Uncertainty Principles

Lecture 16

Physics 342
Quantum Mechanics I

Monday, March 3rd, 2008

We saw, last time, that commuting observables (i.e. Hermitian operators, A and B with $[A, B] = 0$) had compatible eigenstates, and so a "determinate state" of A was also a determinate state of B. There are a few examples of such commuting observables that we have encountered, but the most familiar operators, x, p and H do not commute, so we can ask the natural question: "If we know the variance of one operator, what can we say about the variance of another?".

This is a natural question only within the context of what we know about linear algebra – from a physics point of view, it is an insanity. The idea that measuring one thing implies anything whatsoever about measuring another thing is not the stuff of everyday experience. Nevertheless, we know, experimentally (although not from macroscopic experiments), that there is always a mechanism for the uncertainty principle, and so it must be built in to our mathematical formulation.

16.1 Generalized Uncertainty

We want to relate variances to failed commutativity. Start by defining the operator $\Delta Q \equiv Q - \langle Q \rangle$, "subtracting off the mean" of the operator Q. Then we see that the variance of Q can be written as $\langle (\Delta Q)^2 \rangle$, as shown below

$$\langle (\Delta Q)^2 \rangle = \langle Q^2 \rangle - Q \langle Q \rangle - \langle Q \rangle Q + (\langle Q \rangle)^2 \rangle = \langle Q^2 \rangle - \langle Q \rangle^2. \tag{16.1}$$

Given two Hermitian operators P and Q, we can form the operator $\Delta P \, \Delta Q$, and this object can be partitioned (trivially) into a commutator and anti-

commutator[1]

$$\Delta P\,\Delta Q = \frac{1}{2}\,[\Delta P, \Delta Q] + \frac{1}{2}\,\{\Delta P, \Delta Q\}. \tag{16.2}$$

We are making progress – the left hand side of the above has a product of operators related to the variances, and the commutator on the right is equal to $[P, Q]$ (keep in mind that $\langle Q\rangle$ is just a number, so commutes with anything). Since P and Q are Hermitian, we know that their commutator is anti-Hermitian (meaning that the Hermitian conjugate is the *negative* of the operator):

$$([P, Q])^\dagger = (P\,Q - Q\,P)^\dagger = Q\,P - P\,Q = -[P, Q], \tag{16.3}$$

while the anti-commutator is Hermitian (a sum of Hermitian operators).

Consider the expectation value of $\Delta P\,\Delta Q$ (remember, we want to relate the variances of P and Q to their commutator):

$$\langle \Delta P\,\Delta Q\rangle = \frac{1}{2}\,\langle [P, Q]\rangle + \frac{1}{2}\,\langle \{\Delta P, \Delta Q\}\rangle. \tag{16.4}$$

Now, we know that Hermitian operators, like the anticommutator above, have real expectation value. Similarly, it is easy to show that anti-Hermitian operators (like the commutator above) have imaginary expectation value. Then we have, on the right, a purely real and purely imaginary part, like $u + i\,v$, so the magnitude squared of both sides gives

$$|\langle \Delta P\,\Delta Q\rangle|^2 = \frac{1}{4}\,|\langle [P, Q]\rangle|^2 + \frac{1}{4}\,|\langle \{\Delta P, \Delta Q\}\rangle|^2. \tag{16.5}$$

Recall the Schwarz inequality, for two kets $|a\rangle$ and $|b\rangle$, $\langle a|a\rangle\ \langle b|b\rangle \geq |\,\langle a|b\rangle\,|^2$[2]. If we set $|a\rangle = \Delta P\ |X\rangle$ and $|b\rangle = \Delta Q\ |X\rangle$ for any $|X\rangle$, then

$$\langle \Delta P^2\rangle\langle\,\Delta Q^2\rangle \geq |\langle \Delta P\,\Delta Q\rangle|^2 = \frac{1}{4}\,|\langle [P, Q]\rangle|^2 + \frac{1}{4}\,|\langle \{\Delta P, \Delta Q\}\rangle|^2. \tag{16.7}$$

Of course, since both terms on the right are positive, dropping the anti-commutator only strengthens the inequality, and the term on the left is just $\sigma_P\,\sigma_Q$, so

$$\boxed{\sigma_P^2\,\sigma_Q^2 \geq \frac{1}{4}\,|\langle [P, Q]\rangle|^2.} \tag{16.8}$$

[1] The anticommutator of two operators is $\{P, Q\} = P\,Q + Q\,P$.

[2] This is "just" the infinite dimensional generalization of the familiar projector interpretation of the dot product for real vectors – take $\mathbf{a}$, $\mathbf{b} \in \mathbb{R}^3$, then:

$$\mathbf{a}\cdot\mathbf{b} = |\mathbf{a}|\,|\mathbf{b}|\,\cos\theta \longrightarrow |\mathbf{a}|\,|\mathbf{b}| \geq |\mathbf{a}\cdot\mathbf{b}|, \tag{16.6}$$

since $|\cos\theta| \in [0, 1]$.

This gives us a bound on the variance of the P (or Q) operator, given the variance of the Q (or P) operator and the commutator $[P, Q]$. Again, if $[P, Q] = 0$, the two Hermitian operators commute, and determinate states are shared, meaning that we can measure property P and Q simultaneously.

16.2 Position-Momentum Uncertainty Relation

As an example, consider the position-momentum uncertainty relation implied by the above. We have the commutator of x and p: $[x, p] = i\,\hbar$, so

$$\sigma_x^2\,\sigma_p^2 \geq \frac{1}{4}\,\hbar^2 \longrightarrow \sigma_x\,\sigma_p \geq \frac{\hbar}{2}. \tag{16.9}$$

This is supposed to hold for any state. We have a bunch of examples of states at our disposal – why not check a few of them? For the harmonic oscillator, we calculated the variance of x for the eigenstate (of the Hamiltonian) $|n\rangle$:

$$\sigma_x^2 = \frac{(2\,n+1)\,\hbar}{2\,m\,\omega}. \tag{16.10}$$

We can find the variance of the momentum operator for this state via $p = i\,\sqrt{\frac{\hbar\,m\,\omega}{2}}\,(a_+ - a_-)$ – we clearly have $\langle p\rangle = 0$, but

$$\begin{aligned}
\langle n|\,p^2\,|n\rangle &= -\frac{\hbar\,m\,\omega}{2}\,\langle n|\,(a_+^2 - a_+\,a_- - a_-\,a_+ + a_-^2)\,|n\rangle \\
&= \frac{\hbar\,m\,\omega}{2}\,(\langle n|\,a_+ a_-\,|n\rangle + \langle n|\,a_-\,a_+\,|n\rangle) \\
&= \frac{\hbar\,m\,\omega}{2}\,(n + (n+1)) \\
&= \frac{\hbar\,m\,\omega\,(2\,n+1)}{2}.
\end{aligned} \tag{16.11}$$

Here, we have

$$\sigma_x^2\,\sigma_p^2 = \frac{\hbar^2\,(2\,n+1)^2}{4}, \tag{16.12}$$

and for $n = 0$, the ground state, we actually achieve the lower bound. What type of object is this? The ground state of the harmonic oscillator, appropriately normalized, was

$$\psi_0(x) = \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{1/4}\,e^{-\frac{m\,\omega\,x^2}{2\,\hbar}}, \tag{16.13}$$

a Gaussian distribution with mean zero. That is interesting – we encountered the same type of object when we looked at zero-potential Gaussian wave packets. That's when we first observed that, mathematically, there was some relation between the variance of position and momentum.

16.2.1 Minimum Uncertainty States

In our derivation of the uncertainty relation, we used the Schwarz inequality and dropped an anticommutator to introduce the final inequality. We will return now and try to get the lower bound by constructing relations that will achieve equality. We want to minimize the Schwarz inequality – the $\mathbb{R}^3$ version reads:

$$\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}|\,|\mathbf{b}|\,\cos\theta \tag{16.14}$$

for two vectors $\mathbf{a}$ and $\mathbf{b}$ with $\cos\theta$ the angle between them. Squaring both sides, we get

$$(\mathbf{a} \cdot \mathbf{b})^2 = (\mathbf{a} \cdot \mathbf{a})\,(\mathbf{b} \cdot \mathbf{b})\,\cos^2\theta \leq (\mathbf{a} \cdot \mathbf{a})\,(\mathbf{b} \cdot \mathbf{b}), \tag{16.15}$$

where $\leq$ follows because $\cos^2\theta \in [0,1]$. Equality can be achieved when the two vectors are parallel, that is, when $\mathbf{b} = \alpha\,\mathbf{a}$. The same is true for our complex form , so we are looking for a particular state $|\psi\rangle$ such that $\Delta Q\,|\psi\rangle = \alpha\,\Delta P\,|\psi\rangle$, that will make:

$$\langle \Delta P^2 \rangle\,\langle \Delta Q^2 \rangle = |\langle \Delta P\,\Delta Q \rangle|^2 \tag{16.16}$$

Returning to the exact statement

$$|\langle \Delta P\,\Delta Q \rangle|^2 = \frac{1}{4}\,|\langle [P,Q] \rangle|^2 + \frac{1}{4}\,|\langle \{\Delta P, \Delta Q\} \rangle|^2 \tag{16.17}$$

we let $P = x$, $Q = p$ – we dropped the anticommutator in going from (16.7) to (16.8). We could recover equality if the anticommutator were itself zero, in this setting, if:

$$\langle \{\Delta x, \Delta p\} \rangle = 0. \tag{16.18}$$

Since we are assuming, for the purposes of Schwarz *equality* that $|\psi\rangle$ has $\Delta p\,|\psi\rangle = \alpha\,\Delta x\,|\psi\rangle$, the anticommutator has expectation value

$$\langle \psi|\,(\Delta x\,\Delta p + \Delta p\,\Delta x)\,|\psi\rangle = \alpha\,\langle \psi|\,\Delta x^2\,|\psi\rangle + \langle \psi|\,\Delta p\,\Delta x\,|\psi\rangle\,, \tag{16.19}$$

and using the commutator, $[\Delta x, \Delta p] = [x, p] = i\,\hbar$, we can write $\Delta p\,\Delta x = \Delta x \Delta p - \imath\,\hbar$. Inputting this above, we have

$$\langle\psi|\,(\Delta x\,\Delta p + \Delta p\,\Delta x)\,|\psi\rangle = 2\,\alpha\,\langle\psi|\,\Delta x^2\,|\psi\rangle - i\,\hbar. \tag{16.20}$$

We want this to vanish, which tells us instantly that α is purely complex (to cancel the $\hbar$). Let $\alpha = i\,a$ for $a \in \mathbb{R}$, then the defining equation of interest to us is

$$\Delta p\,|\psi\rangle = i\,a\,\Delta x\,|\psi\rangle\,, \tag{16.21}$$

or, in position space, where we can actually carry out the computation:

$$\left(\frac{\hbar}{i}\frac{d}{dx} - \langle p\rangle\right)\psi(x) = i\,a\,(x - \langle x\rangle)\,\psi(x). \tag{16.22}$$

Keep in mind that $\langle p\rangle$ and $\langle x\rangle$ are just numbers, the target mean and variance of the state $\psi(x,t)$. The solution to the above is

$$\psi(x) = \left(\frac{a}{\hbar\,\pi}\right)^{1/4} e^{-\frac{a\,(x-\langle x\rangle)^2}{2\,\hbar}}\,e^{i\,\frac{\langle p\rangle\,x}{\hbar}}. \tag{16.23}$$

This was our traveling wave packet example, it has nonzero expectation value for both position and momentum.

Keep in mind that all of this talk of Gaussians is more of a statement about the Fourier transform, which takes Gaussians to Gaussians. That's the basic relation between the position space wavefunction and the momentum space one, they are Fourier transforms of each other, and a sharply peaked Gaussian on one side becomes broader on the other side of the transform. The most extreme case is the delta function – for $\delta(x)$, the Fourier transform has $|\tilde{\delta}(k)|^2 = \frac{1}{2\,\pi}$, which is "very broad" (in fact, flat).

16.3 Energy-Time "Uncertainty Relation"

In classical mechanics, the time derivative of a function $J(x,p,t)$ along a dynamical trajectory (meaning one that correctly solves the equations of motion for some potential) can be written as:

$$\frac{dJ}{dt} = [J, H] + \frac{\partial J}{\partial t}. \tag{16.24}$$

This is an immediate consequence of the definition of Poisson bracket:

$$[H, J] = \frac{\partial H}{\partial x^\alpha}\frac{\partial J}{\partial p_\alpha} - \frac{\partial J}{\partial x^\alpha}\frac{\partial H}{\partial p_\alpha} \tag{16.25}$$

and the Hamiltonian equations of motion:

$$\dot{x}^\alpha = \frac{\partial H}{\partial p_\alpha} \qquad \dot{p}_\alpha = -\frac{\partial H}{\partial x^\alpha}. \tag{16.26}$$

So the total time derivative is

$$\begin{aligned} \frac{dJ}{dt} &= \frac{\partial J}{\partial x^\alpha}\,\dot{x}^\alpha + \frac{\partial J}{\partial p_\alpha}\,\dot{p}_\alpha + \frac{\partial J}{\partial t} \\ &= \frac{\partial J}{\partial x^\alpha}\frac{\partial H}{\partial p_\alpha} - \frac{\partial J}{\partial p_\alpha}\frac{\partial H}{\partial x^\alpha} + \frac{\partial J}{\partial t} \\ &= [J, H] + \frac{\partial J}{\partial t}, \end{aligned} \tag{16.27}$$

and this relation is used, when J is not explicitly a function of time ($J(x, p, t) = J(x, p)$ only) to establish that functions whose Poisson bracket with H vanish are conserved, $\frac{dJ}{dt} = 0$ along the trajectory.

A very similar result holds in quantum mechanics, w.r.t. expectation values. Consider an operator $\hat{Q}(x, p, t)$ – then the total time derivative of its expectation value is:

$$\frac{d}{dt}\,\langle\Psi|\,\hat{Q}\,|\Psi\rangle = \left\langle\dot{\Psi}\right|\hat{Q}\,|\Psi\rangle + \langle\Psi|\,\frac{\partial\hat{Q}}{\partial t}\,|\Psi\rangle + \langle\Psi|\,\hat{Q}\left|\dot{\Psi}\right\rangle \tag{16.28}$$

with $\left|\dot{\Psi}\right\rangle \equiv \frac{d}{dt}\,|\Psi\rangle$. We know, from Schrödinger's equation, that

$$i\,\hbar\,\frac{d}{dt}\,|\Psi\rangle = \hat{H}\;|\Psi\rangle \tag{16.29}$$

and, similarly, taking the Hermitian conjugate of both sides (and using $\hat{H}^\dagger = \hat{H}$):

$$-i\,\hbar\,\left\langle\dot{\Psi}\right| = \langle\Psi|\,\hat{H}, \tag{16.30}$$

so inputting this into the total time derivative of $\hat{Q}$ gives:

$$\boxed{\begin{aligned}\frac{d}{dt}\langle\hat{Q}\rangle &= -\frac{1}{i\,\hbar}\,\langle\Psi|\,\hat{H}\,\hat{Q}\,|\Psi\rangle + \langle\Psi|\,\frac{\partial\hat{Q}}{\partial t}\,|\Psi\rangle + \frac{1}{i\,\hbar}\,\langle\Psi|\,\hat{Q}\,\hat{H}\,|\Psi\rangle \\ &= \frac{1}{i\,\hbar}\,\langle[\hat{Q},\hat{H}]\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle.\end{aligned}} \tag{16.31}$$

This result can be used to calculate the time-dependence for a number of interesting quantities – in particular, if we take $\hat{Q} = p$, we recover Ehrenfest's theorem.

As with $J(x,p)$, we see that for $\hat{Q}(x,p,t) = \hat{Q}(x,p)$, if the commutator of $\hat{H}$ and $\hat{Q}$ vanishes (really, its expectation value), then $\langle\hat{Q}\rangle$ is a constant of the motion. The simplest example is $\hat{H}$ itself for time-independent potentials – the energy is a constant in time. Indeed, this was what allowed separation and the development of the time-independent Schrödinger equation in the first place.

Now, consider the relation (16.31), with the commutator in place (and no explicit time-dependence), in light of the generalized uncertainty relation (16.8) with $P = \hat{H}$, $Q = \hat{Q}$:

$$\sigma_H^2\,\sigma_Q^2 \geq \frac{1}{4}\,|\langle[H,Q]\rangle|^2 = \frac{\hbar^2}{4}\left|\frac{d\langle\hat{Q}\rangle}{dt}\right|^2. \tag{16.32}$$

Define the time Δt to be the time it takes the expectation value of the operator $\hat{Q}$ to change by one standard deviation (i.e. σ_Q):

$$\left|\frac{d\langle\hat{Q}\rangle}{dt}\right|\Delta t = \sigma_Q, \tag{16.33}$$

so Δt is a natural timescale induced by the measurement properties of the operator $\hat{Q}(x,p)$. If we, somewhat sloppily, refer to the standard deviation of the Hamiltonian as ΔE (sloppy in the sense that we are referring to the temporal evolution of the expectation value of an operator with Δt, and the necessarily constant expectation value of energy with that same Δ notation), then we can write (16.32) as

$$\Delta E\,\Delta t \geq \frac{\hbar}{2}. \tag{16.34}$$

This is called the "energy-time" uncertainty relation. It relates the spread in momentum *to the time it takes a particular observable to change by one*

standard deviation. We must always be careful to define the observable we have in mind. But, quite broadly, it says that if the energy of a state is sharply peaked (so that ΔE is small), then no observable has expectation value that changes "quickly".

In particular, it refers implicitly to some measure of temporal change in the system, via an (often undisclosed) expectation value of some operator.

Homework

Reading: Griffiths, pp. 106–118.

Problem 16.1

Consider the two matrices:

$$\mathbb{A} \doteq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \mathbb{B} \doteq \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \tag{16.35}$$

These clearly commute: $[\mathbb{A}, \mathbb{B}] = 0$, since $\mathbb{A}$ is the identity matrix. This problem is meant to show you that we cannot take just *any* eigenvectors of $\mathbb{A}$ and expect them to be eigenvectors of $\mathbb{B}$.

a. Show that $\mathbf{v}_1 \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\mathbf{v}_2 \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ are eigenvectors of $\mathbb{A}$, and find the eigenvalues. Are these eigenvectors of $\mathbb{B}$?

b. Find the eigenvectors and eigenvalues of $\mathbb{B}$, show that *these are* eigenvectors of $\mathbb{A}$.

Conclusion: We can *find* simultaneous eigenvectors of $\mathbb{A}$ and $\mathbb{B}$ (since they commute), but we are not guaranteed that any set of eigenvectors are simultaneous eigenvectors.

Problem 16.2

Show that an operator $\hat{Q}$ that is *anti*-Hermitian:

$$\int_{-\infty}^{\infty} \psi^*(x)\, \hat{Q}\, \psi(x)\, dx = -\int_{-\infty}^{\infty} \left(\hat{Q}\, \psi(x)\right)^* \psi(x)\, dx \tag{16.36}$$

has purely imaginary expectation values: $\langle \hat{Q} \rangle$ is imaginary.

Problem 16.3

Our choice of basis is important when finding expectation values, and, even earlier, when we solve Schrödinger's equation (think of the position ver-

sus momentum representation). Suppose we take the abstract form of Schrödinger's equation:

$$\hat{H}\ |\Psi(t)\rangle = i\,\hbar\,\frac{\partial}{\partial t}\ |\Psi(t)\rangle \tag{16.37}$$

and expand $|\Psi(t)\rangle$ in the natural basis defined by $\hat{H}$ (i.e. it's eigenstates).

a. Assume we have a complete, continuous set of eigenstates of $\hat{H}$ indexed by k:

$$\hat{H}\ |\psi_k\rangle = E(k)\ |\psi_k\rangle \tag{16.38}$$

where $E(k)$ is a real number that is a function of k. In addition, we know that $\langle\psi_{k'}|\psi_k\rangle = \delta(k-k')$. The expansion, as a function of time of a general state $|\Psi(t)\rangle$ can be accomplished using the time-dependent decomposition coefficients $\phi(k,t)$ in:

$$|\Psi(t)\rangle = \int_{-\infty}^{\infty} \phi(k,t)\ |\psi_k\rangle\ dk \tag{16.39}$$

(so that the decomposition varies in time, but at each time t, we can represent the ket $|\Psi(t)\rangle$ in terms of the basis $|\psi_k\rangle$). Input this into (16.37), and simplify.

b. Now hit both sides of your result from part a. with $\langle\psi_{k'}|$ and use the orthonormality relation to solve for $\phi(k',t)$.