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**Question wise Mark Summary**

**Q.No Mark Q.No Mark Q.No Mark Q.No Mark**

1A 4/5

1B 4/5

1C 4/5

1D 4/5

1E 4/5

1F 4/5

1G 4/5

1H 4/5

1I 3/5

2 9/15

3 0/15

4 0/15

5 0/15

6 0/15

7 11/15

8 0/15

9 0/15



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1. Read the instructions carefully given on the answer script and admit card.
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3. As shown in the example below blacken the circles completely.

Correct method



Incorrect method



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1. The Roll No. and Answer Book no. found elsewhere or any other symbol found in the answer book will be treated as unfair means.
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3. Do Not bring the materials like slip of paper/mobile/digital diaries/ study material/ revision notes in examination hall. Possession of the mobiles/ digital diaries/ electronic watch and any other electronic gadget except memory less scientific calculator shall be considered as UFM case.
4. Do not keep or paste currency note in answer script it shall be consider as UFM.

### अनुचित साधन से बचने हेतु:

1. उत्तर पुस्तिका के निर्देशित स्थान को छोड़कर अनुक्रमांक एवं उत्तरपुस्तिका का क्रमांक कहीं और न लिखें तथा कोई भी चिह्न न बनायें क्योंकि यह अनुचित साधन प्रयोग की परिधि में आता है।
2. उत्तर पुस्तिका के बारकोड अथवा उत्तर पुस्तिका संख्या पर छेड़ करने पर अनुचित साधन प्रयोग माना जायेगा।
3. परीक्षा कक्ष में बिना वस्तुएं साथ न लाये, जैसे लिखे हुए कामज के टुकड़े, मॉबाइल, डिजिटल डायरी, कोपी, पुस्तक यह सभी वस्तुएं जो अनुचित साधन के अन्तर्गत आती है। केवल संबंधित प्रश्नपत्र में ही मेमोरी लेस साइट्रॉनिक कैल्कुलेटर ले जाने की अनुमति होगी।
4. उत्तर पुस्तिकाओं में रूपये न रखें न ही उत्तर पुस्तिका में चिपकायें। ऐसा करना अनुचित साधन प्रयोग की परिधि में आता है।

### परीक्षार्थी के लिए निर्देश

1. प्रवेश पत्र एवं उत्तर पुस्तिका पर दिये गये निर्देशों को ध्यान से पढ़ें।
2. कवर पृष्ठ के दूसरी तरफ कुछ न लिखें।
3. उत्तर पुस्तिका के पृष्ठों पर दोनों तरफ लिखें।
4. प्रश्न पत्र पर अपने अनुक्रमांक के अतिरिक्त कुछ न लिखें।
5. प्रश्न पत्र कोड एवं प्रश्न पत्र कोड साक्यानी पूर्णक लिखें।
6. अपनी स्थिति स्पष्ट लिखें।
7. उत्तर पुस्तिका के पृष्ठों की संख्या देखें। अगर उत्तर पुस्तिका में पृष्ठ (1-24) से कम है या कटे हुए हैं, तो परीक्षा शुरू होने के पूर्व दूसरी उत्तर पुस्तिका ले लें।
8. प्रश्नपत्र को देख, यदि प्रश्नपत्र के विषय कोड, विषय का नाम तथा प्रश्न में कोई त्रुटि है तो उसके परीक्षा शुरू होने के 30 मिनट के अन्दर कक्षा निरीक्षक को तत्काल सूचित करें, उसके बाद विश्वविद्यालय द्वारा कोई कार्रवाई नहीं की जायेगी।
9. प्रश्नों के उत्तर लिखने के लिये पेंसिल का प्रयोग न करें।
10. B कोपी या अतिरिक्त शॉफ नहीं दिया जायेगा।

### INSTRUCTIONS TO THE CANDIDATE

1. Read the instructions carefully given on the Question Paper, Admit Card & Answer Script.
2. Do not write anything on back side of the cover page.
3. Write on both sides of pages of answer book.
4. Do not write anything on question paper except Roll Number.
5. Write Paper Code & Question Paper Id carefully.
6. CHECK the number of pages (1-32) or any other kind of damage in your answer script, if found than change the answer script immediately before the commencement of examination.
7. CHECK the Question Paper for any kind of discrepancy e.g. Subject Code, Subject Name and Question of the Question Paper during first THIRTY MINUTES of the commencement of the exam, so that it can be corrected in TIME. After that no corrections shall be entertained by the university.
8. Do not use pencil for answering the question.
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10. No supplementary answer book & graph paper will be provided.

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2. Use blue or black ball point pen for filling the circles.

	1	8	1	5	4	3	2	1	6	9
0	0	0	0	0	0	0	0	0	0	0
1	●	1	●	1	1	1	1	●	1	1
2	2	2	2	2	2	2	●	2	2	2
3	3	3	3	3	3	●	3	3	3	3
4	4	4	4	4	●	4	4	4	4	4
5	5	5	5	●	5	5	5	5	5	5
6	6	6	6	6	6	6	6	6	●	6
7	7	7	7	7	7	7	7	7	7	7
8	8	●	8	8	8	8	8	8	8	8
9	9	9	9	9	9	9	9	9	9	●

Note - If your Roll No. is of 10 digits. Please leave first three columns



Paper Code

B 0 1 0 9 0 2 T



01

Section - AShort Answer Type QuestionAnswer no. 1 (A)

given.

an harmonic oscillator  $\therefore$  mass =  $m$ angular frequency =  $\omega$ 

potential  $V(x) = \frac{1}{2} m \omega^2 x^2 + b x^4$

ground state wave

function:  $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$

First order energy

correction

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle \quad \text{--- (1)}$$

for the ground state  $E_0^1 = \langle \psi_0 | H' | \psi_0 \rangle$ 

$$E_0^1 = \langle \psi_0 | b x^4 | \psi_0 \rangle \quad \text{--- (2)}$$

here,

 $b$  is independent of  $x$ so,  $E^1 \neq 0$ 

we know

$$\langle 0 | x^4 | 0 \rangle = 3 \left(\frac{\hbar}{2m\omega}\right)^2 \quad \text{--- (3)}$$

use ground state wave function in eq. (2), we get

$$E_0^1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} \cdot \frac{b}{m^2\omega^2} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} \quad \text{--- (4)}$$



on solving equation (4)  
we get

$$E_0' = \sqrt{\frac{m\omega}{\pi\hbar}} \frac{3e^2 b}{4m^2\omega^2} e^{-\frac{m\omega x^2}{2\hbar}}$$

$$E_0' = \frac{3}{4} \sqrt{\frac{m\omega}{\pi\hbar}} \frac{e^2 b}{m^2\omega^2} e^{-\frac{m\omega x^2}{2\hbar}}$$

also

$$b \langle 0 | x^2 | 0 \rangle = b \cdot 3 \left( \frac{\hbar}{2m\omega} \right)^2$$

Answer no. 1 (B)

For H-atom

To show,  $E^z = 0$

Let intensity of electric field  $E$   
and corresponding energy in the  
form of work done.

$$W = Fd \quad \text{--- (1)}$$

$$W = qEz$$

change in direction of  $z$

$$W = -eEz \cos\theta$$

for  $n=2$

$$W = eEz \quad \text{--- (2)}$$



Hamiltonian of system is  $H$

$$H = \frac{p^2}{2u} + V(u) \quad \text{--- (3)}$$

for the ground state

$$n = 1$$

$$l = n - 1 = 0$$

$$m = -l \text{ to } +l = 0$$

By using the selection rule,

$$\Delta m = 0 \quad \text{and}$$

$$\Delta l = \pm 1 \quad \text{--- (4)}$$

are not followed, the energy correction of first order for H-atom

$$E^1 = \langle \psi^0 | H^1 | \psi^0 \rangle$$

$\Delta m \neq 0$  for first order energy correction for ground state

hence,

$$\boxed{E^1 = 0} \quad \text{proved}$$

There is no first order energy correction to the ground state of hydrogen atom due to symmetry and parity



Answer no. 1 (C)

Validity condition of WKB approximation

There are some condition that tells the accurate approximation

- 1) The potential  $V$  scattered waves are small compared to the kinetic energy of incident wave.

$$\left| \frac{1}{4\pi} \int e^{ik_0 r'} V(r') dr' \right| \ll 1$$

- 2) The magnitude of intensity of scattered wave is small compared to incident wave

$$\left| \frac{2m}{\hbar^2 k} \int r V(r) \sin(k_0 r) dr \right| \ll 1$$

- 3) This approximation applied only for low potential energy scattering.

- 4) Transition probability: must occur when  $E_f - E_i = \hbar\omega$

$$T_{if} = \frac{2\pi}{\hbar} |V_{fi}|^2 \rho(E)$$

- 5) It must follow energy conservation

$$E_f = E_i + \hbar\omega$$

- 6) Amplitude must small

$$C_f(\hat{x}) = -\frac{i}{\hbar} \int_{-\infty}^{\infty} e^{i\omega t} V(r') dr'$$

Do Not Write anything in this Portion



Answer no. 1 (D)

Given,

H-atom with atomic number  $z$

$ze \rightarrow (z-1)e$  nuclear charge

wave function

$$\psi_0 = \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0}\right)^{3/2} \exp\left(-\frac{zr}{a_0}\right) \quad (1)$$

So,

probability for new Hamiltonian after change nuclear charge

$$P(x,t) = \int \psi^* H \psi d\tau \quad (2)$$

$$= \int \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0}\right)^{3/2} e^{-(zr/a_0)} H \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0}\right)^{3/2} e^{-(zr/a_0)}$$

after nuclear charge changes

probability will be

$$P(x,t) = \int \frac{1}{\sqrt{\pi}} \left(\frac{z-1}{a_0}\right)^{3/2} e^{-(\frac{z-1}{a_0}r)} H \frac{1}{\sqrt{\pi}} \left(\frac{z-1}{a_0}\right)^{3/2} e^{-(\frac{z-1}{a_0}r)}$$

$$P(x,t) = \frac{1}{\sqrt{\pi}} \int \left(\frac{z-1}{a_0}\right)^{3/2} e^{-(\frac{z-1}{a_0}r)} \cdot e^z d\tau$$

when nuclear charge are change then probability also changes from  $z$  to  $(z-1)e$



## Answer no. 1 (E)

Einstein Coefficients - The Albert Einstein gives the some absorption and emission coefficient to describe the transition between two energy levels or state.

### Absorption Coefficient ( $B_{12}$ )

When atom in ground energy state after absorbing radiation it jumps to higher energy state with emitting photon of frequency  $\nu$ .

### Stimulated emission ( $B_{21}$ )

Atom is placed in higher energy state and fall down during absorption of radiation and emit a photon of energy  $h\nu$ .

### Spontaneous emission ( $A_{21}$ )

Atom in higher energy state falls down to lower energy state with taking the incident energy and emits a photon of energy same  $h\nu$ .

### Relation between coefficients

There are two transition associates with



absorption coefficient and stimulated emission of radiation

$$B_{12} = B_{21}$$

and

$$\frac{A_{21}}{B_{21}} = \frac{8\pi h \nu^3}{c^3}$$

absorption coefficient and stimulated emission are related as above expression for the radiation where,

$\nu$  = frequency of incident photon

$c$  = speed of light

$B_{21}$  = stimulated emission coefficient

$h$  = plank's constant

### Answer no. 1 (F)

Optical Theorem  $\rightarrow$  The optical theorem relates the scattering amplitude's imaginary part and total cross-section.

Proof - Scattering amplitude for partial wave analysis approximation is given by

$$f(\theta, \phi) = \sum_k \left( \frac{2k+1}{k} \right) e^{i\delta_k} \sin \delta_k (P_k) \cos \theta$$



for  $\theta = 0$

scattering amplitude becomes-

$$f(\theta) = \sum_k \left( \frac{2l+1}{k} \right) e^{i\delta_l} \sin \delta_l P_l(\cos \theta) \quad \text{--- (3)}$$

for low energy  
scattering

$$P_l(x) = 1$$

$$\therefore \cos \theta = 1$$

expand  $e^{i\delta_l}$  then equation (3) becomes

$$f(\theta) = \left( \frac{2l+1}{k} \right) (i\delta_l + \cos \delta_l) \sin \delta_l$$

taking only imaginary part

$$\text{Im}g. f(\theta) = \left( \frac{2l+1}{k} \right) \sin^2 \delta_l \quad \text{--- (3)}$$

The differential cross-section for partial wave ( $l=0$ )

$$\sigma_T = \frac{4\pi}{k^2} (2l+1) \sin^2 \delta_l \quad \text{--- (4)}$$

substituting equation (4) in equation (3) we get

$$\sigma_T = \frac{4\pi}{k^2} \text{Im}g[f(\theta)]$$

This is the expression for optical Theorem which relates imaginary part of scattering and total differential cross-section.

Answer no. 1 (6)

Phase Shift - In Quantum scattering the phase shift describes that how the scattered wave delayed in phase compared to the incident wave due to the use of potential.

If scattering occurs then how the scattered wave is shifted due to potential then corresponding wave function  $\psi$  is

$$\psi(r) \sim \left( \sin kr + \frac{\pi}{2} + \delta_l \right) \quad \text{--- (1)}$$

where,

$l$  = angular quantum number

$\psi$  = wave function

$\delta_l$  = phase shift by scattered wave

Nature of phase shift - This is based upon the given potential in scattering.

for low scattering  $l=0$

so,

$$\frac{\delta_0}{k} = \frac{\tan(k_0 a) - k_0 a}{k^2} \quad \text{--- (2)}$$

when repulsive potential applied then nature of phase shift changes

from equation (2)



due to potential

differential cross-section is expressed as.

$$\sigma_T = \frac{\pi}{k} \left[ \frac{\tan(k_0 a) - k_0 a}{k} \right]^2$$

This is the expression for cross-section due to phase shift of attractive and repulsive potential

Answer no. 1 (H)

### Klein-Gordon Equation

For non-relativistically case.

The Klein-Gordon equation is given by

$$\left( \square^2 - \frac{m^2 c^2}{\hbar^2} \right) \psi = 0 \quad \text{--- (1)}$$

where,

$\square^2 = \text{D'Alembert operator}$

Schrodinger equation for this case

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\nabla^2 \psi + \beta \cdot mc^2 \psi \quad \text{--- (2)}$$



For non-relativistic case

position probability density

$$P(\vec{r}, t) = |\psi|^2 \quad \text{--- (3)}$$

Probability current density

$$J(\vec{r}, t) = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) \quad \text{--- (4)}$$

On solving the Schrodinger relativistic equation which is equation (2)

we get, after comparing with continuity equation

$$\frac{\partial P(\vec{r}, t)}{\partial t} + \nabla \cdot \vec{J}(\vec{r}, t) = 0 \quad \text{--- (5)}$$

we get

$$P(\vec{r}, t) = \frac{i\hbar}{2mc^2} \left( \psi \frac{\partial \psi^*}{\partial t} - \psi^* \frac{\partial \psi}{\partial t} \right) \quad \text{--- (6)}$$

$$J(\vec{r}, t) = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) \quad \text{--- (7)}$$

again

we get

$$P(\vec{r}, t) \neq |\psi|^2$$

$$J(\vec{r}, t) \neq J(\vec{r}, t)$$

now take

$$P(\vec{r}, t) = \frac{i\hbar}{2mc^2} \frac{\partial}{\partial t} (\psi \frac{\partial \psi^*}{\partial t} - \psi^* \frac{\partial \psi}{\partial t})$$

$$\text{put } \vec{E} = i\hbar \frac{\partial}{\partial t}$$

$$P = \frac{E}{2mc^2} (2\psi^* \psi)$$

$$\therefore \psi \psi^* = 1$$

$$\frac{E}{mc^2}$$



means

E is positive then probability  
is +ve value

if E is -ve then probability is -vely  
value of  $\psi^*$

This is the big drawback of Klein-Gordon equation.

Answer no. 1 (I)

given

$$\sigma' = \begin{bmatrix} \sigma & 0 \\ 0 & \sigma \end{bmatrix}$$

⊕

Direct  
matrices are

$$\alpha_x = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

⊗

and

Pauli matrix is

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\alpha_y = \begin{bmatrix} 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \\ i & 0 & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix}$$

⊗



To find

$$[A] \sigma_x^2 [B] \cdot [\sigma_x, \sigma_x]$$

$$A \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}^2 B \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \text{--- (4)}$$

Pauli matrix is order of  $2 \times 2$   
which is solvable

but Dirac matrix is order of  $4 \times 4$

on solving equation (4),  
we get

$$[A] \begin{bmatrix} \sigma & 0 \\ 0 & \sigma \end{bmatrix} [B] \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = 0$$

we get the zero.

Section - CLong Answer Type QuestionAnswer no. 7

part (a) →

For scattering amplitude use  
Schrödinger's time independent equation

$$\frac{-\hbar^2 \nabla^2 \psi}{2\mu} + V\psi = E\psi \quad \text{--- (1)}$$

For incident wave ( $x \rightarrow -\infty$ )

potential is zero  $V(x) = 0$

$$\frac{-\hbar^2 \nabla^2 \psi}{2\mu} + V\psi = E\psi$$

$$\nabla^2 \psi + k^2 \psi = E\psi \quad \text{--- (2)}$$

has a solution

$$\psi_{inc} = e^{ikz}$$

For scattering region ( $x \neq 0$ ) Schrödinger's  
equation becomes

$$\nabla^2 \psi + k^2 \psi = 0 \quad \text{--- (3)}$$

For a particle at a large distance ( $x \rightarrow +\infty$ )

$$\nabla^2 \psi + k^2 \psi = V\psi \quad \text{--- (4)}$$



Scattered wave is spherical so it depends on  $\theta$  and  $\phi$

total wave function is

$$\psi = \psi_{inc} + \psi_{scattered}$$

$$\psi = e^{ikz} + \frac{e^{ikr}}{r} f(\theta, \phi) \quad (3)$$

Apply perturbation approaches.

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + V(\mathbf{r}) \quad (4)$$

eq. (4) put in (3) we get

$$\nabla^2 e^{i\mathbf{k}\cdot\mathbf{r}} + \nabla^2 V(\mathbf{r}) + k^2 e^{i\mathbf{k}\cdot\mathbf{r}} + k^2 V(\mathbf{r}) = V \cdot V(\mathbf{r}) + V \cdot e^{i\mathbf{k}\cdot\mathbf{r}} \quad (5)$$

potential is small so  $V(\mathbf{r}) \rightarrow 0$

inhomogeneous solution of eq. (5) is

$$V(\mathbf{r}) = \int G(\mathbf{r}, \mathbf{r}') F(\mathbf{r}') d\mathbf{r}'$$

use Green function

$$\therefore G(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \int \frac{e^{i\mathbf{k}\cdot\mathbf{r} - \omega|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$

then equation (5) can be written as

$$V(\mathbf{r}) = -\frac{1}{4\pi} \int \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}') - \omega|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') d\mathbf{r}' \quad (6)$$



$$\therefore |\omega - \omega'| = \omega$$

On comparing eq. (5) and (6) we get

$$\psi(\omega) = e^{ikz} + \frac{e^{ikz}}{i} f(\theta, \phi)$$

$$V(\omega) = -\frac{1}{4\pi} \int e^{ikr'} V(\omega') d\omega'$$

we get

$$f(\theta, \phi) = -\frac{1}{4\pi} \int e^{ik(z' - \omega z')} V(\omega') d\omega'$$

$$\omega z'$$

$$z' - \omega z' = k_0 - k = k$$

$$f(\theta, \phi) = -\frac{1}{4\pi} \int V(\omega') d\omega' \quad \text{--- (9)}$$

This is the scattering amplitude for Born approximation

eq. (9) also written as

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int e^{ik\omega'} V(\omega) d^3\omega \quad \text{--- (10)}$$

part (b)

$$f(\theta, \phi) = ?$$

given,  $V(\omega) = -\left(\frac{Ze^2}{\omega}\right) \exp(-\alpha\omega)$



by using fourier transform

$$\int e^{ikx} e^{-ax} = \frac{4\pi}{k^2 + a^2} \quad \text{--- (1)}$$

putting this value in equation (1)

$$= \int e^{ikx} V(x) d^3x$$

$$= \int e^{ikx} \left( \frac{-Ze^2}{r} \right) d^3x$$

by using eq. (1)

$$= -Ze^2 \int e^{ikx} e^{-ax} d^3x$$

$$= -Ze^2 \cdot \frac{4\pi}{k^2 + a^2}$$

then  $f(\theta, \phi)$  becomes

$$f(\theta, \phi) = \frac{-m}{2\pi\hbar^2} \left[ \frac{-Ze^2 \cdot 4\pi}{k^2 + a^2} \right]$$

$$f(\theta, \phi) = \left[ \frac{-m}{\hbar^2} \cdot \frac{1}{k^2 + a^2} \right] \quad \text{--- (2) ans.}$$

This is the required result for given potential  $V(x)$  which is Coulomb potential.



part (c) →

Rutherford's Formula - It is used for alpha scattering for Coulomb potential.

which is defined as-

$$\frac{d\sigma}{d\Omega} = \left| \frac{1}{4\pi\epsilon_0} \cdot \frac{Z_1 Z_2 e^2}{4E} \cdot \frac{1}{\sin^2(\theta/2)} \right|^2 \quad \text{--- (14)}$$

where,

$Z_1$  and  $Z_2$  = charges

$E$  = kinetic field

$e$  is charge of particle

$\theta$  is angle between scattered and incident beam

$\epsilon_0$  is permittivity

Equation (14) is expression for Rutherford scattering.

Do Not Write anything in this Portion



## Section - B

### Long Answer Type Question

Answer no. 2.

Variational Principle - Variation principle is used for system of Schrodinger equation which is not solved by approximation method.

It states that "For a given trial wave function the expectation value of the energy state is always greater than the energy of ground state level."  $\langle E \rangle \geq E_0$

This method is used to calculate ground state energy of the system

$$\langle E \rangle = \langle \psi | H | \psi \rangle$$

$$\langle E \rangle = \frac{\int \psi^* H \psi d\tau}{\langle \psi | \psi \rangle} \geq E_0 \quad \text{--- (1)}$$

#### Steps involving variation method

- 1) Take the trial wave function  $\psi$
- 2) minimize the Hamiltonian with respect to variable parameter say  $\lambda$



$$\frac{d\langle H \rangle}{dA} = 0$$

- 3) Minimise the Hamiltonian
- 4) Get the expectation energy is greater than ground state energy

For Ground-State Energy -

particle of upper bound  $x_0$  with mass  $m$  and wave function  $\psi$

then  $E = \langle \psi | H | \psi \rangle$

$$\langle E \rangle = \frac{\int \psi^* H \psi d\tau}{\langle \psi | \psi \rangle} \quad \text{--- (2)}$$

If the wave function does not equal

$$\psi_0 \neq \psi$$

then the

$$\phi = \int a_n \phi_n \quad \text{--- (3)}$$

$$\phi = \int a_m a_m^* \psi^* \psi d\tau$$

then for perturbation energy becomes,

$$E = \int \psi^* \psi d\tau \quad \text{--- (4)}$$

where,  $\psi^* \psi = 1$



from equation (2)

$$\langle E \rangle = \sum |a_n|^2 \phi_m E \quad \text{--- (5)}$$

Subtracting (5) on both sides we get

$$\langle E \rangle - E_0 = \sum |a_n|^2 E - E_0 \quad \text{--- (6)}$$

we get the  $\langle E \rangle - E_0 > 0$

Here  $a_n$  is a positive negligible quantity and for  $E$  its value is 1 for the trial wave function so,

we can write it as

$$\langle E \rangle > E_0$$

hence

It showed that expectation value of energy is always greater than ground state energy.

Eigen values of hydrogen atom -

Variation is used for upper bound state to the energy so we can write as.

$$\frac{d\langle H \rangle}{d\lambda_1}, \frac{d\langle H \rangle}{d\lambda_2}, \frac{d\langle H \rangle}{d\lambda_3} \dots$$



for Hydrogen atom upper bound is valid for variation principle method.

Limitation ✓ Variational principle-

The variation method used only for upper bound state not the lower bound state of the quantum system.

It is used ✓ for atom, molecules or system where state are bound and system does not solve by time independent Schrodinger equation.

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