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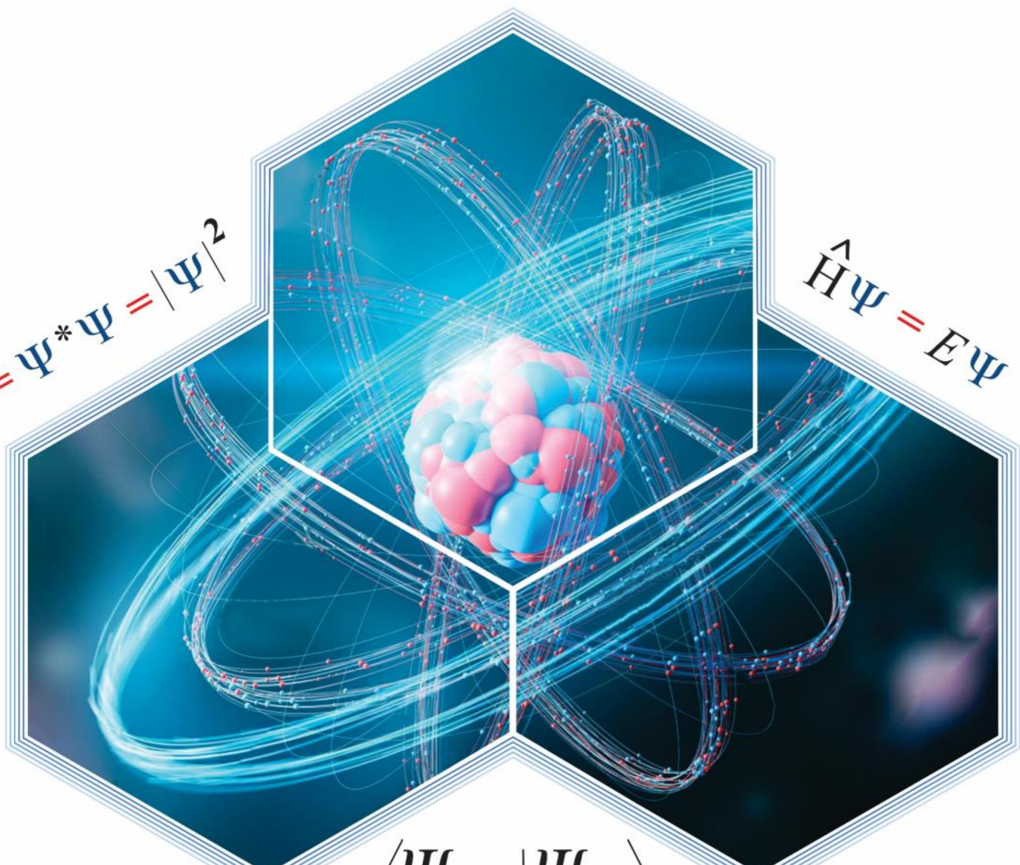
QUANTUM MECHANICS - I

For BS/M.Sc Physics Programme

4th Edition

$P = \Psi^*\Psi = |\Psi|^2$

$\hat{H}\Psi = E\Psi$



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Dr. Syed Hamad Bukhari
Hafiz Umer Farooq

TEACH YOURSELF

QUAMTUM MECHANICS-I

4th Edition

For **BS/M.Sc Physics** students of all Pakistani Universities

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Chapter 1

Origins of Quantum Mechanics

SOLVED PROBLEMS

Problem: 1.1- How much energy is required to remove an electron from the n= 8 state of a hydrogen atom?

Solution

Energy of the $n = 8$ state of hydrogen atom is

$$E_n = \frac{-13.6\ eV}{n^2} \implies E_8 = \frac{-13.6\ eV}{8^2} = -0.21\ eV$$

Problem: 1.2- Calculate the maximum wavelength that hydrogen in its ground state can absorb.

Solution

Maximum wavelength correspond to minimum energy. Hence the jump from ground state to first excited state gives the maximum λ. Energy can be calculated from

$$E_n = \frac{-13.6\ eV}{n^2}$$

Energy of the ground state $(n = 1) = -13.6\ eV$

Energy of the first excited state $(n = 2) = -13.6/4 = -3.4\ eV$

Maximum wavelength corresponds to the energy $-3.4 - (-13.6) = 10.2\ eV$

$$c = f\lambda \implies \lambda = \frac{c}{f} = \frac{hc}{E} \qquad \because E = hf \text{ and } f = \frac{E}{h}$$

$$\text{Maximum wavelength } \lambda = \frac{hc}{E}$$
$$= \frac{(6.626\times10^{-34}Js)\times(3.0\times10^{8}m/s)}{(10.2)(1.6\times10^{-19}J)}$$
$$\lambda = 122\times10^{-9}m \ = \ 122\ nm$$

Problem: 1.3- An electron in the $n = 2$ state of hydrogen remains there on the average of about 10^{-8} s, before making a transition to n = 1 state.

(i) Estimate the uncertainty in the energy of the n=2 state.

(ii) What fraction of the transition energy is this?

Solution

$$(i) \qquad \Delta E \geq \frac{h}{4\pi\Delta t} = \frac{6.626\times10^{-34}\text{Js}}{4\pi\times10^{-8}\text{s}}$$
$$= 0.527\times10^{-26}\text{J} = 3.29\times10^{-8}\text{eV}$$

(ii) Energy of $n = 2 \rightarrow n = 1$transition

$$= -3.4 - (-13.6) = 10.2\text{eV}$$
$$\text{Fraction } = \frac{\Delta E}{E} = \frac{3.29\times10^{-8}\text{eV}}{10.2\text{eV}} = 3.23\times10^{-9}$$

Problem: 1.4- The uncertainty in the velocity of a particle is equal to its velocity. If $\Delta p\cdot\Delta x \cong h$, show that the uncertainty in its location is its de Broglie wavelength.

Solution

Given $\Delta v = v$ Then,

$$\Delta p = m\Delta v = mv = p$$
$$\Delta x\times\Delta p \cong h \quad \text{or} \quad \Delta x\cdot p \cong h$$
$$\Delta x \cong \tfrac{h}{p} = \lambda$$

Problem: 1.5- Calculate the probability of finding the particle in the region $-1 \leq x \leq 1$, represented by the wavefunction

$$\psi(x) = \frac{1}{\sqrt{\pi}}\frac{1}{\sqrt{x^2+1}}$$

Solution

probability of finding the particle in the region $-1 \leq x \leq 1$ is given by

$$P = \int_{-1}^{+1} |\psi(x)|^2 \, dx = \int_{-1}^{+1} \frac{1}{\pi} \frac{1}{x^2+1} \, dx$$

$$P = \frac{1}{\pi} \left| \tan^{-1} x \right|_{-1}^{1} = \frac{1}{\pi} \left(\frac{\pi}{4} + \frac{\pi}{4} \right)$$

$$P = \frac{1}{\pi} \left(\frac{\pi}{2} \right) = \frac{1}{2}.$$

Chapter 2

Mathematical Tools of Quantum Mechanics

SOLVED PROBLEMS

Problem: 2.1- Consider the states $|\psi\rangle = 3i|\phi_1\rangle - 7i|\phi_2\rangle$ and $|\chi\rangle = -|\phi_1\rangle + 2i|\phi_2\rangle$ where $|\phi_1\rangle$ and $|\phi_2\rangle$ are orthonormal. Calculate $|\psi + \chi\rangle$ and $\langle\psi + \chi|$

Solution

The calculation of $|\psi + \chi\rangle$ is straightforward:

$$\begin{aligned}|\psi + \chi\rangle &= |\psi\rangle + |\chi\rangle = (3i|\phi_1\rangle - 7i|\phi_2\rangle) + (-|\phi_1\rangle + 2i|\phi_2\rangle) \\ &= (-1 + 3i)|\phi_1\rangle - 5i|\phi_2\rangle\end{aligned}$$

This leads to the expression $\langle\psi + \chi|$

$$\begin{aligned}\langle\psi + \chi| &= (-1 + 3i)^*\langle\phi_1| + (-5i)^*\langle\phi_2| \\ &= (-1 - 3i)\langle\phi_1| + 5i\langle\phi_2|\end{aligned}$$

Problem: 2.2- Find the Hermitian adjoint of $f(\hat{A}) = \left(1 + i\hat{A} + 3\hat{A}^2\right)\left(1 - 2i\hat{A} - 9\hat{A}^2\right)/(5 + 7\hat{A})$

Solution

Since the Hermitian adjoint of an operator function $f(\hat{A})$ is given by $f^\dagger(\hat{A}) = f\left(\hat{A}^\dagger\right)$, we can write

$$\left(\frac{\left(1 + i\hat{A} + 3\hat{A}^2\right)\left(1 - 2i\hat{A} - 9\hat{A}^2\right)}{5 + 7\hat{A}}\right)^\dagger = \frac{\left(1 + 2i\hat{A}^\dagger - 9\hat{A}^{2\dagger}\right)\left(1 - i\hat{A}^\dagger + 3\hat{A}^{2\dagger}\right)}{5 + 7\hat{A}^\dagger}$$

Problem: 2.3- Show that the operator $|\psi\rangle\langle\psi|$ is a projection operator only when $|\psi\rangle$ is normalized.

Solution

It is easy to ascertain that the operator $|\psi\rangle\langle\psi|$ is Hermitian, since $(|\psi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\psi|$. As for the square of this operator, it is given by

$$(|\psi\rangle\langle\psi|)^2 = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi|$$

Thus, if $|\psi\rangle$ is normalized, we have $(|\psi\rangle\langle\psi|)^2 = |\psi\rangle\langle\psi|$. In sum, if the state $|\psi\rangle$ is normalized, the product of the ket $|\psi\rangle$ with the bra $\langle\psi|$ is a projection operator.

Problem: 2.4- Show that the commutator of two Hermitian operators is anti-Hermitian.

Solution

If $\hat{A}$ and $\hat{B}$ are Hermitian, we can write

$$[\hat{A}, \hat{B}]^\dagger = (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger = \hat{B}^\dagger\hat{A}^\dagger - \hat{A}^\dagger\hat{B}^\dagger = \hat{B}\hat{A} - \hat{A}\hat{B} = -[\hat{A}, \hat{B}]$$

that is, the commutator of $\hat{A}$ and $\hat{B}$ is anti-Hermitian: $[\hat{A}, \hat{B}]^\dagger = -[\hat{A}, \hat{B}]$

Problem: 2.5- Show that if $\hat{A}^{-1}$ exists, the eigenvalues of $\hat{A}^{-1}$ are just the inverse of those of $\hat{A}$.

Solution

Since $\hat{A}^{-1}\hat{A} = \hat{I}$ we have on the one hand

$$\hat{A}^{-1}\hat{A}|\psi\rangle = |\psi\rangle$$

and on the other hand

$$\hat{A}^{-1}\hat{A}|\psi\rangle = \hat{A}^{-1}(\hat{A}|\psi\rangle) = a\hat{A}^{-1}|\psi\rangle$$

Combining the previous two equations, we obtain

$$a\hat{A}^{-1}|\psi\rangle = |\psi\rangle$$

hence

$$\hat{A}^{-1}|\psi\rangle = \frac{1}{a}|\psi\rangle$$

This means that $|\psi\rangle$ is also an eigenvector of $\hat{A}^{-1}$ with eigenvalue $1/a$. That is, if $\hat{A}^{-1}$ exists, then

$$\hat{A}|\psi\rangle = a|\psi\rangle \quad \Longrightarrow \quad \hat{A}^{-1}|\psi\rangle = \frac{1}{a}|\psi\rangle$$

Chapter 3

Fundamentals of Quantum Mechanics

SOLVED PROBLEMS

Problem: 3.1- Can we measure the kinetic and potential energies of a particle simultaneously with arbitrary precision?

Solution

The operator for kinetic energy, $T = -\left(\hbar^2/2m\right)\nabla^2$. The Operator for potential energy, $V = V(r)$. Hence,

$$\left[-\frac{\hbar^2}{2m}\nabla^2, \dot{V}\right]\psi = -\frac{\hbar^2}{2m}\nabla^2(\mathrm{V}\psi) - V\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi$$
$$= -\frac{\hbar^2}{2m}\left(\nabla^2 V\right)\psi \neq 0$$

since the operators of the two observables do not commute, simultaneous measurement of both is not possible. Simultaneous measurement is possible if V is constant or linear in coordinates.

Problem: 3.2- Show that the operator $U = \frac{1+iA}{1-iA}$ is unitary. Provided A is Hermitian.

Solution

$$U^\dagger U = \left(\frac{1+iA}{1-iA}\right)^\dagger \left(\frac{1+iA}{1-iA}\right) = \left(\frac{1-iA^\dagger}{1+iA^\dagger}\right)\left(\frac{1+iA}{1-iA}\right)$$
$$U^\dagger U = \left(\frac{1-iA}{1+iA}\right)\left(\frac{1+iA}{1-iA}\right) \qquad \because \quad A^\dagger = A$$
$$U^\dagger U = I$$

Similarly, $UU^\dagger = I$. Hence U is unitary operator.

Problem: 3.3- If A and B are Hermitian operators, show that $(AB + BA)$ is Hermitian i.e. $\{A, B\}^\dagger = \{A, B\}$.

Solution

Since A and B are Hermitian, we have $A^\dagger = A$ and $B^\dagger = B$. So,

$$\begin{aligned}\{A, B\}^\dagger &= (AB + BA)^\dagger \\ &= B^\dagger A^\dagger + A^\dagger B^\dagger = BA + AB \\ &= AB + BA \\ &= \{A, B\}\end{aligned}$$

Problem: 3.4- Consider a system whose state is given in terms of an orthonormal set of three vectors: $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$ as:

$$|\psi\rangle = \frac{\sqrt{3}}{3}|\phi_1\rangle + \frac{2}{3}|\phi_2\rangle + \frac{\sqrt{2}}{3}|\phi_3\rangle$$

verify that $|\psi\rangle$ is normalized. Then calculate the probability of finding the system in any one of the state $|\phi_1\rangle, |\phi_2\rangle$, and$|\phi_3\rangle$. Verify that total probability is equal to one.

Solution

Using the orthonormality condition $\langle\phi_j|\phi_k\rangle = \delta_{jk}$ where $j, k = 1, 2, 3$ we can verify that $|\psi\rangle$ is normalized.

$$\langle\psi|\psi\rangle = \frac{1}{3}\langle\phi_1|\phi_1\rangle + \frac{4}{9}\langle\phi_2|\phi_2\rangle + \frac{2}{9}\langle\phi_3|\phi_3\rangle = \frac{1}{3} + \frac{4}{9} + \frac{2}{9} = 1$$

Since, $|\psi\rangle$ is normalized, the probability of finding the system in $|\phi_1\rangle$ is given by

$$P_1 = |\langle\phi_1|\psi\rangle|^2 = \left|\frac{\sqrt{3}}{3}\langle\phi_1|\phi_1\rangle + \frac{2}{3}\langle\phi_1|\phi_2\rangle + \frac{\sqrt{2}}{3}\langle\phi_1|\phi_3\rangle\right|^2 = \frac{1}{3}$$

Since, $\langle\phi_1|\phi_1\rangle = 1$ and $\langle\phi_1|\phi_2\rangle = \langle\phi_1|\phi_3\rangle = 0$. Similarly, from the relations $\langle\phi_2|\phi_2\rangle = 1$ and $\langle\phi_2|\phi_1\rangle = \langle\phi_2|\phi_3\rangle = 0$, we obtain the probability of finding the system in $|\phi_2\rangle$:

$$P_2 = |\langle\phi_2|\psi\rangle|^2 = \left|\frac{2}{3}\langle\phi_2|\phi_2\rangle\right|^2 = \frac{4}{9}$$

As for $\langle\phi_3|\phi_3\rangle = 1$ and $\langle\phi_3|\phi_1\rangle = \langle\phi_3|\phi_2\rangle = 0$, they lead to the probability of finding the system in $|\phi_3\rangle$:

$$P_3 = |\langle\phi_3|\psi\rangle|^2 = \left|\frac{\sqrt{2}}{3}\langle\phi_3|\phi_3\rangle\right|^2 = \frac{2}{9}$$

As expected, the total probability is equal to one

$$P = P_1 + P_2 + P_3 = \frac{1}{3} + \frac{4}{9} + \frac{2}{9} = 1$$

Problem: 3.5- Give the mathematical representation of a spherical wave traveling outward from a point and evaluate its probability current density.

Solution

The mathematical representation of a spherical wave travelling outwards from a point is given by

$$\psi(r) = \frac{A}{r}\exp(ikr)$$

where A is a constant and k is the wave vector. The probability current density

$$\begin{aligned}
j &= \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right) \\
&= \frac{i\hbar}{2m}|A|^2\left[\frac{e^{ikr}}{r}\nabla\left(\frac{e^{-ikr}}{r}\right) - \frac{e^{-ikr}}{r}\nabla\left(\frac{e^{ikr}}{r}\right)\right] \\
&= \frac{i\hbar}{2m}|A|^2\left[\frac{e^{ikr}}{r}\left(-\frac{ik}{r}e^{-ikr} - \frac{e^{-ikr}}{r^2}\right) - \frac{e^{-ikr}}{r}\left(\frac{ik}{r}e^{ikr} - \frac{e^{ikr}}{r^2}\right)\right] \\
&= \frac{i\hbar}{2m}|A|^2\left(\frac{-2ik}{r^2}\right) = \frac{\hbar k}{mr^2}|A|^2
\end{aligned}$$

Chapter 4

One-Dimensional Problems

SOLVED PROBLEMS

Problem: 4.1- For an electron in a one-dimensional infinite potential well of width 1 Å, calculate the separation between the two lowest energy levels

Solution

$$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2} \qquad \because a = 1\text{Å} = 10^{-10}\text{m}$$

$$E_2 - E_1 = \frac{3\pi^2\hbar^2}{2ma^2} = \frac{3\times\pi^2\times(1.055\times10^{-34}Js)^2}{2\,(9.1\times10^{-31}\text{kg})\,10^{-20}\text{m}^2}$$

$$= 1.812\times10^{-17}\text{J} = 113.27\text{eV}$$

Problem: 4.2- An electron in a one-dimensional infinite potential well, defined by $V(x) = 0$ for $-a \le x \le a$ and $V(x) = \infty$ otherwise, goes from the $n = 4$ to the $n = 2$ level. The frequency of the emitted photon is 3.43 $\times 10^{14}$ Hz. Find the width of the box.

Solution

As we know that

$$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}$$

$$E_4 - E_2 = \frac{12\pi^2\hbar^2}{2ma^2} = 2\pi\hbar v \quad \because \quad E_4 - E_2 = 16E_1 - 4E_1$$

$$a^2 = \frac{6\pi^2\hbar^2}{2\pi m\hbar v}$$

$$a^2 = \frac{3\pi\hbar}{mv} = \frac{3\,(1.055\times10^{-34}\text{Js})\times3.14}{(9.1\times10^{-31}\text{kg})\,(3.43\times10^{14}\text{s}^{-1})}$$

$$a^2 = 79.6\times10^{-20}\text{m}^2$$

$$a = 8.92\times10^{-10}\text{m or } 2a = 17.84\times10^{-10}\text{m}$$

Problem: 4.3- The wave function of a particle confined in a box of length a is

$$\psi = \sqrt{\frac{2}{a}}\; sin(\frac{\pi x}{a})$$

Calculate the probability of finding the particle in the region $0 < x < a/2$.

Solution

The required probability is

$$\begin{aligned} P &= \frac{2}{a}\int_0^{a/2} \sin^2\frac{\pi x}{a}dx \\ &= \frac{1}{a}\int_0^{a/2}\left(1-\cos\frac{2\pi x}{a}\right)dx \\ &= \frac{1}{a}\int_0^{a/2}dx - \frac{1}{a}\int_0^{a/2}\cos\frac{2\pi x}{a}dx = \frac{1}{2} \end{aligned} \tag{4.1}$$

Problem: 4.4- Consider the ket $|\psi\rangle = \begin{pmatrix} -i \\ 3 \\ 4i \end{pmatrix}$. (a) Find $|\psi\rangle^*$ and $\langle\psi|$. (b) is $|\psi\rangle$ normalized? If not normalized it

Solution

(a) The expression of $|\psi\rangle^*$ and $\langle\psi|$ are give by

$$|\psi\rangle^* = \begin{pmatrix} -i \\ 3 \\ 4i \end{pmatrix} \quad \text{and} \quad \langle\psi| = \begin{pmatrix} i & 3 & -4i \end{pmatrix}$$

It is clear that $|\psi\rangle^* \neq \langle\psi|$.

(b) The norm of $|\psi\rangle$ is given by

$$\langle\psi|\psi\rangle = \begin{pmatrix} i & 3 & -4i \end{pmatrix} \begin{pmatrix} -i \\ 3 \\ 4i \end{pmatrix}$$
$$= (i)(-i) + (3)(3) + (-4i)(4i)$$
$$= -i^2 + 9 - 16i^2 = 26$$

Thus $|\psi\rangle$ is not normalized. However, if we multiply it with $\frac{1}{\sqrt{26}}$, it becomes normalized

$$|\psi\rangle = \frac{1}{\sqrt{26}} \begin{pmatrix} -i \\ 3 \\ 4i \end{pmatrix}$$

Problem: 4.5- Electrons with energies 1 eV are incident on a barrier 5 eV high 0.4 nm wide. Evaluate the transmission probability.

Solution

The transmission probability T is given by

$$T = e^{-2\alpha a}, \quad \alpha = \frac{\sqrt{2m\,(V_0 - E)}}{\hbar}$$

$$\alpha = \frac{\sqrt{2\,(9.1 \times 10^{-31}\text{kg})\,(4\text{eV})\,(1.6 \times 10^{-19}\text{J/eV})}}{(1.054 \times 10^{-34}\text{Js})}$$

$$\alpha = 10.24 \times 10^{9}\text{m}^{-1}$$

$$\alpha a = \left(10.24 \times 10^{9}\text{m}^{-1}\right)\left(0.4 \times 10^{-9}\text{m}\right) = 4.096$$

$$T = \frac{1}{e^{2\alpha a}} = \frac{1}{e^{8.192}} = 2.77 \times 10^{-4}$$

Chapter 5

Angular Momentum

SOLVED PROBLEMS

Problem: 5.1- Evaluate the commutator $[\hat{L}_x, \hat{L}_y]$ in the momentum representation.

Solution

$$[L_x, L_y] = [yp_z - zp_y, zp_x - xp_z] = [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z]$$
$$= yp_x [p_z, z] - 0 - 0 + p_y x [z, p_z]$$

In the momentum representation $[z, p_z] = i\hbar$

$$[L_x, L_y] = i\hbar (xp_y - yp_x) = i\hbar L_z$$

Problem: 5.2- Find the energy level of a spin $s = 3/2$ particle whose Hanmiltonian is given by

$$\hat{H} = \frac{\alpha}{\hbar^2} (\hat{S}_x^2 + \hat{S}_y^2 - 2\hat{S}_z^2) - \frac{\beta}{\hbar} \hat{S}_z$$

where α and β are constants. Are these levels degenerate?

Solution

Rewriting $\hat{H}$ in the form,

$$\hat{H} = \frac{\alpha}{\hbar^2} (\hat{S}^2 - 3\hat{S}_z^2) - \frac{\beta}{\hbar} \hat{S}_z \qquad \because \quad \hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 - \hat{S}_z^2$$

We see that $\hat{H}$ is diagonal in the $\{|s,m\rangle\}$ basis:

$$\begin{aligned}E_m = \langle s,m|\hat{H}|s,m\rangle &= \langle s,m|\frac{\alpha}{\hbar^2}(\hat{S}^2 - 3\hat{S}_z^2)|s,m\rangle - \langle s,m|\frac{\beta}{\hbar}\hat{S}_z|s,m\rangle \\ &= \frac{\alpha}{\hbar^2}\left[\hbar^2 s(s+1) - 3\hbar^2 m^2\right] - \frac{\beta}{\hbar}\hbar m \\ &= \alpha\frac{3}{2}\left(\frac{3}{2}+1\right) - 3\alpha m^2 + \beta m \\ &= \frac{15}{4}\alpha - m(3\alpha m + \beta)\end{aligned}$$

where the quantum number m takes any of the four values $m = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$. Since, E_m depends on m, the energy levels of this particle are thus four fold degenerate.

Problem: 5.3- $Y_{lm_l}(\theta,\phi)$ form a complete set of orthonormal functions of (θ,ϕ). Prove that $\sum_l \sum_{m_l=-l}^{l} |Y_{lm_l}\rangle \langle Y_{lm_l}| = 1$.

Solution

On the basis of expansion theorem, any function of θ and ϕ may be expanded in the form

$$\psi(\theta,\phi) = \sum_l \sum_{m_l} C_{lm_l} Y_{lm_l}(\theta,\phi)$$

In Dirac's notation,

$$|\psi\rangle = \sum_l \sum_{m_l} C_{lm_l} |Y_{lm_l}\rangle$$

Operating from left by $\langle Y_{l'm_l'}|$ and using the orthonormality relation

$$\langle Y_{l'm'}|Y_{lm_l}\rangle = \delta_{l'l}\delta_{m_l m_l'} \quad ; \quad C_{lm_l} = \langle Y_{lm_l}|\psi\rangle$$

Substituting this value of C_{lm_l}, we obtain

$$|\psi\rangle = \sum_l \sum_{m_l=-l}^{l} |Y_{lm_l}\rangle \langle Y_{lm_l}|\psi\rangle$$

From this relation it follows that

$$\sum_l \sum_{m_l=-l}^{l} |Y_{lm_l}\rangle \langle Y_{lm_l}| = 1$$

Problem: 5.4- In the $|jm_j\rangle$ basis formed by the eigenkets of J^2 and J_z, show that

$$\langle jm_j |J_- J_+| jm_j\rangle = (j - m_j)(j + m_j + 1)\hbar^2$$

Solution

$$\begin{aligned} J_- J_+ &= J^2 - J_z^2 - \hbar J_z \\ \langle jm_j |J_- J_+| jm_j\rangle &= \left\langle jm_j \left|J^2 - J_z^2 - hJ_z\right| jm_j\right\rangle \\ &= \left[j(j+1) - m_j^2 - m_j\right] \hbar^2 \langle jm_j|jm_j\rangle \end{aligned}$$

since $\langle jm_j|jm_j\rangle = 1$

$$\begin{aligned} \langle jm_j |J_- J_+| jm_j\rangle &= \left[j^2 - m_j^2 + j - m_j\right] \hbar^2 \\ &= [(j + m_j)(j - m_j) + (j - m_j)]\hbar^2 \\ &= (j - m_j) + (j + m_j + 1)\hbar^2 \end{aligned}$$

Problem: 5.5- For Pauli's matrices, prove that (i) $[\sigma_x, \sigma_y] = 2i\sigma_z$, (ii) $\sigma_x\sigma_y\sigma_z = i$.

Solution

(i) We have

$$\mathbf{S} = \frac{1}{2}\hbar\sigma, \quad [S_x, S_y] = i\hbar S_z$$

Substituting the values of S_x, S_y and S_z, we get

$$\begin{aligned} \left[\frac{1}{2}\hbar\sigma_x, \frac{1}{2}\hbar\sigma_y\right] &= i\hbar\frac{1}{2}\hbar\sigma_z \\ \frac{1}{4}\hbar^2 \left[\sigma_x, \sigma_y\right] &= i\hbar^2\frac{1}{2}\sigma_z \\ [\sigma_x, \sigma_y] &= 2\text{i}\sigma_z \end{aligned}$$

(ii)

$$\begin{aligned} \sigma_x\sigma_y\sigma_z &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} = i \end{aligned}$$

Chapter 6

Three-Dimensional Problems

SOLVED PROBLEMS

Problem: 6.1- For the ground state of the hydrogen atom, evaluate the expectation value of the radius vector r of the electron.

Solution

The wave function of the ground state is given by

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} \exp\left(\frac{-r}{a_0}\right)$$

$$\langle r \rangle = \int \psi_{100}^{*} r \psi_{100} d\tau = \frac{1}{\pi a_0^3} \int_0^{\infty} r^3 \exp\left(-\frac{2r}{a_0}\right) dr \int_0^{\pi 2\pi} \int_0^{\pi 2\pi} \sin\theta d\theta d\phi$$

Problem: 6.2- What is the probability of finding the ls-electron of the hydrogen atom at distance (i) 0.5 $a_\circ$, (ii) 0.9 $a_\circ$ (iii) $a_\circ$ (iv) 1.2 $a_\circ$ from the nucleus? Comment on the result.

Solution

The radial probability density $P_{nl}(r) = |R_{nl}|^2 r^2$. Then

$$R_{10} = \frac{2}{a_0^{3/2}} \exp\left(-\frac{r}{a_0}\right), \quad P_{10}(r) = \frac{4r^2}{a_0^3} \exp\left(-\frac{2r}{a_0}\right)$$

(i) $P_{10}(0.5a_0) = \frac{e^{-1}}{a_0} = \frac{0.37}{a_0}$

(ii) $P_{10}(0.9a_0) = \frac{4(0.9)^2}{a_0}e^{-1.8} = \frac{0.536}{a_0}$

(iii) $P_{10}(a_0) = \frac{4e^{-2}}{a_0} = \frac{0.541}{a_0}$

(iv) $P_{10}(1.2a_0) = \frac{4(1.2)^2}{a_0} = \frac{0.523}{a_0}$

$P_{10}(r)$ increases as r increases from 0 to a_0 and then decreases, indicating a maximum at $r = a_0$. This is in conformity with Bohr's picture of the hydrogen atom.

Problem: 6.3- A positron and an electron form a short lived atom called positronium before the two annihilate to produce gamma rays. Calculate, in electron volts, the ground state energy of positronium.

Solution

The positron has a charge $+e$ and mass equal to the electron mass. The mass μ in the energy expression of hydrogen atom is the reduced mass which, for the positronium atom, is

$$\frac{m_{\mathrm{e}} \cdot m_{\mathrm{e}}}{2m_{\mathrm{e}}} = \frac{m_{\mathrm{e}}}{2}$$

where m_{e} is the electron mass. Hence the energy of the positronium atom is half the energy of hydrogen atom.

$$E_n = -\frac{k^2 m_e e^4}{4\hbar^2 n^2}, \quad n = 1, 2, 3, \ldots$$

Then the ground state energy is

$$-\frac{13.6}{2}\mathrm{eV} = -6.8\mathrm{eV}$$

Problem: 6.4- A quark having one-third the mass of a proton is confined in a cubical box of side 1.8×10^{-15} m. Find the excitation energy in MeV from the first excited state to the second excited state.

Solution

As we know that

$$E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2ma^2}\left(n_1^2 + n_2^2 + n_3^2\right)$$

First excited state: $E_{211} = E_{121} = E_{112} = \frac{6\pi^2\hbar^2}{2ma^2}$

Second excited state: $E'_{221} = E_{212} = E_{122} = \frac{9\pi^2\hbar^2}{2ma^2}$

$$m = \frac{1.67262 \times 10^{-27}\text{kg}}{3} = 0.55754 \times 10^{-27}\text{kg}$$

$$\begin{aligned}\Delta E &= \frac{3\pi^2\hbar^2}{2ma^2} \\ &= \frac{3\pi^2 \left(1.05 \times 10^{-34}\text{Js}\right)^2}{2\left(0.55754 \times 10^{-27}\text{kg}\right)\left(1.8 \times 10^{-15}\text{m}\right)^2} \\ &= 9.0435 \times 10^{-11}\text{J} = \frac{9.0435 \times 10^{-11}\text{J}}{1.6 \times 10^{-19}\text{J/eV}} \\ &= 565.2\text{MeV}\end{aligned}$$

Problem: 6.5- An electron of mass m and charge $-e$ moves in a region where a uniform magnetic field $\vec{B} = \vec{\nabla} \times \vec{A}$ exists in the z-direction. Write the Hamiltonian operator of the system.

Solution

Given $\vec{B} = \vec{\nabla} \times \vec{A}$. We have

$$\vec{B} = \hat{i}\left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right) + \hat{j}\left(\frac{\partial A_k}{\partial z} - \frac{\partial A_z}{\partial x}\right) + \hat{k}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)$$

since the field is in the z-direction,

$$\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} = 0$$

$$\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} = 0$$

$$\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} = 0$$

On the basis of these equations, we can take

$$A_x = A_z = 0, \quad A_y = Bx \text{ or } A = Bx\hat{j}$$

The Hamiltonian operator

$$
\begin{aligned}
H &= \frac{1}{2m}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2, \quad p = -i\hbar\nabla \\
&= \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2 + \frac{e^2}{c^2}A^2 + \frac{e}{c}\vec{p}\cdot\vec{A} + \frac{e}{c}\vec{A}\cdot\vec{p}\right) \\
&= \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2 + \frac{e^2B^2x^2}{c^2} + \frac{e}{c}p_yBx + \frac{e}{c}Bxp_y\right) \\
&= \frac{1}{2m}\left[p_x^2 + \left(p_y + \frac{eBx}{c}\right)^2 + p_z^2\right]
\end{aligned}
$$

where p_x, p_y, p_z are operators.


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