &= \left(\sum_m c_m^* \langle\psi_m| e^{iE_m t/\hbar}\right)\left(\sum_n c_n |\psi_n\rangle e^{-iE_n t/\hbar}\right) & (20)\\
&= \sum_m \sum_n c_m^* c_n \langle\psi_m|\psi_n\rangle e^{iE_m t/\hbar} e^{-iE_n t/\hbar} & (21)\\
&= \sum_m \sum_n c_m^* c_n \delta_{mn} e^{iE_m t/\hbar} e^{-iE_n t/\hbar} & (22)\\
&= \sum_n c_n^* c_n e^{iE_n t/\hbar} e^{-iE_n t/\hbar} & (23)\\
&= \sum_n |c_n|^2 = 1 & (24)
\end{aligned}$$

Thus, it is indeed normalized.

Earlier, we showed that the wave function with arbitrary time is completely determined once we know c_n. So, how can we obtain c_n, given the initial wave function (i.e., when $t = 0$)? If we multiply (16) on the left by $\langle\psi_m|$, we get

$$\langle\psi_m|\psi(0)\rangle = \sum_n c_n \langle\psi_m|\psi_n\rangle = \sum_n c_n \delta_{mn} = c_m \tag{25}$$

In other words, c_n can be obtained by

$$c_n = \langle\psi_n|\psi(0)\rangle = \int \psi_n^*(x)\psi(x,0)dx \tag{26}$$

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 (4) and (5) into this equation, we get:

$$v = \frac{\omega}{k} = \frac{\hbar\omega}{\hbar k} = \frac{E}{p} = \frac{\frac{1}{2}mv^2}{mv} = \frac{v}{2} \tag{27}$$

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 4. Let's say $\psi_n(x)$ satisfies the time-independent Schrödinger equation (13). Supposing that the wave function at $t = 0$ is given by $\Psi(x, t = 0) = \frac{1}{\sqrt{2}}(\psi_1(x) + i\psi_2(x))$, obtain $\Psi(x, t)$ for arbitrary t. Express your answer in terms of $\psi_1(x)$, $\psi_2(x)$, E_1 and E_2.

Problem 5. By using (15) and (17), obtain an expression for the expectation value of the Hamiltonian and check that it does not change over time, as long as the Hamiltonian operator H is Hermitian. This result shows the conservation of energy.

Problem 6. 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 7. Assume that a state is in a linear combination of the state with energy E_1 and the state with energy E_2. Then, the expectation value of its position x oscillates. What is the period of this oscillation? Notice that expectation value of any observable oscillates with the same period, as the probability density oscillates in this period. (Remark. Physically similar thing is happening in "neutrino oscillation," except that a neutrino is a linear combination of three eigenstates of energy. We will talk more about neutrino oscillation in a later article.)

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

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

- A general solution to the time-dependent Schrödinger equation is given by

$$\psi(x, t) = \sum_n c_n\psi_n(x)e^{-iE_nt/\hbar}$$

where

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n(x)}{\partial x^2} + V(x)\psi_n(x) = E_n\psi_n(x)$$

- c_n can be obtained by

$$c_n = \langle\psi_n|\psi(0)\rangle = \int\psi_n^*(x)\psi(x, 0)dx$$