General Uncertainty Principle

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Uncertainty and Non-Commutation

As we discussed in the Linear Algebra lecture, if two physical variables correspond to *commuting* Hermitian operators, they can be diagonalized simultaneously—that is, they have a common set of eigenstates. In these eigenstates *both* variables have precise values at the same time, there is no "Uncertainty Principle" requiring that as we know one of them more accurately, we increasingly lose track of the other. For example, the energy and momentum of a free particle can both be specified exactly. More interesting examples will appear in the sections on angular momentum and spin.

But if two operators do *not* commute, in general one *cannot* specify both values precisely. Of course, such operators could still have *some* common eigenvectors, but the interesting case arises in attempting to measure A and B simultaneously for a state $|\psi\rangle$ in which the commutator $[A,B]$ has a nonzero expectation value, $\langle\psi|[A,B]|\psi\rangle \neq 0$.

A Quantitative Measure of "Uncertainty"

Our task here is to give a *quantitative* analysis of how accurately noncommuting variables can be measured together. We found earlier using a semi-quantitative argument that for a free particle, $\Delta p \cdot \Delta x \sim \hbar$ at best. To improve on that result, we need to be precise about the uncertainty ΔA in a state $|\psi\rangle$.

We *define* ΔA as the root mean square deviation:

$$(\Delta A)^2 = \langle\psi|\left(A-\langle A\rangle\right)^2|\psi\rangle, \text{ where } \langle A\rangle = \langle\psi|A|\psi\rangle.$$

To make the equations more compact, we define $\hat{a}$ by

$$A = \langle A\rangle + \hat{a}.$$

(We'll put a caret (a hat) on the $\hat{a}$ to remind ourselves it's an operator—and, of course, it's a *Hermitian* operator, like A.) We also drop the ψ bra and ket, on the understanding that this whole argument is for a particular state. Now

$$(\Delta A)^2 = \left\langle\left(A-\langle A\rangle\right)^2\right\rangle = \left\langle\hat{a}^2\right\rangle.$$

Introduce an operator B in exactly similar fashion, $B = \langle B\rangle + \hat{b}$, having the property that $\langle\psi|[A,B]|\psi\rangle \neq 0$.

The Generalized Uncertainty Principle

The quantitative measure of how the combined "uncertainty" of measuring two variables relates to their lack of commutativity is most simply presented as a

Theorem:

$$(\Delta A)^2(\Delta B)^2 \geq \tfrac{1}{4}\langle i[A,B]\rangle^2 .$$

(*Remark*: remember that for A, B Hermitian, $[A,B]$ is *anti*Hermitian: so $\langle i[A,B]\rangle$ is real! To make this clear, take adjoints: if H is hermitian then $(\langle\psi|H|\psi\rangle)^* = \langle\psi|H^\dagger|\psi\rangle = \langle\psi|H|\psi\rangle$, so $\langle\psi|H|\psi\rangle$ is real. If K is *anti* Hermitian, $K^\dagger = -K$, then $(\langle\psi|K|\psi\rangle)^* = \langle\psi|K^\dagger|\psi\rangle = -\langle\psi|K|\psi\rangle$, from which $\langle\psi|K|\psi\rangle$ is *pure imaginary*.)

Proof of the Theorem:

Define

$$|\psi_a\rangle = \hat{a}|\psi\rangle, \quad |\psi_b\rangle = \hat{b}|\psi\rangle .$$

Then

$$(\Delta A)^2(\Delta B)^2 = \langle\psi|\hat{a}^2|\psi\rangle\langle\psi|\hat{b}^2|\psi\rangle = \langle\psi_a|\psi_a\rangle\langle\psi_b|\psi_b\rangle$$

Using Schwartz's inequality

$$\langle\psi_a|\psi_a\rangle\langle\psi_b|\psi_b\rangle \geq |\langle\psi_a|\psi_b\rangle|^2$$

gives immediately

$$(\Delta A)^2(\Delta B)^2 \geq |\langle\psi_a|\psi_b\rangle|^2 = |\langle\psi|\hat{a}\hat{b}|\psi\rangle|^2 .$$

The operator $\hat{a}\hat{b}$ is neither Hermitian nor antiHermitian. To evaluate the mod squared of its expectation value, we break the amplitude into real and imaginary parts:

$$\langle\psi|\hat{a}\hat{b}|\psi\rangle = \langle\psi|\tfrac{1}{2}(\hat{a}\hat{b}+\hat{b}\hat{a})|\psi\rangle + \langle\psi|\tfrac{1}{2}[\hat{a},\hat{b}]|\psi\rangle .$$

(The first term on the right-hand side is the expectation value of a Hermitian matrix, and so is real, the second term is the expectation value of an antiHermitian matrix, so is pure imaginary.)

It follows immediately that

$$\left|\langle\psi|\hat{a}\hat{b}|\psi\rangle\right|^2 \;\geq\; \left|\langle\psi|\tfrac{1}{2}\left[\hat{a},\hat{b}\right]|\psi\rangle\right|^2.$$

But $[A,B]=[\hat{a},\hat{b}]$, so

$$(\Delta A)^2(\Delta B)^2 \;\geq\; \tfrac{1}{4}\langle i[A,B]\rangle^2.$$

Minimizing the Uncertainty

For a particle in one dimension denote

$$A=x,\quad B=p=-i\hbar\frac{d}{dx},\ \text{so}\ [A,B]=-i\hbar\left(x\frac{d}{dx}-\frac{d}{dx}x\right)=i\hbar.$$

(It important in that last step to understand that the operator $\frac{d}{dx}$ operates on everything to its right, and, as we are always finding matrix elements of operators, there will be a following ket it operates on, so $\frac{d}{dx}x=1+x\frac{d}{dx}$.)

We conclude that

$$(\Delta x)^2(\Delta p)^2 \;\geq\; \tfrac{1}{4}\hbar^2.$$

Question: *Is there a wavefunction for which this inequality becomes an equality?*

That would require $\left|\langle\psi_a|\psi_b\rangle\right|^2=\langle\psi_a|\psi_a\rangle\langle\psi_b|\psi_b\rangle$, which can only be true if the two vectors are parallel, $|\psi_b\rangle=\lambda|\psi_a\rangle$, or, written explicitly,

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

Actually , that's not enough: we *also* need $\langle\psi|\tfrac{1}{2}\left(\hat{a}\hat{b}+\hat{b}\hat{a}\right)|\psi\rangle$ to be zero. (Look at the equation above giving $\langle\psi|\hat{a}\hat{b}|\psi\rangle$ in terms of its real and imaginary parts, and how we used it to establish the inequality.)

Writing $|\psi_b\rangle=\lambda|\psi_a\rangle$ as $\hat{b}|\psi\rangle=\lambda\hat{a}|\psi\rangle$ and $\langle\psi|\hat{b}=\lambda^*\langle\psi|\hat{a}$ we find

$$\langle\psi|\tfrac{1}{2}\left(\hat{a}\hat{b}+\hat{b}\hat{a}\right)|\psi\rangle=\left(\lambda+\lambda^*\right)\langle\psi|\hat{a}^2|\psi\rangle,$$

so this will be zero *if and only if* λ *is pure imaginary*.

Turning to the differential equation, we first take the simplest case where $\langle x\rangle$ and $\langle p\rangle$ are both zero. The first requirement just sets the origin, but the second stipulates that our wave function has no net momentum.

For this simple case, $|\psi_b\rangle = \lambda|\psi_a\rangle$ becomes

$$-i\hbar\frac{d\psi(x)}{dx} = \lambda x\psi(x)$$
$$\frac{d\psi}{\psi} = \frac{i\lambda}{\hbar}xdx$$
$$\psi = Ce^{i\lambda x^2/2\hbar}$$

and recalling that λ is pure imaginary, this is a Gaussian wave packet! It is straightforward to check that the solution with $\langle x\rangle$ and $\langle p\rangle$ nonzero is

$$\psi(x) = Ce^{i<p>x/\hbar}e^{-\alpha(x-<x>)^2/2\hbar}$$

where $\alpha = -i\lambda$ is real, and C is the usual Gaussian normalization constant.

Exercise: check this.

The conclusion is then that the Gaussian wave packet gives the optimum case for minimizing the joint uncertainties in position and momentum.

Note that the condition $\hat{b}|\psi\rangle = \lambda\hat{a}|\psi\rangle$ does *not* mean that $|\psi\rangle$ is an eigenstate of either $\hat{a}$ or $\hat{b}$, but it *is* an eigenstate of the *nonHermitian* operator $\hat{b}-\lambda\hat{a} = \hat{b}+i\alpha\hat{a}$, with eigenvalue zero. We shall soon see that this nonHermitian operator and its adjoint play important roles in the quantum mechanics of the simple harmonic oscillator.