Physics 342 Lecture 12

At the end of the previous lecture, we had identified the fascinating property that the position and momentum operators do not commute:

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}x = i\hbar.$$

This is called the canonical commutation relation as it has profound consequences for physical consequences in quantum mechanics. Actually, if you are familiar with Poisson brackets in the Hamiltonian formulation of classical mechanics, you might remember that the poisson bracket of x and p is:

$$\{x, p\} = \frac{dx}{dx}\frac{dp}{dp} - \frac{dx}{dp}\frac{dp}{dx} = 1,$$

which is the same as the commutation relation, up to $i\hbar$. As operators, the mathematizal interpretation of $[\hat{x}, \hat{p}] \neq 0$ is the following. If the eigenstates of $\hat{x}$ and $\hat{p}$ were identical, i.e., for some set of states $\{|v_i\rangle\}_i$, we would have

$$\hat{x}|v_i\rangle = x_i|v_i\rangle \quad \underline{\text{and}} \quad \hat{p}|v_i\rangle = p_i|v_i\rangle$$

then $\hat{x}$ and $\hat{p}$ would commute:

$$\hat{x}\hat{p}|v_i\rangle = x_i p_i |v_i\rangle = \hat{p}\hat{x}|v_i\rangle.$$

However, because $[\hat{x}, \hat{p}] \neq 0$, this is not possible: the eigenstates of $\hat{x}$ and $\hat{p}$ cannot be the same and therefore when thought of as matrices, $\hat{x}$ and $\hat{p}$ cannot be <u>simultaneously</u> <u>digonalized</u>.

If we express the Hilbert space with the basis of eigenstates of momentum, for example, then necessarily the eigenstates of position will be non-trivial linear combinations of states of different momentum, and vice-versa.

In this lecture, we'll provide a bit more physical understanding of this non-commutitivity. To do this, let's consider two Hermitian operators, A and B, and we will calculate the expectation value of their commutation relation on some state $|\psi\rangle$ in the Hilbert space:

$$\langle\psi|[A,B]|\psi\rangle \equiv \langle[A,B]\rangle.$$

Expanding this out, we can write it as

$$\langle[A,B]\rangle = \langle AB - BA\rangle = \langle AB\rangle - \langle BA\rangle$$

$$= \Big(\langle AB\rangle - \langle A\rangle\langle B\rangle\Big) - \Big(\langle BA\rangle - \langle A\rangle\langle B\rangle\Big).$$

I have added and subtracted $\langle A\rangle\langle B\rangle$ with benefit of malevolent forethought. Note that, by Hermitivity of A, B, their individual expectation values are real:

$\langle A\rangle, \langle B\rangle \in \mathbb{R}$, and $\langle AB\rangle, \langle BA\rangle$ are complex conjugates:

$$\langle AB\rangle^* = \langle BA\rangle.$$

Thus, if we call $z \equiv \langle AB\rangle - \langle A\rangle\langle B\rangle$, then this is just:

$$\langle[A,B]\rangle = z - z^* = 2i\,\mathrm{Im}\,z = 2i\,\mathrm{Im}\Big(\langle AB\rangle - \langle A\rangle\langle B\rangle\Big),$$

the imaginary part of the complex number $z = \langle AB \rangle - \langle A \rangle \langle B \rangle$. Rearranging we have

$$\mathrm{Im}\left(\langle AB \rangle - \langle A \rangle \langle B \rangle\right) = \frac{\langle AB \rangle - \langle BA \rangle}{2i}$$

Next, as a complex number z can be expressed as:

$$z = \mathrm{Re}(z) + i\,\mathrm{Im}(z), \text{ and has magnitude}$$

$$|z|^2 = z z^* = \mathrm{Re}(z)^2 + \mathrm{Im}(z)^2 \geq \mathrm{Im}(z)^2,$$

we can bound this commutator expectation value from above by:

$$\left(\frac{\langle AB \rangle - \langle BA \rangle}{2i}\right)^2 \leq \mathrm{Re}\left(\langle AB \rangle - \langle A \rangle \langle B \rangle\right)^2 + \mathrm{Im}\left(\langle AB \rangle - \langle A \rangle \langle B \rangle\right)^2.$$

The real part of $\langle AB \rangle - \langle A \rangle \langle B \rangle$ is:

$$\mathrm{Re}\left(\langle AB \rangle - \langle A \rangle \langle B \rangle\right) = \frac{\langle AB \rangle - \langle A \rangle \langle B \rangle + \langle BA \rangle - \langle A \rangle \langle B \rangle}{2}$$

$$= \frac{\langle AB \rangle + \langle BA \rangle}{2} - \langle A \rangle \langle B \rangle$$

We actually won't use this directly, but it's good to see it explicitly. Now, note that this complex number can be written as:

$$\langle AB \rangle - \langle A \rangle \langle B \rangle = \langle \psi | (A - \langle A \rangle)(B - \langle B \rangle) | \psi \rangle.$$

To see this, expand out the right side:

$$\langle\psi|(A-\langle A\rangle)(B-\langle B\rangle)|\psi\rangle = \langle\psi|AB|\psi\rangle - \langle A\rangle\langle\psi|B|\psi\rangle - \langle B\rangle\langle\psi|A|\psi\rangle + \langle A\rangle\langle B\rangle\langle\psi|\psi\rangle$$

$$= \langle AB\rangle - \langle A\rangle\langle B\rangle,$$ because both $\langle A\rangle$ and $\langle B\rangle$ are just ~~complex~~ real numbers.

With this identification, we can now interpret the two parts of this inner product as follows. Call

$$(A-\langle A\rangle)|\psi\rangle = |f\rangle \quad \text{and} \quad (B-\langle B\rangle)|\psi\rangle = |g\rangle.$$

Then, we have established that:

$$\left(\frac{\langle[A,B]\rangle}{2i}\right)^2 \leq |\langle f|g\rangle|^2.$$

If $\langle f|g\rangle$ represented the dot product of two, ordinary, vectors, then we would have:

$$|\langle f|g\rangle|^2 = \langle f|f\rangle\langle g|g\rangle \cos^2\theta.$$

However, $\cos^2\theta \leq 1$ for all θ, so we have another inequality:

$$|\langle f|g\rangle|^2 \leq \langle f|f\rangle\langle g|g\rangle.$$

This is called the Schwartz Inequality, and can be proved for general states and inner product (which we won't do here). So, we now have the inequality:

$$\left(\frac{\langle [A,B] \rangle}{2i}\right)^2 \leq \langle (A - \langle A \rangle)(A - \langle A \rangle) \rangle \langle (B - \langle B \rangle)(B - \langle B \rangle) \rangle$$

Let's figure out what these expectation values are. For A, we have

$$\begin{aligned} \langle (A - \langle A \rangle)(A - \langle A \rangle) \rangle &= \langle A^2 \rangle - \langle A \rangle^2 - \langle A \rangle^2 + \langle A \rangle^2 \\ &= \langle A^2 \rangle - \langle A \rangle^2 \end{aligned}$$

This quantity is also called the <u>variance</u> of A on the state $|\psi\rangle$. The term variance connotes, and practically means that it is a measure of how the value of A on the state $|\psi\rangle$ varies about its mean, $\langle A \rangle$. Because the quantity

$$\langle \psi | (A - \langle A \rangle)(A - \langle A \rangle) | \psi \rangle \geq 0$$

is the magnitude squared of the state $|(A - \langle A \rangle)\psi\rangle$, the variance is always non-negative. The variance is <u>only</u> 0 if and only if the state $|\psi\rangle$ is an eigenstate of A. For example, let's assume that our Hilbert space is two dimensional and we use the eigenvectors of A as the basis, $\{|v_i\rangle\}_{i=1}^{2}$, where

$A|v_1\rangle = \lambda_1 |v_1\rangle$, $A|v_2\rangle = \lambda_2 |v_2\rangle$, and so the state $|\psi\rangle$ can be expressed as

$|\psi\rangle = \alpha_1 |v_1\rangle + \alpha_2 |v_2\rangle$, where $\alpha_1, \alpha_2 \in \mathbb{C}$.

Then, $\langle A \rangle = \langle \psi | A | \psi \rangle = \left(\langle v_1 | \alpha_1^* + \langle v_2 | \alpha_2^* \right)\left(\alpha_1 \lambda_1 |v_1\rangle + \alpha_2 \lambda_2 |v_2\rangle \right)$

$$= \lambda_1 |\alpha_1|^2 + \lambda_2 |\alpha_2|^2.$$

Also, $\langle A^2\rangle = \langle\psi|A^2|\psi\rangle = \left(\langle v_1|\alpha_1^* + \langle v_2|\alpha_2^*\right)\left(\alpha_1\lambda_1^2|v_1\rangle + \alpha_2\lambda_2^2|v_1\rangle\right)$

$$= \lambda_1^2|\alpha_1|^2 + \lambda_2^2|\alpha_2|^2,$$

and we us orthonormality of $|v_1\rangle$, $|v_2\rangle$:

$$\langle v_1|v_1\rangle = \langle v_2|v_2\rangle = 1, \quad \langle v_1|v_2\rangle = 0.$$

Then, the variance of such a state is:

$$\langle A^2\rangle - \langle A\rangle^2 = \lambda_1^2|\alpha_1|^2 + \lambda_2^2|\alpha_2|^2 - \left(\lambda_1|\alpha_1|^2 + \lambda_2|\alpha_2|^2\right)^2$$

$$= \lambda_1^2\left(|\alpha_1|^2 - |\alpha_1|^4\right) + \lambda_2^2\left(|\alpha_2|^2 - |\alpha_1|^4\right)$$

$$- 2\lambda_1\lambda_2|\alpha_1|^2|\alpha_2|^2$$

Without loss of generality, we can assume that one of the eigenvalues, say λ_2, is 0: $\lambda_2 = 0$. (Why is that? For example, is the absolute energy meaningful?) Then, the variance is:

$\langle A^2\rangle - \langle A\rangle^2 = \lambda_1^2|\alpha_1|^2\left(1 - |\alpha_1|^2\right)$, which clearly

only vanishes if $|\alpha_1|^2 = 1,0$ or that $|\psi\rangle = |v_1\rangle$ or $|v_2\rangle$. This can be generalized, but the idea still holds: for a general state $|\psi\rangle$, the variance of A is non-zero.

All the same statements can be made for B. We compactly denote the variance of A as σ_A^2 (and correspondingly for B), so we can express this inequality as:

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{\langle [A,B] \rangle}{2i} \right)^2$$, or, removing squares:

$$\boxed{\sigma_A \sigma_B \geq \left| \frac{\langle [A,B] \rangle}{2i} \right|}$$

This is called the generalized uncertainty principle. Recall that σ_A^2, σ_B^2 is a measure of how close to an eigenstate of A or B the state $|\psi\rangle$ is. If the commutator of A and B is non-zero, then $|\psi\rangle$ cannot be an eigenstate of A and B simultaneously; that is, if $[A,B] \neq 0$, then σ_A and σ_B cannot both be 0.

For the particular identification of $A = \hat{x}$ and $B = \hat{p}$, we have

$[\hat{x}, \hat{p}] = i\hbar$, and so

$$\boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}}$$

This is called the Heisenberg uncertainty relation. A generic state $|\psi\rangle$ cannot be an eigenstate of $\hat{x}$ and $\hat{p}$, simultaneously.

This means that there is necessarily uncertainty (i.e., variance) of an objects position and momentum. Colloquially, we can say that if we know a particle's momentum, then it is in an eigenstate of $\hat{p}$, so that $\sigma_p = 0$. However, for the uncertainty relation to hold, we must have ~~$\sigma_x = \infty$~~ $\sigma_x = \infty$; the position of the particle is completely unknown! This is very unlike classical mechanics in which we can know arbitrary data to arbitrary precision of any object. The consequences of this uncertainty relation will be explored throughout this class.

Finally, just to connect the variance to something a bit more familiar, let's calculate it for a fair die. The expression of the variance for the outcome of rolls of the die would be:

$$\sigma^2_{die} = \sum_{i=1}^{6} p_i i^2 - \left(\sum_{i=1}^{6} p_i i\right)^2$$

$$= \frac{1}{6}(1+4+9+16+25+36) - \frac{1}{36}(1+2+3+4+5+6)^2$$

$$= \frac{1}{6}\frac{6(6+1)(2\cdot 6+1)}{6} - \frac{1}{36}\frac{6^2(6+1)^2}{4}$$

$$= \frac{91}{6} - \frac{49}{4} = \frac{35}{12} \cong 2.92$$

The square-root of the variance is called the <u>standard deviation</u> and we find for this case:

$$\sigma_{die} \cong 1.71$$

The interpretation of the standard deviation is that on any given roll, you expect to be approximately within one σ_{die} of the mean. Recall that the mean for the outcome of the roll of the die is

$$\langle roll \rangle = \frac{7}{2} = 3.5.$$

Being within one σ_{die} of this value means that your roll is in the range:

$$roll \in [3.5 - 1.71, 3.5 + 1.71] = [1.79, 5.21],$$

which is true for all possible rolls, except 1 and 6.

Thus 2/3 of the time (for rolls of 2, 3, 4, or 5) are you withing one σ_{die} of <roll>. This is indeed "most" of the time (i.e., larger than 50%).

Okay, enough abstractness. Next week we will begin studying some concrete examples to see how all of this works.