A short introduction to quantum mechanics III: the equivalence between Heisenberg's matrix method and Schrödinger's differential equation

In the article "A short introduction to quantum mechanics I: observables and eigenvalues," I explained that Heisenberg's quantum mechanics is based on the formula $XP - PX = i\hbar$, where X is the position operator and P is the momentum operator, while Schrödinger's quantum mechanics is based on the idea that the energy matrix is $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$. I claimed, without proof, that the two formalisms are equivalent. In this article, I will concretely show that they are indeed equivalent.

The key idea to understanding this is that $XP - PX = i\hbar$ can be satisfied if the position operator X corresponds to multiplying the wave function by x, while the momentum operator P corresponds to $-i\hbar\frac{\partial}{\partial x}$(differentiating with respect to x and multiplying by $-i\hbar$). Now, let's see how this corresponds to Heisenberg's quantum mechanics. If we apply the momentum operator P to the vector $\psi(x)$, we get $P\psi(x) = -i\hbar\frac{\partial\psi(x)}{\partial x}$. If we then apply the position operator X to this, we get $-i\hbar x\frac{\partial\psi(x)}{\partial x}$. In other words:

$$XP\psi(x) = -i\hbar x\frac{\partial\psi(x)}{\partial x} \tag{1}$$

Similarly we can easily obtain

$$X\psi(x) = x\psi(x) \tag{2}$$

$$PX\psi(x) = P(X\psi(x)) = -i\hbar\frac{\partial(x\psi(x))}{\partial x} = -i\hbar(\psi(x) + x\frac{\partial\psi(x)}{\partial x}) \tag{3}$$

One more step forward, we get:

$$(XP - PX)\psi(x) = i\hbar\psi(x) \tag{4}$$

In other words, $XP - PX = i\hbar$. This is Heisenberg's matrix method. Indeed the condition $XP - PX = i\hbar$ is equal to the condition that the position operator X corresponds to multiplying the wave function by x and the momentum operator P corresponds to $-i\hbar\dfrac{\partial}{\partial x}$.

Now, let's derive Schrödinger's equation. In classical mechanics, mechanical energy is

$$E = \frac{1}{2}mv^2 + V(x) = \frac{(mv)^2}{2m} + V(x) = \frac{p^2}{2m} + V(x) \tag{5}$$

Putting this into the language of operators, p^2 means applying P twice to the vector $\psi(x)$, while $V(x)$ means multiplying $\psi(x)$ by $V(x)$. In other words, p^2 is $-\hbar^2\dfrac{\partial^2}{\partial x^2}$ If we divide this by $2m$ and add $V(x)$ we obtain the energy matrix. If we then apply the energy matrix to the vector $\psi(x)$, we get:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) \tag{6}$$

We can get the eigenvalues and the eigenvectors of this energy matrix by solving the equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x) \tag{7}$$

where E is the eigenvalue.

At this point, we would like to introduce commutator. A commutator of A and B is defined by $AB - BA$ and denoted as $[A, B]$, For example, our earlier formula can be re-written as follows:

$$[X, P] = i\hbar \tag{8}$$

So far we have considered a 1-dimensional problem. But in reality, a particle can move in three dimensions, on which we will now focus. In this case, we have the position operators X, Y, Z, which act by multiplying x, y, z respectively. Also, we now have three momentum operators: the x,y,z-components of momentum, which we denote by P_x,P_y,P_z. Naturally, they act by $-i\hbar\dfrac{\partial}{\partial x}$,$-i\hbar\dfrac{\partial}{\partial y}$,$-i\hbar\dfrac{\partial}{\partial z}$. With this information, it is easy to check the following:

$$[X, P_x] = [Y, P_y] = [Z, P_z] = i\hbar \tag{9}$$

$$[Y, P_x] = [Z, P_x] = [X, P_y] = [Z, P_y] = [X, P_z] = [Y, P_z] = 0 \tag{10}$$

$$[X, Y] = [Y, Z] = [Z, X] = 0 \tag{11}$$

$$[P_x, P_y] = [P_y, P_z] = [P_z, P_x] = 0 \tag{12}$$

The last one can be shown from the fact that partial derivatives commute. On the other hand, (5) is given by:

$$E = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x, y, z) \tag{13}$$

which implies

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

Problem 1. Check $[Y, P_x] = 0$ using Leibniz rule and the property of partial derivatives. (Hint[1])

Problem 2. Prove the followings

$$[A, B] = -[B, A], \qquad [A, A] = 0 \tag{15}$$

$$[AB, C] = A[B, C] + [A, C]B \tag{16}$$

$$[D, EF] = [D, E]F + E[D, F] \tag{17}$$

Problem 3. Using (16) and (17), prove the followings:

$$[X^2, P_x] = 2i\hbar X \tag{18}$$

$$[X, P_x^2] = 2i\hbar P_x \tag{19}$$

Problem 4. Using Leibniz rule and $P\psi(x) = -i\hbar\frac{\partial\psi(x)}{\partial x}$, prove the following:

$$[f(X), P_x] = i\hbar\frac{\partial f(x)}{\partial x} \tag{20}$$

(Hint[2]) Notice that we could have obtained (18) using the above formula.

Summary

- A commutator of A and B is defined by $AB - BA$ and denoted as $[A, B]$.
- $[X, P] = i\hbar$.
- The position operator X acts by multiplying x.
- The momentum operator P_x acts by $-i\hbar\frac{\partial}{\partial x}$.
- $[A, B] = -[B, A], \qquad [A, A] = 0$
- $[AB, C] = A[B, C] + [A, C]B$
- $[D, EF] = [D, E]F + E[D, F]$

[1] Show $[Y, P_x]\psi = 0$

[2] Show $[f(X), P_x]\psi = i\hbar\frac{\partial f(x)}{\partial x}\psi$