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Lecture - 29

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- So, we recollect today some of the topics that we have examined in the previous class
 - In the previous class we have discussed superposition principle. We were considering a case of, a situation in which the problem we are considering is conservative and the total energy is not known.
 - So we use the most general form of the wavefunction superposition of monochromatic components and we have given a name to this superposition which is **Wavepacket**.
This is the same name which is analogous in EM Theory i.e. the superposition of EM waves.
- Note: The **Wavefunction** is not Electromagnetic, it is a **Probability density**.
- From the practical standpoint the wave packet is useful because by suitably

combining the coefficients of superposition, we can construct a wavepacket i.e energetically

Non zero in a limited region of space and goes to zero outside the region. In this sense

→ We may assume that the particle stays in a region of SPACE where localization probability is zero. It does not stay in the remaining part of the SPACE.

→ Obviously the wavepacket moves in Space so the position of the centre of the wave packet changes with time.

Note: This description is very useful because it allows us to reconstruct the Dynamics of the wavepacket that is similar in some sense to the dynamics of a classical particle.

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Wave Packet — I

- The general solution of the time-dependent Schrödinger equation, depending whether the spectrum is discrete or continuous, has the form

$$\psi(\mathbf{r}, t) = \sum_n c_n w_n(\mathbf{r}) \exp(-jE_n t/\hbar), \text{ discrete}$$

$$\psi(\mathbf{r}, t) = \int_k c_k w_k(\mathbf{r}) \exp(-jE_k t/\hbar) d^3k, \text{ continuous}$$

- For a free particle the continuous case holds, with

$$w_k(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \exp(j\mathbf{k} \bullet \mathbf{r}), \quad \xrightarrow{3D}$$

$$E_k = \frac{\hbar^2}{2m} (k_1^2 + k_2^2 + k_3^2), \quad \xrightarrow{3D}$$

and $-\infty < k_i < +\infty$. The order of degeneracy of E_k is thus ∞^3 . Letting $\omega \doteq E_k/\hbar = \hbar k^2/(2m)$ and taking any \mathbf{k}_0 , the following holds: $k_i^2 = (k_{0i} - k_{0i} + k_i)^2 = k_{0i}^2 + 2k_{0i}(k_i - k_{0i}) + (k_i - k_{0i})^2$, whence

$$\omega = \frac{\hbar}{2m} k_0^2 + \frac{\hbar}{m} \mathbf{k}_0 \bullet (\mathbf{k} - \mathbf{k}_0) + \frac{\hbar}{2m} |\mathbf{k} - \mathbf{k}_0|^2.$$

- Taking $t = 0$ one sees that

$$c_k = \langle w_k | \psi \rangle_{t=0} = (2\pi)^{-3/2} \int_r \exp(-j\mathbf{k} \bullet \mathbf{r}) \psi(\mathbf{r}, 0) d^3r,$$

namely, c_k is the Fourier transform of $\psi(\mathbf{r}, 0)$.

↓ Scalar product of Eigenfunction (w_i) & wave function (ψ)

Note: till so far we have not introduced any approximations.

∴ The values of ' \mathbf{k} ' near ' \mathbf{k}_0 ' are important

∴ $\mathbf{k} - \mathbf{k}_0$ is very small

∴ $|\mathbf{k} - \mathbf{k}_0|^2$ can be ignored

$w_n(\mathbf{r})$: Eigen function

E_n : Eigen value

c_n : coefficient

They can be calculated provided the initial condition

if we assume there is a peak wrt \mathbf{k}_0

Wave Packet — II

- As the expansion of ψ is made in terms of the eigenfunctions of momentum, $w_k = \exp(j\mathbf{k} \bullet \mathbf{r})$, the probability of finding \mathbf{k} within d^3k , assuming that ψ is normalized, is $|c_k|^2 d^3k$.
- Let the width of c_k be small, and let \mathbf{k}_0 correspond to the center of c_k . For all the significant \mathbf{k} s one can then neglect the quadratic term of ω :

$$\omega \simeq \omega_0 + \mathbf{u}_g \bullet (\mathbf{k} - \mathbf{k}_0), \quad \omega_0 \doteq \frac{\hbar}{2m} k_0^2, \quad \mathbf{u}_g \doteq \frac{\hbar}{m} \mathbf{k}_0,$$

Group Velocity

where \mathbf{u}_g is the group velocity. The approximation holds as long as $\hbar|\mathbf{k} - \mathbf{k}_0|^2 t / (2m) \ll 2\pi$. Letting $\Phi_0 \doteq \mathbf{k}_0 \bullet \mathbf{r} - \omega_0 t$, the expression of ψ then becomes

$$\psi(\mathbf{r}, t) \simeq \exp(j\Phi_0) \int_k \frac{c_k}{(2\pi)^{3/2}} \exp[j(\mathbf{r} - \mathbf{u}_g t) \bullet (\mathbf{k} - \mathbf{k}_0)] d^3k.$$

- Defining the envelope function

$$A(\mathbf{r} - \mathbf{u}_g t; \mathbf{k}_0) \doteq \int_k \frac{c_k}{(2\pi)^{3/2}} \exp[j(\mathbf{r} - \mathbf{u}_g t) \bullet (\mathbf{k} - \mathbf{k}_0)] d^3k,$$

it follows $\psi = \exp(j\Phi_0) A(\mathbf{r} - \mathbf{u}_g t; \mathbf{k}_0)$, whence $|\psi|^2 = |A|^2$.

localization
of the particle
is given only by
square modulus

Q) How is the motion of Envelope function in space?

Ans

'A' depends on $\mathbf{r} - \underline{\mathbf{u}_g t}$

\therefore Envelope function moves rigidly with \mathbf{u}_g

→ ' u_g ' allows us to ascribe a velocity to the wavepacket as if it were a particle

we can ascribe a Momentum by considering

Momentum associated to

k_0

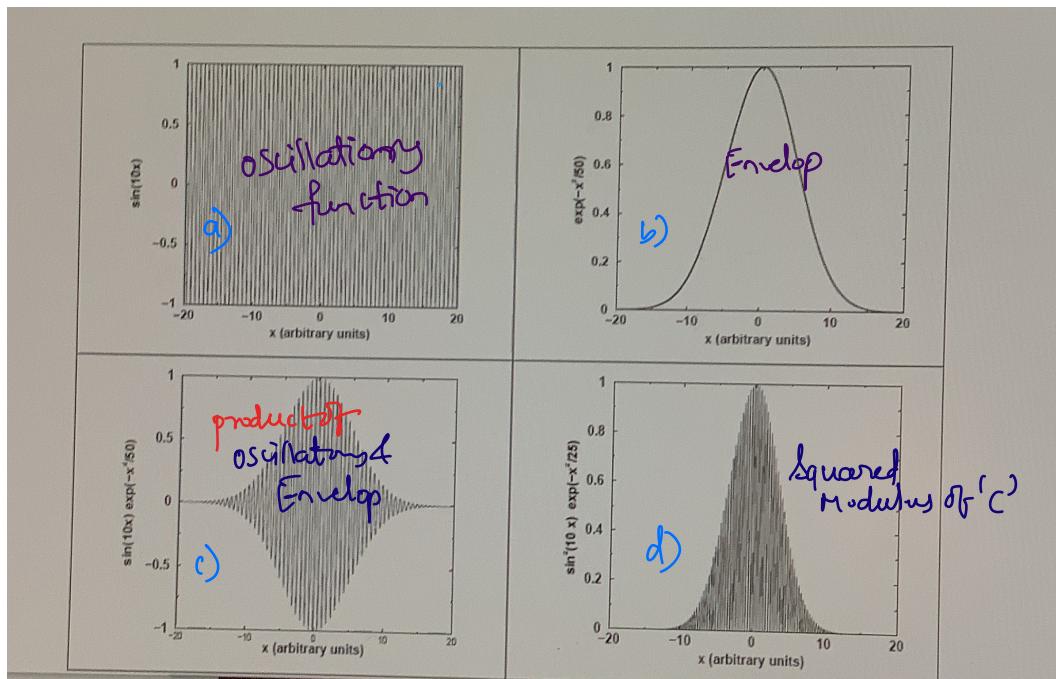
The central point
of the wave packet
in k -space

we can also ascribe a Position because WP

is also limited in the Physical space because

Norm of FT is equal to the Normalization Function

we also use the same concept in the propagation
of wavefunction in a crystal because of its
periodicity we can approximate the description.



In general when we want to describe a particle with a WP we use a Gaussian wavepacket because of its properties.

(i) Minimum uncertainty WP

→ So far we have considered only one possible eqⁿ in QM \rightarrow it is built up with Hamiltonian operator (it is the Quantum counterpart of Hamiltonian function in CM)

Hamiltonian function } is correlated with Energy of the particle

~~Sol~~ Solⁿ of Schrodinger eqⁿ provides with the Eigen values & Eigen functions associated with Energy

Q) In CM we have many other Dynamic quantities Position, Momentum, Angular Momentum etc. What should we do if we want to investigate other Dynamic properties?

Any

We extend the concept we considered for
SE and we do it by stating a number
of postulates if they are consistent with the
reality!

General Methods of Quantum Mechanics — I

The conclusions reached so far are:

- ▷ The only energy values allowed for a particle subject to a conservative force are the eigenvalues of the time-independent equation $\mathcal{H}\psi = E\psi$, where \mathcal{H} is derived from the classical Hamiltonian by replacing p_i with $-j\hbar\partial/\partial x_i$. *Momentum operator*
- ▷ The wave function of a conservative case (taking discrete eigenvalues) is $\psi = \sum_n c_n w_n \exp(-jE_n t/\hbar)$. The particle's localization is given by $|\psi|^2$; an energy measurement that finds E_m forces c_n to become δ_{nm} .
- ▷ The time evolution of ψ in the general case is given by the time-dependent Schrödinger equation $j\hbar \partial\psi/\partial t = \mathcal{H}\psi$. *This is true also in the Non-conservative case*

Q)

However, some important issues are still to be understood: ?

- ◀ How can one calculate the probability that an energy measurement finds the eigenvalue E_m ? Hp: such probability is related to $|c_m|^2$. *(from Parseval's Theorem)*
- ◀ How can one calculate the probability to find, by means of a suitable measurement, a value of another dynamical quantity (e.g., p_i, M_i)? Hp: by analogy, one should solve an eigenvalue equation.

$\xrightarrow{*}$) How do we find the Eigen value & qⁿ of the required Dynamical Quantity (P_i, M_i etc) ?

Ans We proceed in the same way we did in the Hamiltonian

- We start with the Classical expression of the Dynamical Quantity & we look whether in this expression & then look for the components of the Momentum.
- We have to write it in terms of in general Momentum & Positional co-ordinates.
They should be replaced by Momentum Operators

~~* For this to be possible Eigenvalues must be REAL.~~

Eigen values will be Real only if the Operator is Hermitian.

General Methods of Quantum Mechanics — II

Postulates of Quantum Mechanics

- Given a physical quantity A (also called *observable*), an operator \mathcal{A} is associated to it. It is found by expressing A in terms of canonical coordinates and replacing p_i with $-j\hbar\partial/\partial q_i$ in such a way that \mathcal{A} is Hermitian.
- The eigenvalue equation $\mathcal{A}\psi = E\psi$ is formed, where the set of eigenfunctions is orthogonal and complete (to be checked case by case). The equation is subject to the same boundary or asymptotic conditions as $\mathcal{H}w = Ew$. Thanks to completeness, the wave function can be written

$$\psi = \sum_n a_n(t) v_n(\mathbf{r}) \quad \text{or} \quad \psi = \int_{\beta} a_{\beta}(t) v_{\beta}(\mathbf{r}) d\beta,$$

where n, β indicate sets of discrete or continuous indices, and

Coefficients $\Rightarrow a_n = \langle v_n | \psi \rangle \quad \text{or} \quad a_{\beta} = \langle v_{\beta} | \psi \rangle$.

- If ψ is normalizeable it is $\sum_n |a_n|^2 = 1$ or $\int_{\beta} |a_{\beta}|^2 d\beta = 1$.

Parseval's

Theorem

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General Methods of Quantum Mechanics — III

Postulates of Quantum Mechanics (cont.)

- ▷ The eigenvalues A_n or A_β are the only values that a measure of the physical quantity A can find.
- ▷ Taking a normalizable ψ , if the eigenvalues are discrete then the probability that a measurement finds A_n is $P_n = |a_n|^2$. If they are continuous, the infinitesimal probability that A_β is found in the interval $d\beta$ around β is $dP = |a_\beta|^2 d\beta$.
- ▷ As the eigenvalues represent a physical quantity, they must be real. This happens iff A is Hermitian, as is easily demonstrated. It is worth adding that the property of being Hermitian must be checked: for instance, the observable $A = xp_x$ can be written in equivalent ways as

$$xp_x, \quad p_x x, \quad (xp_x + p_x x)/2.$$

- However, the quantum counterparts A

$$-j\hbar x \frac{\partial}{\partial x}, \quad -j\hbar \frac{\partial}{\partial x} x, \quad -j\hbar \frac{1}{2} \left(x \frac{\partial}{\partial x} + \frac{\partial}{\partial x} x \right)$$

are different, and only the third one is Hermitian.

different ways of
expressing the physical
quantity using
canonical coordinates
A Momentum
Operator

Eigenvalues of Hermitian Operators

According to the basic postulates, the eigenvalues of an operator \mathcal{A} are the only possible values of the observable A to which \mathcal{A} is associated. For \mathcal{A} to be acceptable, the following hold:

- \mathcal{A} must have a complete set of eigenfunctions.
- The eigenvalues of \mathcal{A} must be real, since they correspond to possible values of the physical quantity A .

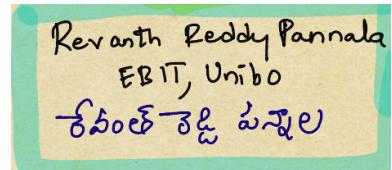
The following theorems hold: *If \mathcal{A} is an Hermitian operator, then its eigenvalues are real.* Assuming by way of example a discrete spectrum, for any eigenfunction v_n it is

$$\langle v_n | \mathcal{A}v_n \rangle = \langle \mathcal{A}v_n | v_n \rangle \implies A_n \langle v_n | v_n \rangle = A_n^* \langle v_n | v_n \rangle$$

whence $A_n = A_n^*$. *If the eigenfunctions form a complete set, then an operator whose eigenvalues are real is Hermitian:*

$$\begin{aligned} \langle g | \mathcal{A}f \rangle - \langle \mathcal{A}g | f \rangle &= \sum_n \sum_m g_n^* f_m [\langle v_n | \mathcal{A}v_m \rangle - \langle \mathcal{A}v_n | v_m \rangle] = \\ &= \sum_n \sum_m g_n^* f_m \langle v_n | v_m \rangle (A_m - A_n^*) = \sum_n g_n^* f_n (A_n - A_n^*) = 0, \end{aligned}$$

which holds $\forall f, g$ because all A_n are real.



→ Issue of Separability of the Operator.

Operator Properties — I

- Let \mathcal{A} an operator acting only on the coordinate x . Similarly, let \mathcal{B} and \mathcal{C} two operators acting only on y and z , respectively. The eigenvalue equations for the discrete-spectrum case read

$$\mathcal{A}u_k = A_k u_k, \quad \mathcal{B}v_m = B_m v_m, \quad \mathcal{C}w_n = C_n w_n.$$

where $u_k(x)$, $v_m(y)$, and $w_n(z)$ are the three sets of eigenfunctions. Given $f(x, y, z)$, thanks to the completeness of the three sets it turns out

$$\begin{aligned} f &= \sum_n a_n(x, y) w_n = \sum_n \left[\sum_m b_{mn}(x) v_m \right] w_n = \\ &= \sum_n \left\{ \sum_m \left[\sum_k c_{kmn} u_k \right] v_m \right\} w_n = \sum_{kmn} c_{kmn} u_k v_m w_n, \end{aligned}$$

showing that the set $u_k v_m w_n$ is complete. Also, for any linear combination of the above operators, with a, b, c arbitrary vectors, it is

operator is separable eigenvalues are individual Eigen values

$$(a \mathcal{A} + b \mathcal{B} + c \mathcal{C}) u_k v_m w_n = (a A_k + b B_m + c C_n) u_k v_m w_n,$$

that is, $u_k v_m w_n$ is an eigenfunction corresponding to eigenvalue $a A_k + b B_m + c C_n$.



Operator Properties — II

Examples of Operators and Eigenfunctions

1. The operator corresponding to $\mathbf{r} = x_1 \mathbf{i}_1 + x_2 \mathbf{i}_2 + x_3 \mathbf{i}_3$ is \mathbf{r} itself, with eigenvalue equation $\mathbf{r} f(\mathbf{r}) = \mathbf{r}_0 f(\mathbf{r})$. The eigenvalue equation for x_i reads

$$x_i v_i(x_i) = x_{i0} v_i(x_i) \Rightarrow (x_i - x_{i0}) v_i(x_i) = 0 \quad \forall x_i \neq x_{i0}.$$

Then $v_i = \delta(x_i - x_{i0})$, whence $\mathbf{r}_0 = x_{10} \mathbf{i}_1 + x_{20} \mathbf{i}_2 + x_{30} \mathbf{i}_3$ and

$$f(\mathbf{r}) = \delta(x_1 - x_{10}) \delta(x_2 - x_{20}) \delta(x_3 - x_{30}) = \delta(\mathbf{r} - \mathbf{r}_0) \Rightarrow \text{Eigen function here is a Dirac Delta function}$$

2. The operator corresponding to $\mathbf{p} = p_1 \mathbf{i}_1 + p_2 \mathbf{i}_2 + p_3 \mathbf{i}_3$ is

$$-j\hbar \left(i_1 \frac{\partial}{\partial x_1} + i_2 \frac{\partial}{\partial x_2} + i_3 \frac{\partial}{\partial x_3} \right) = -j\hbar \text{grad},$$

and the eigenvalue equation reads $-j\hbar \text{grad } f = \mathbf{p}_0 f$. Separation yields for the i th eigenvalue equation, with $v_i = v_i(x_i)$,

$$-j\hbar v'_i = p_{i0} v_i \Rightarrow v_i = (2\pi)^{-1/2} \exp(jk_i x_i),$$

with $k_i = p_{i0}/\hbar$, whence $\mathbf{k} = \mathbf{p}/\hbar = k_1 \mathbf{i}_1 + k_2 \mathbf{i}_2 + k_3 \mathbf{i}_3$ and

$$f = f_k(\mathbf{r}) = (2\pi)^{-3/2} \exp(j\mathbf{k} \cdot \mathbf{r}).$$

Eigen function by definition is Notequal to zero!

$$-j\hbar v'_i = p_{i0} v_i$$

$$p_{i0} = k_i \hbar$$

$$\Rightarrow -j \frac{\hbar}{2\pi} \frac{d v_i}{d x_i} = k_i \hbar v_i$$

$$\Rightarrow \frac{d v_i}{v_i} = j k_i dx_i$$

TOPS

$$\Rightarrow \log v_i = \sum k_i x_i$$

$$v_i = e^{\sum k_i x_i}$$



Operator Properties -- III

- A conservative system of N interacting particles is described by the wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N, t)$ such that, assuming that ψ is normalizeable,

$$|\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N, t)|^2 d^3 r_1 d^3 r_2 \dots d^3 r_N$$

is the probability of simultaneously localizing the 1st, 2nd, ..., N th particle within the elementary volumes $d^3 r_1, d^3 r_2, \dots, d^3 r_N$ centered at r_1, r_2, \dots, r_N , respectively. The quantum Hamiltonian is derived by replacing $p_i^2 = p_{ix}^2 + p_{iy}^2 + p_{iz}^2$ with $-\hbar^2/(2m_i) \nabla_i^2$ in the classical one:

$$H = \sum_{i=1}^N \frac{p_i^2}{2m_i} + V \quad \Leftarrow \quad \mathcal{H} = \sum_{i=1}^N -\frac{\hbar^2}{2m_i} \nabla_i^2 + V$$

where $V = V(\mathbf{r}_1, \dots, \mathbf{r}_N)$ and $-\nabla_i^2 = \partial^2/\partial x_i^2 + \partial^2/\partial y_i^2 + \partial^2/\partial z_i^2$. In a state of definite and constant energy E_S ,

$$\psi = w \exp(-jE_S t/\hbar), \quad w = w(\mathbf{r}_1, \dots, \mathbf{r}_N),$$

where E_S is an eigenvalue of $\mathcal{H}w = Ew$.

unfortunately
Potential Energy
is Not
Separable
*(However there may
be situations where
it is separable)*
ex: Periodic Crystal



Operator Properties — IV

Separable Systems (a)

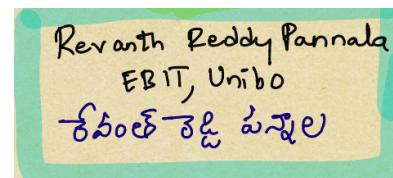
A conservative system of N interacting particles is *separable* if $V = \sum_i V_i(\mathbf{r}_i)$, whence the Hamiltonian has the form

$$\mathcal{H} = \sum_{i=1}^N \left(-\frac{\hbar^2}{2m_i} \nabla_i^2 + V_i(\mathbf{r}_i) \right) \doteq \sum_i \mathcal{H}_i$$

Assuming discrete eigenvalues, the i th Hamiltonian gives rise to the equation

$$\mathcal{H}_i w_{n_i} = E_{n_i} w_{n_i},$$

where index n_i denotes the n th eigenvalue (eigenfunction) of the i th particle. From the general properties of operators it follows that the eigenfunction of the whole system is the product of eigenfunctions like w_{n_i} , and the eigenvalue is the sum of eigenvalues like E_{n_i} . The eigenvalues are such that their sum provides the prescribed value E_S .





Eigenfunctions of Commuting Operators

- The following theorems hold: If two operators \mathcal{A} and \mathcal{B} have a common complete set of eigenfunctions, then they commute. Assuming by way of example a discrete spectrum, for any eigenfunction v_n it is

$$\mathcal{AB}v_n = \mathcal{AB}_n v_n = B_n \mathcal{A}v_n = B_n A_n v_n$$

$$\mathcal{BA}v_n = \mathcal{BA}_n v_n = A_n \mathcal{B}v_n = A_n B_n v_n$$

hence \mathcal{A} and \mathcal{B} commute for all v_n . As a consequence,

$$\begin{aligned}\mathcal{AB}f &= \mathcal{AB} \sum_n f_n v_n = \sum_n f_n \mathcal{AB}v_n = \sum_n f_n \mathcal{BA}v_n = \\ &= \mathcal{BA} \sum_n f_n v_n = \mathcal{BA}f\end{aligned}$$

holds $\forall f$. In turn: If two operators \mathcal{A} and \mathcal{B} commute, then they have a common complete set of eigenfunctions:

$$\left. \begin{array}{l} \mathcal{AB}v_n = \mathcal{BA}v_n \\ \mathcal{Av}_n = A_n v_n \end{array} \right\} \Rightarrow \mathcal{AB}v_n = \mathcal{BA}_n v_n \Rightarrow \mathcal{Ag}_n = A_n g_n$$

with $g_n \doteq \mathcal{B}v_n$. Hence g_n belongs to the same eigenvalue as v_n . If the eigenvalue is not degenerate it must be $g_n \propto v_n$: letting $g_n = B_n v_n$, it follows $\mathcal{B}v_n = B_n v_n$. The theorem holds in the degenerate case as well.

Ex:
 Energy
 &
 Momentum
 have common
 set of eigen
 functions

Q) Knowing whether two operators have common sets of Eigenfunctions?

Ans: If we measure Momentum (P), we indirectly measure energy (E)

$$E = \frac{P^2}{2m}$$

That means in this case we do not have the problem of measuring position & velocity as in the case of (Bud Tennis Ball) where measuring one dynamic quantity perturbs another dynamic quantity.

- But for $P \& E$ there is **NO** perturbation.

Expectation Value — I

Let \mathcal{A} be the Hermitian operator associated to an observable A , and ψ a normalizable wave function: $\langle \psi | \psi \rangle = 1$. The expectation value of A is defined as

$$\text{Expectation of } A \Rightarrow \langle A \rangle \doteq \langle \psi | \mathcal{A} | \psi \rangle.$$

It is easily seen that such definition provides the average value of the eigenvalues of \mathcal{A} . Taking a discrete spectrum, i.e., $\mathcal{A}v_n = A_n v_n$, the wave function can be expanded as $\psi = \sum_n c_n v_n$, with $c_m \doteq \langle v_m | \psi \rangle$. The probability of finding the n th eigenvalue is $P_n = |c_n|^2$. The following holds:

$$\begin{aligned} \sum_n |c_n|^2 A_n &= \sum_n \left(\sum_m c_m^* \delta_{mn} \right) c_n A_n = \sum_n \left(\sum_m c_m^* \langle v_m | v_n \rangle \right) c_n A_n = \\ &= \left\langle \sum_m c_m v_m \middle| \sum_n c_n A_n v_n \right\rangle = \left\langle \sum_m c_m v_m \middle| \sum_n c_n \mathcal{A} v_n \right\rangle = \langle \psi | \mathcal{A} | \psi \rangle \end{aligned}$$

Average value of the Eigenvalues

The average of the A_n s is then (with \mathcal{I} the identity operator)

$$\frac{\sum_n P_n A_n}{\sum_n P_n} = \frac{\sum_n |c_n|^2 A_n}{\sum_n |c_n|^2} = \frac{\langle \psi | \mathcal{A} | \psi \rangle}{\langle \psi | \mathcal{I} | \psi \rangle} = \langle A \rangle.$$

Expectation Value — II

The same calculation holds for continuous eigenvalues:

$$\frac{\int_{\alpha} P_{\alpha} A_{\alpha} d\alpha}{\int_{\alpha} P_{\alpha} d\alpha} = \frac{\int_{\alpha} |c_{\alpha}|^2 A_{\alpha} d\alpha}{\int_{\alpha} |c_{\alpha}|^2 d\alpha} = \frac{\langle \psi | \mathcal{A} | \psi \rangle}{\langle \psi | \mathcal{I} | \psi \rangle} = \langle A \rangle,$$

where

$$\int_{\alpha} |c_{\alpha}|^2 A_{\alpha} d\alpha = \int_{\alpha} \left(\int_{\beta} c_{\beta}^* \delta(\beta - \alpha) d\beta \right) c_{\alpha} A_{\alpha} d\alpha.$$

Using again the discrete spectrum, the calculation of the average value can be extended to the powers of the eigenvalues, A_n^2, A_n^3, \dots .

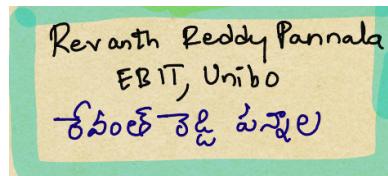
Observing that $\mathcal{A}^2 v_n \doteq \mathcal{A}(\mathcal{A}v_n) = \mathcal{A}\mathcal{A}_n v_n = A_n^2 v_n$, one finds

$$\langle A^2 \rangle \doteq \langle \psi | \mathcal{A}^2 | \psi \rangle = \int_{\tau} \psi^* \mathcal{A} \mathcal{A} \psi d\tau = \langle \mathcal{A} \psi | \mathcal{A} \psi \rangle \geq 0.$$

The variance of the eigenvalues is given by

$$(\Delta A)^2 \doteq \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 - 2\langle A \rangle A + \langle A \rangle^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2.$$

As $(\Delta A)^2 \geq 0$, it follows $\langle A^2 \rangle \geq \langle A \rangle^2$. The standard deviation $\Delta A = \sqrt{(\Delta A)^2} \geq 0$ is also called uncertainty.



Heisenberg Uncertainty Relation — I

Given two Hermitian operators \mathcal{A} , \mathcal{B} , the covariance of the eigenvalues is given by

$$\begin{aligned}\langle (A - \langle A \rangle)(B - \langle B \rangle) \rangle &= \langle AB - \langle A \rangle B - \langle B \rangle A + \langle A \rangle \langle B \rangle \rangle = \\ &= \langle AB \rangle - \langle A \rangle \langle B \rangle.\end{aligned}$$

The operators $\mathcal{A}_0 = \mathcal{A} - \langle A \rangle$ and $\mathcal{B}_0 = \mathcal{B} - \langle B \rangle$ are also Hermitian; defining the complex functions $f \doteq \mathcal{A}_0\psi$ and $g \doteq \mathcal{B}_0\psi$, and introducing a real parameter λ , let $\sigma \doteq f + j\lambda g$. It is found:

$$\begin{aligned}\langle \sigma | \sigma \rangle \geq 0 &\implies \int_{\tau} [f^*f + j\lambda(f^*g - g^*f) + \lambda^2 g^*g] d\tau \geq 0, \\ \int_{\tau} [\psi^* \mathcal{A}_0^2 \psi + j\lambda \psi^* (\mathcal{A}_0 \mathcal{B}_0 - \mathcal{B}_0 \mathcal{A}_0) \psi + \lambda^2 \psi^* \mathcal{B}_0^2 \psi] d\tau &\geq 0.\end{aligned}$$

The commutator of \mathcal{A}_0 and \mathcal{B}_0 is the operator \mathcal{C}_0 such that

$$j\mathcal{C}_0 = \mathcal{A}_0\mathcal{B}_0 - \mathcal{B}_0\mathcal{A}_0.$$

It is easily seen that, if \mathcal{A}_0 and \mathcal{B}_0 are Hermitian, then \mathcal{C}_0 is also Hermitian, whence its eigenvalues are real. From the above

$$\langle \mathcal{A}_0^2 \rangle - \lambda \langle \mathcal{C}_0 \rangle + \lambda^2 \langle \mathcal{B}_0^2 \rangle \geq 0.$$

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