Lecture 7 - Momentum operator

What's important:
- momentum operator
- commutation relations
- Hermitian operators

Text: Gasiorowicz, Chap. 3.

Momentum operator

Once we have solved the Schrödinger equation

$$i\hbar \frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} \qquad (1)$$

for some particular condition (we'll introduce the form of the SE which includes interactions in a moment) then we can calculate the mean position and its dispersion from quantities like

$$<x> = \int \psi^* \, x \, \psi \, dx \quad \text{and} \quad <x^2> = \int \psi^* \, x^2 \, \psi \, dx. \qquad (2)$$

Given the form of the wavepackets described earlier, it's obvious how to do the mathematics of Eq. (1) - one just integrates over some functions which depend on *x* and *t*. But what about a quantity like the momentum *p*? What is the meaning of the expression

$$<p> = \int \psi^* \, p \, \psi \, dx \; ?$$

An appealing starting point is to return to the classical definition

$$p = mv = m \, dx/dt$$

and PROPOSE

$$<p> = m \, d<x>/dt. \qquad (3)$$

We'll provide the motivation for this in a later lecture on the classical limit of ψ. Thus,

$$<p> = m \, (d/dt) \int \psi^* \, x \, \psi \, dx. \qquad (4)$$

The wavefunction is time-dependent, so taking the time derivative inside the integral will yield terms like $d\psi/dt$. However, there is no time-dependence to *x*: it's just an integration variable, not a function of *t* [that is, it is NOT the trajectory *x*(*t*)]. Then

$$<p> = m\int_{-\infty}^{\infty} \left(\frac{\partial\psi^*}{dt} x\psi + \psi^* x \frac{\partial\psi^*}{dt} \right) dx.$$

We can now use the free-particle Schrödinger equation, Eq. (1), to replace the time derivative of ψ with a spatial derivative, so all the variables in the integral are consistent. This yields

$$< p >= -\frac{i\hbar}{2}\int_{-\infty}^{\infty}\left(\frac{\partial^2\psi^*}{dx^2}x\psi - \psi^* x\frac{\partial^2\psi}{dx^2}\right)dx \quad (5)$$

Note the relative minus sign arising from the complex conjugate.

The next few steps in evaluating the integral are not obvious. We're looking for a way of replacing the second order derivative with something like $\partial/\partial x$ (function), which we can evaluate at the integration limits of $|x| = \infty$. The steps are as follows:

1. Use the replacement

$$\frac{\partial^2\psi^*}{\partial x^2}x\psi = \frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x}x\psi\right) - \frac{\partial\psi^*}{\partial x}\psi - \frac{\partial\psi^*}{\partial x}x\frac{\partial\psi}{\partial x}. \quad (6)$$

2. For the second term on the RHS, use the replacement

$$\frac{\partial\psi^*}{\partial x}\psi = \frac{\partial}{\partial x}(\psi^*\psi) - \psi^*\frac{\partial\psi}{\partial x} \quad (7)$$

3. For the third term on the RHS, use the replacement

$$\frac{\partial\psi^*}{\partial x}x\frac{\partial\psi}{\partial x} = \frac{\partial}{\partial x}\left(\psi^* x\frac{\partial\psi}{\partial x}\right) - \psi^*\frac{\partial\psi}{\partial x} - \psi^* x\frac{\partial^2\psi}{\partial x^2} \quad (8)$$

Watch the minus signs in making the replacements! The integrand becomes (after accounting for the signs, the last term in (8) cancels the second term in the integral):

$$\frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x}x\psi - \psi^* x\frac{\partial\psi}{\partial x} - \psi^*\psi\right) + 2\psi^*\frac{\partial\psi}{\partial x}. \quad (9)$$

How does this help? The first part of (9) has the form df/dx, so that it contributes

$$\int_{-\infty}^{\infty}(df/dx)\, dx \quad (10)$$

to the integral. If f is square integrable (integral of f^*f is finite when integrated over x), then the integral of its derivative must vanish. Thus, (10) vanishes, as does the integral of the first term in (9). Substituting into Eq. (5) gives us:

$$< p >= -i\hbar\int_{-\infty}^{\infty}\psi^*\frac{\partial}{\partial x}\psi dx \quad (11)$$

The mathematical steps to solve Eq. (11) are now clear once $\psi(x,t)$ is known. More importantly, Eq. (11) suggests a way of representing the momentum and its square:

$$p = -i\hbar \frac{\partial}{\partial x} \quad \text{and} \quad p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2} \qquad (12)$$

This is an **operator** representation of *p*: is has the effect of doing something to the function $\psi(x,t)$ to its right.

The **position** operator as seen for wavefunctions $\psi(p,t)$ has a similar form. See Chap. 3 of Gasiorowicz.

Commutation relations

The fact that the momentum operator involves a derivative with respect to position means that an attempt to find the expectation of *x* and *p* requires a specification of the order in which the measurement taken. This is best summarized by evaluating the commutator

$$[A,B] = AB - BA \qquad (13)$$

familiar from linear algebra. Placing an "op" on *p* to explicitly mean

$$p_{op} = -i\hbar\, \partial/\partial x \qquad (14)$$

we find

$$[x, p_{op}]\,\psi(x,t) = x\{-i\hbar\, \partial\psi(x,t)/\partial x\} - \{-i\hbar\, \partial/\partial x(x\,\psi(x,t))\}$$
$$= -i\hbar x \bullet \partial\psi(x,t)/\partial x + i\hbar\psi(x,t) + i\hbar x \bullet \partial\psi(x,t)/\partial x$$
$$= i\hbar\psi(x,t).$$

Just taking the operators by themselves, this means

$$[x, p_{op}] = +i\hbar. \qquad (15)$$

We could equally well work with momentum-space wavefunctions $\psi(p,t)$, where

$$x_{op} = +i\hbar\, \partial/\partial p$$

to find

$$[x_{op}, p] = i\hbar.$$

The fact that *x* and *p* **DON'T** commute is at the heart of Heisenberg's uncertainty principle: measurement of one of these quantities affects the "value" of the other.

Hermitian operators

Should it bother us that the operator representation of momentum is complex? No, as can be seen by comparing $\langle p \rangle$ with its complex conjugate:

$$\langle p \rangle - \langle p \rangle^*,$$

which, by explicit substitution is:

$$< p > - < p > * = -i\hbar \int \psi * \frac{\partial \psi}{\partial x} dx - (+i\hbar) \int \psi \frac{\partial \psi *}{\partial x} dx$$

$$= -i\hbar \int \frac{\partial}{\partial x} (\psi * \psi) dx$$

The integral is evaluated at -∞ and +∞, where $\psi^*\psi$ vanishes if $\int \psi^*\psi \, dx$ is to be finite (*i.e.*, if the wavefunction is square integrable). Thus,

$$<p> - <p>^* = 0$$

and $<p>$ is real.

Operators whose expectations are real are called *Hermitian* operators. In matrix language, a Hermitian matrix is one which is equal to its complex transpose:

$$A = (A^*)^T. \tag{16}$$