

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:

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

Similarly we can easily obtain

$$X\psi(x) = x\psi(x) \quad (2)$$

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

One more step forward, we get:

$$(XP - PX)\psi(x) = i\hbar\psi(x) \quad (4)$$

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 $-i\hbar \frac{\partial}{\partial x}$.

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

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

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 $-\hbar^2 \frac{\partial^2}{\partial x^2}$. 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:

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

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

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

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:

$$[X, P] = i\hbar \quad (8)$$

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 $-i\hbar \frac{\partial}{\partial x}, -i\hbar \frac{\partial}{\partial y}, -i\hbar \frac{\partial}{\partial z}$. With this information, it is easy to check the following:

$$[X, P_x] = [Y, P_y] = [Z, P_z] = i\hbar \quad (9)$$

$$[Y, P_x] = [Z, P_x] = [X, P_y] = [Z, P_y] = [X, P_z] = [Y, P_z] = 0 \quad (10)$$

$$[X, Y] = [Y, Z] = [Z, X] = 0 \quad (11)$$

$$[P_x, P_y] = [P_y, P_z] = [P_z, P_x] = 0 \quad (12)$$

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

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

which implies

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

Problem 1. Check $[Y, P_x] = 0$ using Leibniz rule and the property of partial derivatives. (Hint¹)

Problem 2. Prove the followings

$$[A, B] = -[B, A], \quad [A, A] = 0 \quad (15)$$

$$[AB, C] = A[B, C] + [A, C]B \quad (16)$$

$$[D, EF] = [D, E]F + E[D, F] \quad (17)$$

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

$$[X^2, P_x] = 2i\hbar X \quad (18)$$

$$[X, P_x^2] = 2i\hbar P_x \quad (19)$$

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

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

(Hint²) Notice that we could have obtained (18) using the above formula.

¹Show $[Y, P_x]\psi = 0$

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