The Cauchy-Schwarz inequality

Consider the usual n-dimensional vector space. In this space we have two vectors v and u. The Cauchy-Schwarz inequality states that

$$|\langle v|u\rangle|^2 \leq \langle v|v\rangle \langle u|u\rangle$$

where $\langle \, | \, \rangle$ stands for an inner (scalar) product. Moreover the two sides of the above equation are equal only when $v = \lambda u$ (i.e. v and u are linearly dependent)

For finite n we can easily show that the above inequality holds true. If we introduce

$$w = u - \frac{\langle u|v\rangle}{\langle v|v\rangle} v$$

then by linearity of the inner product

$$\langle w|v\rangle = \left\langle u - \frac{\langle u|v\rangle}{\langle v|v\rangle} v \,\middle|\, v \right\rangle = \langle u|v\rangle - \frac{\langle u|v\rangle}{\langle v|v\rangle}\langle v|v\rangle = 0$$

vector w is orthogonal to v. Then the norm of

$$u = \frac{\langle u|v\rangle}{\langle v|v\rangle} v + w$$

can be computed easily given this orthogonality of w and v:

$$\|u\|^2 = \left|\frac{\langle u|v\rangle}{\langle v|v\rangle}\right|^2 \|v\|^2 + \|w\|^2 = \frac{|\langle u|v\rangle|^2}{\|v\|^2} + \|w\|^2 \geq \frac{|\langle u|v\rangle|^2}{\|v\|^2}$$

Multiplying by $\|v\|^2$ on both sides yields the Cauchy-Schwarz inequality

It turns out the Cauchy-Schwarz inequality also takes place when we deal with a Hilbert space.

If the inner product of two functions is defined as

$$\langle f|g\rangle = \int_a^b f(x)^* g(x)\, dx$$

and if both $f(x)$ and $g(x)$ are square-integrable, then

$$\left| \int_a^b f(x)^* g(x) dx \right| \leq \sqrt{\int_a^b |f(x)|^2 dx} \sqrt{\int_a^b |g(x)|^2 dx}$$

The uncertainty principle

Back several lectures ago we considered the Heisenberg uncertainty principle for the momentum and position. Let us now prove this very important principle in a more general form.

Suppose we have two observables with corresponding operators $\hat{A}$ and $\hat{B}$.

Recall that

$$(\Delta A)^2 = \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle = \langle \Psi | (\hat{A} - \langle \hat{A} \rangle)^2 \Psi \rangle \overset{\hat{A} \text{ is hermitian}}{=\!=\!=}$$

$$= \langle (\hat{A} - \langle A \rangle) \Psi | (\hat{A} - \langle A \rangle) \Psi \rangle$$

or, if we denote $f \equiv (A - \langle A \rangle) \Psi$,

$$(\Delta A)^2 = \langle f | f \rangle$$

In a similar way

$$(\Delta B)^2 = \langle g | g \rangle \quad \text{where} \quad g \equiv (\hat{B} - \langle B \rangle) \Psi$$

Then

$$(\Delta A)^2 (\Delta B)^2 = \langle f | f \rangle \langle g | g \rangle \underset{\text{Cauchy-Schwarz}}{\geq} |\langle f | g \rangle|^2$$

For any complex number z the following is true

$$|z|^2 = (\operatorname{Re} z)^2 + (\operatorname{Im} z)^2 \geq (\operatorname{Im} z)^2 = \left[\frac{1}{2i} (z - z^*) \right]^2$$

Now, if we take $z = \langle f|g\rangle$ we obtain

$$(\Delta A)^2(\Delta B)^2 \geq \left[\frac{1}{2i}\left(\langle f|g\rangle - \langle g|f\rangle\right)\right]^2 \qquad (*)$$

On the other hand,

$$\langle f|g\rangle = \left\langle (\hat{A} - \langle\hat{A}\rangle)\Psi \,\middle|\, (\hat{B} - \langle\hat{B}\rangle)\Psi \right\rangle = \langle\Psi|(\hat{A} - \langle A\rangle)(B - \langle B\rangle)|\Psi\rangle =$$

$$= \langle\Psi|(\hat{A}\hat{B} - \hat{A}\langle\hat{B}\rangle - \hat{B}\langle\hat{A}\rangle + \langle A\rangle\langle B\rangle)\Psi\rangle =$$

$$= \langle\Psi|\hat{A}\hat{B}\Psi\rangle - \langle\hat{B}\rangle\langle\Psi|\hat{A}\Psi\rangle - \langle A\rangle\langle\Psi|\hat{B}\Psi\rangle + \langle A\rangle\langle B\rangle\langle\Psi|\Psi\rangle =$$

$$= \langle\hat{A}\hat{B}\rangle - \langle\hat{B}\rangle\langle\hat{A}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle + \langle\hat{A}\rangle\langle\hat{B}\rangle$$

$$= \langle\hat{A}\hat{B}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle$$

Similarly

$$\langle g|f\rangle = \langle\hat{B}\hat{A}\rangle - \langle\hat{B}\rangle\langle\hat{A}\rangle$$

Put together these give:

$$\langle f|g\rangle - \langle g|f\rangle = \langle\hat{A}\hat{B}\rangle - \langle\hat{B}\hat{A}\rangle = \langle[\hat{A},\hat{B}]\rangle$$

Going back to equation (*) we now have:

$$(\Delta A)^2(\Delta B)^2 \geq \left[\frac{1}{2i}\langle[A,B]\rangle\right]^2$$

or

$$\Delta A\,\Delta B \geq \frac{1}{2}\left|\langle[\hat{A},\hat{B}]\rangle\right|$$

This is the Robertson relation for the uncertainty principle.

If we recall the familiar fundamental commutation relation, $[\hat{x},\hat{p}] = i\hbar$, then the last formula will give us the traditional form of the uncertainty principle!

$$\Delta x\,\Delta p \geq \frac{1}{2}|i\hbar| = \frac{\hbar}{2}$$

The general form of the uncertainty principle can be used with other observables, not just x and p. For example, it turns out that different components of angular momenta in quantum mechanics do not commute. Hence they cannot be measured simultaneously.

In general a pair of observables is called incompatible if their operators do not commute.

One important fact about the compatible observables is that they have a shared set of eigenfunctions, while incompatible observables cannot have a complete set of common eigenfunctions.

The energ-time uncertainty principle

It turns out there is an uncertainty relation for the energy and time:

$$\Delta t \, \Delta E \geq \frac{\hbar}{2} \qquad (**)$$

which in its appearace is very similat to the well known

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

It should be noted that in nonrelativistic quantum mechanics time, unlike x, is an independent variable. However, the existence of (**) is not completely counter intuitive. We can recall that

$$\hat{p} \Psi = -i\hbar \frac{\partial}{\partial x} \Psi$$

the Schrödinger equation reads

$$H\Psi = i\hbar \frac{\partial}{\partial t} \Psi$$

from where the analogy becomes more visible.

Let us now consider the rate of change of the expectation value of some operator Q

$$\frac{d}{dt}\langle \hat{Q}\rangle = \frac{d}{dt}\langle \Psi|\hat{Q}\Psi\rangle = \langle \frac{\partial \Psi}{\partial t}|\hat{Q}\Psi\rangle + \langle \Psi|\frac{\partial \hat{Q}}{\partial t}\Psi\rangle + \langle \Psi|\hat{Q}\frac{\partial \Psi}{\partial t}\rangle$$

From the Schrödinger equation we have

$$i\hbar\frac{\partial \Psi}{\partial t} = \hat{H}\Psi$$

If we replace $\frac{\partial \Psi}{\partial t}$ with $\frac{1}{i\hbar}\hat{H}\Psi$ in the expression for $\frac{d}{dt}\langle Q\rangle$ we obtain

$$\frac{d}{dt}\langle Q\rangle = -\frac{1}{i\hbar}\langle \hat{H}\Psi|\hat{Q}\Psi\rangle + \langle \frac{\partial \hat{Q}}{\partial t}\rangle + \frac{1}{i\hbar}\langle \Psi|\hat{Q}\hat{H}\Psi\rangle$$

Now since $\hat{H} = \hat{H}^+$ we can rearrange it as follows

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle \Psi|\hat{H}\hat{Q}\Psi\rangle - \frac{i}{\hbar}\langle \Psi|\hat{Q}\hat{H}\Psi\rangle + \langle \frac{\partial Q}{\partial t}\rangle$$

or

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [\hat{H},\hat{Q}]\rangle + \langle \frac{\partial \hat{Q}}{\partial t}\rangle$$

This important relation is known as the generalized Ehrenfest theorem. It tells us, in particular, that if an operator does not depend on time explicitly and it commutes with the Hamiltonian then its expectation value is constant in time. In other words, if $\frac{\partial \hat{Q}}{\partial t} = 0$ and $[\hat{H}, Q] = 0$ then Q is an integral of motion.

Now if we take the generalized uncertainty principle (which was derived in the previous section) and replace $\hat{A}$ with $\hat{H}$ and $\hat{B}$ with $\hat{Q}$, while assuming $\frac{\partial Q}{\partial t} = 0$ we will obtain

$$\Delta H \Delta Q \geq \frac{1}{2} \left| \langle [\hat{H}, \hat{Q}] \rangle \right| = \frac{1}{2} \left| \frac{\hbar}{i} \frac{d\langle Q \rangle}{dt} \right| = \frac{\hbar}{2} \left| \frac{d\langle Q \rangle}{dt} \right|$$

If we define

$$\Delta t \equiv \frac{\Delta Q}{\left| \frac{d\langle Q \rangle}{dt} \right|} \quad \text{or} \quad \Delta Q = \left| \frac{d\langle Q \rangle}{dt} \right| \Delta t$$

then we get the energy-time uncertainty principle in the sought form:

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

Δt here represents here the amount of time it takes the expectation value of Q to change by one standard deviation.

Example 1. If an unstable particle lasts about time Δt before desintegrating then the uncertainty in its energy will be $\Delta E \geq \frac{\hbar}{2\Delta t}$. As we know from special relativity the rest mass is related to the total energy, $E = mc^2$. Thus, if a particle is unstable it is impossible to measure its mass precisely.

Example 2 Spectral lines corresponding to transitions between atomic (or molecular) energy levels are never infinitely sharp. This is because the energy levels above the ground state have a finite lifetime Δt. Hence the transition frequencies have "natural" width of the order

$$\Delta \nu = \frac{\Delta E}{h} \geq \frac{1}{4\pi \Delta t} \approx \frac{1}{\Delta t}$$