Commuting and Non-commuting Operators
Chapter 17

Postulate 3. In any measurement of the observable associated with an operator $\hat{A}$ the only values that will ever be observed are the eigen values, a, which satisfy the eigen value equation;

$$\hat{A}\Psi = a\Psi \qquad \text{e. g. } \hat{H}\Psi_n = E_n\Psi_n.$$

If the system is an eigenstate of $\hat{A}$ with eigenvalue a, then any measurement of the observable quantity A of that state will yield a value a, only.

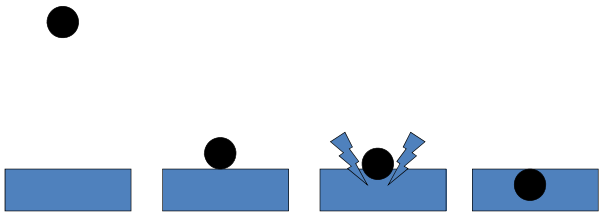
In quantum mechanics two observables A and B of a quantum system can be predicted (found) *exactly* only if the *outcomes of the measurements of the two observables are independent of the order* in which they are determined.

Further, in quantum systems there exists a limitation on the uncertainty associated with *some* simultaneous measurements that can be made, regardless of the methodology employed.

Classical mechanics allows prediction of the information with no limits on the amount of information obtainable.

Classical mechanics

Uncertainty in measurements is only limited by capabilities of technique, measuring instrument precision and the investigator skill.



Quantum mechanics.

Two observables can be known simultaneously with high accuracy (in some cases).

But in other cases the two observables measured would have an innate uncertainty.

This uncertainty cannot be removed by the improvement of the technique of measurement.

If operators $\hat{A}$ and $\hat{B}$ are associated with observed values (measurements) of α and β, they can be measured simultaneously by experiment only *if* the measurement process does not change the system.

If the first measurement changes the *system*, the second measurement will not be performed on the 'same' *system* dealt at the first measurement.

The position (x) of an electron in an atom, if measured by using a probe, such as a light ray will change the velocity of the electron by electron interacting with the light ray. So if the velocity (v), of the electron is measured *after* measuring the position, it is the velocity of a different system!!

Quantum systems are described by a wave function, say $\psi_n(x)$; assume they are eigenfunctions of operators $\hat{A}$ and $\hat{B}$.

The outcome of the measurement of property A followed by measurement of property B would then be as follows; in stages;

$$\hat{B}[\hat{A}\psi_n(x)] \qquad \#$$

i.e. $$\hat{B}[\hat{A}\psi_n(x)] = \hat{B}[\alpha_n\psi_n(x)] = \alpha_n\hat{B}\psi_n(x)$$

$$\hat{B}[\hat{A}\psi_n(x)] = \alpha_n\hat{B}\psi_n(x) = \alpha_n\beta_n\psi_n(x)$$

The second measurement (property *B*) would not change the wave function (i.e. the state of the system) *only if* ψ *is an eigen function* of $\hat{B}$.

Now, $$\hat{B}[\hat{A}\psi_n(x)] = \alpha_n\beta_n\psi_n(x)$$

Reversing the order of operations on ψ yields;

$$\hat{A}[\hat{B}\psi_n(x)] = \hat{A}[\beta_n\psi_n(x)] = \beta_n\hat{A}\psi_n(x) = \beta_n\alpha_n\psi_n(x)$$

i.e. $$\underbrace{\beta_n\alpha_n}\psi_n(x) = \underbrace{\alpha_n\beta_n}\psi_n(x)$$

Making $$\hat{A}[\hat{B}\psi_n(x)] = \hat{B}[\hat{A}\psi_n(x)]$$

$$\hat{A}[\hat{B}\psi_n(x)] = \hat{B}[\hat{A}\psi_n(x)]$$

The above, is made possible because the operators did not change the wavefunction., i.e. the state of the system.

$$\hat{A}\psi_n(x) = a_n\psi_n(x) \qquad \hat{B}\psi_n(x) = b_n\psi_n(x)$$

The second measurement will <u>*change*</u> the wave function (state) *if the wave function is NOT an eigen function* of BOTH operators.

The requirement for being able to be simultaneously measure two observables is that the two operators must be eigen operators of the same wave function.

$$\hat{A}[\hat{B}\psi_n(x)] = \hat{B}[\hat{A}\psi_n(x)]$$

*Test is: $\hat{A}[\hat{B}\,f(x)] - \hat{B}\,[\hat{A}\,f(x)] = 0$

$$\hat{A}[\hat{B}f(x)] - \hat{B}[\hat{A}f(x)] = \hat{A}\hat{B}f(x) - \hat{B}\hat{A}f(x) = [\hat{A}\hat{B} - \hat{B}\hat{A}]f(x) = [\hat{A},\hat{B}]f(x)$$

Commutator of $\hat{A}$ and $\hat{B}$.

If $[\hat{A}\hat{B} - \hat{B}\hat{A}]f(x) = [\hat{A},\hat{B}]f(x) = 0$

$\hat{A}$ and $\hat{B}$ commutes.

$$\hat{A}[\hat{B}f(x)] - \hat{B}[\hat{A}f(x)] = \hat{A}\hat{B}f(x) - \hat{B}\hat{A}f(x)$$

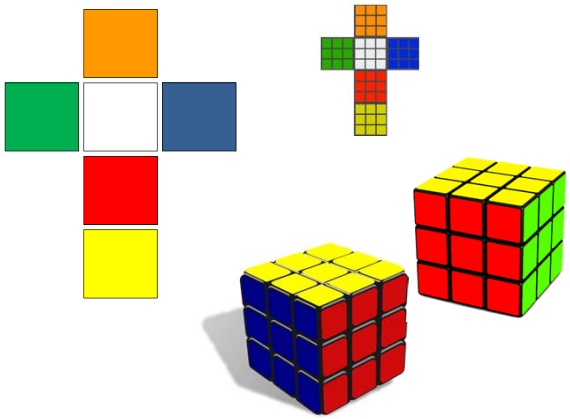
Note; another form

If $\hat{A}[\hat{B}f(x)] - \hat{B}[\hat{A}f(x)] = [\hat{A},\hat{B}]f(x) \neq 0$

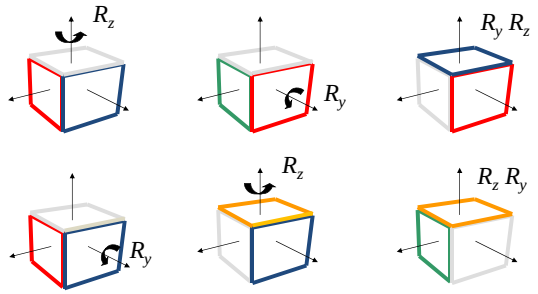
the value of the commutator is *not equal to zero,* values for properties A and B *cannot be measured <u>simultaneously</u>* and exactly (with high accuracy), $\hat{A}$ and $\hat{B}$ are non-commuting operators.

$$[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$$

Study Example Problem 17.1



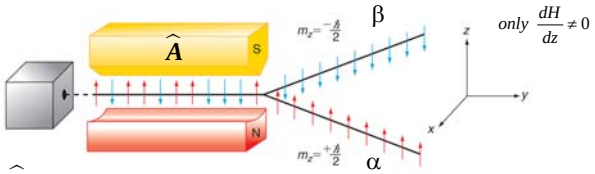
Non-commuting operators - example



$R_y R_z \neq R_z R_y$

$R_y R_z - R_z R_y \neq 0$ $\qquad [R_y, R_z] \neq 0$

Stern-Gerlach Experiment:



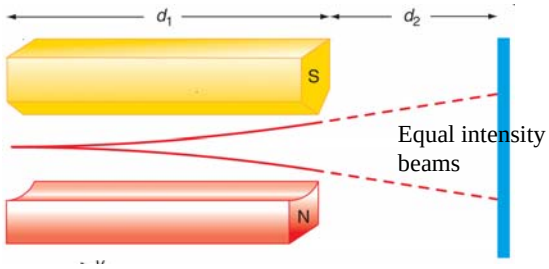
$\hat{A}$ = measuring the z components.

Ag atom has a single unpaired electron – mag. moment **μ**.

Atoms orient only in two directions w.r.t. field.

Measuring **μ** in z direction has only spots, 2 eigen functions, i.e two states.

The two states were described by 2 eigen functions, α and β.



$\hat{A}$ = measuring the z components.

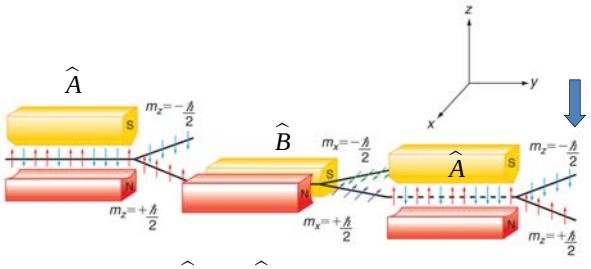
The number of spin states for silver atom are *only* 2, and the complete set has only 2 wave functions α and β.

The initial acceptable wavefunction describing silver atom can be written as;

$$\psi = c_1\alpha + c_2\beta \quad \text{with } |c_1|^2 + |c_2|^2 = 1$$

Equal intensity of beams; $\dfrac{|c_1|^2}{|c_2|^2} = 1$

$$|c_1|^2 = |c_2|^2 = 1/2$$

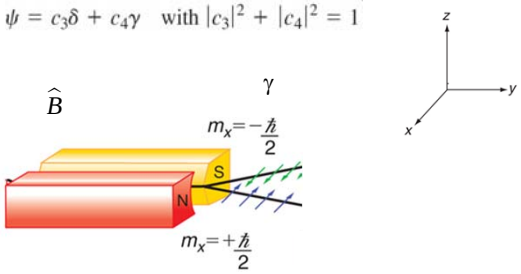


$\hat{A}$ and $\hat{B}$ do not commute.

i.e. operators for components of magnetic moments do not commute.

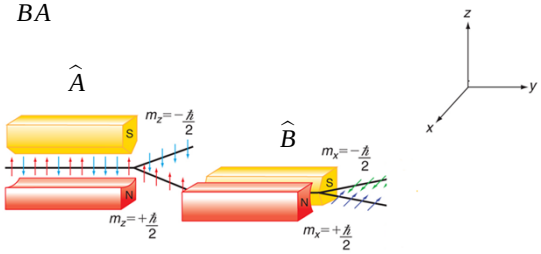
$\hat{B}$ = measuring the x components.

$\psi = c_3\delta + c_4\gamma$ with $|c_3|^2 + |c_4|^2 = 1$

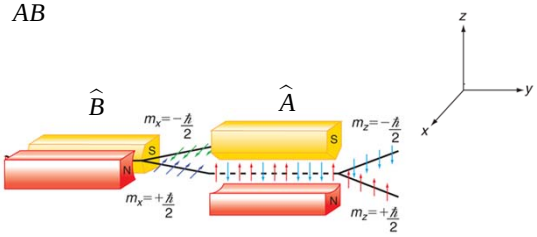


δ

$\hat{B}\hat{A}$

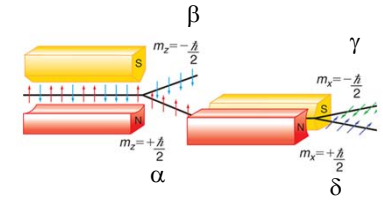


$\hat{A}\hat{B}$

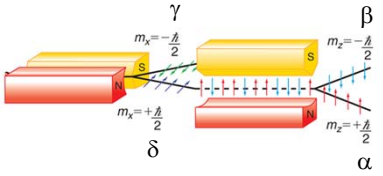


$\hat{A}$ and $\hat{B}$ do not commute.

i.e. operators for components of magnetic moments do not commute.



$$c_2\beta + c_3\delta + c_4\gamma$$



$$c_2\gamma + c_3\alpha + c_4\beta$$

Heisenberg Uncertainty Principle.

A common statement of the uncertainty principle is that the position and momentum of a quantum mechanical particle cannot be known exactly and simultaneously.

It is because; $[\hat{x}, \hat{p}] \neq 0$

A free particle described by $\Psi(x,t) = Ae^{i(kx-\omega t-\phi)}$

Simplified by setting $t = 0$ and $\phi = 0$ $\Psi(x) = Ae^{i(kx)}$

TABLE 14.1 Observables and Their Quantum Mechanical Operators

Observable	Operator	Symbol for Operator
Momentum	$-i\hbar\frac{\partial}{\partial x}$	$\hat{p}_x$
Kinetic energy	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$	$\hat{E}_{kinetic} = \frac{1}{2m}(\hat{p}_x)(\hat{p}_x)$
Position	x	$\hat{x}$
Potential energy	$V(x)$	$\hat{E}_{potential}$
Total energy	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$	$\hat{H}$
Angular momentum	$-i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$	$\hat{l}_x$
	$-i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$	$\hat{l}_y$
	$-i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$	$\hat{l}_z$

For simplicity the property in one direction considered.

Evaluation of commutator $[\hat{x},\hat{p}]$

$$\hat{A}[\hat{B}\psi(x)] - \hat{B}[\hat{A}\psi(x)] = \hat{x}[\hat{p}\psi(x)] - \hat{p}[\hat{x}\psi(x)]$$

$$\hat{p}\psi(x) = i\hbar\frac{d}{dx}Ae^{i(kx)} = \hbar kAe^{i(kx)}$$

$$\hat{x}\psi(x) = xAe^{i(kx)}$$

$$\hat{x}[\hat{p}\psi(x)] - \hat{p}[\hat{x}\psi(x)] =$$

$$\hat{x}[\hbar kAe^{i(kx)}] - \hat{p}[xAe^{i(kx)}] = \hbar kxAe^{i(kx)} - i\hbar\frac{d}{dx}xAe^{i(kx)}$$

$$= \hbar kxAe^{i(kx)} - i\hbar Ae^{i(kx)} - x\hbar kAe^{i(kx)}$$

Heisenberg Uncertainty Principle.

The values determined are not discrete, hence there are built in uncertainties, Δx and Δp, for example.

Uncertainty Principle; $\Delta p \Delta x \geq \frac{\hbar}{2}$

Alternate definition $\sigma_x \sigma_p \geq \frac{\hbar}{2}$ σ = variance

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 \quad \text{and} \quad \sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$$

variance = mean of squares – square of means

variance

(See Example Problem 17.5 for proof)

Illustration of Uncertainty Principle for 1D Box.

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

Normalized wave functions; $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 \quad \text{and} \quad \sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$$

$$\langle p^2 \rangle = \int \psi^*(x) \hat{p}^2 \psi(x) dx \quad \text{and}$$

$$\langle p \rangle^2 = \left(\int \psi^*(x) \hat{p} \psi(x) dx \right)^2$$

$$\sigma_p = \sqrt{\frac{n^2 \pi^2 \hbar^2}{a^2}} = \frac{n\pi\hbar}{a}$$

$$\langle x^2 \rangle = \int \psi^*(x) \hat{x}^2 \psi(x) dx \quad \text{and}$$

$$\langle x \rangle^2 = \left(\int \psi^*(x) \hat{x} \psi(x) dx \right)^2$$

$$\sigma_x = a \sqrt{\left(\frac{1}{12} - \frac{1}{2\pi^2 n^2} \right)}$$

$$\sigma_p \sigma_x = \frac{n\pi\hbar}{a} \sqrt{a^2 \left(\frac{1}{12} - \frac{1}{2\pi^2 n^2} \right)} = \hbar \sqrt{\left(\frac{\pi^2 n^2}{12} - \frac{1}{2} \right)}$$

$$= 0.57\hbar > \frac{\hbar}{2} \quad \text{for } n = 1$$

Note: If a system (a state described by a wavefunction) is an *eigenstate* of the total energy operator (Hamiltonian, $\hat{H}$) and if a property P, of which the operator $\hat{P}$, *does not* commute with $\hat{H}$, then *P* cannot be known accurately for that system.

If an operator $\hat{A}$ does not commute with another operator, $\hat{B}$, then eigenfunctions of $\hat{A}$ are *not eigenfunctions* of $\hat{B}$ and vice versa.

If an operator $\hat{A}$ commutes with another operator, $\hat{B}$, then eigenfunctions of $\hat{A}$ are *eigenfunctions* of $\hat{B}$ and vice versa.

The operators $\hat{A}$ and $\hat{B}$ may differ by a multiplicative factor.