



# ALAGAPPA UNIVERSITY

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KARAIKUDI – 630 003

**DIRECTORATE OF DISTANCE EDUCATION**

**M.Sc. (PHYSICS)**

**III – SEMESTER**

**34532**

**QUANTUM MECHANICS - II**

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# BLOCK I: THEORY OF ANGULAR MOMENTUM

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## UNIT-I ANGULAR MOMENTUM

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### Structure

- 1.1 Angular momentum
- 1.2 Commutation rules for angular momentum
  - 1.2.1 Allowed values of j and m
- 1.3 Check your progress
- 1.4 Unit – End Exercises
- 1.5 Answer to Check your progress
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### 1.1 ANGULAR MOMENTUM

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In Classical mechanics, the angular momentum  $L$  of a particle is defined as the vector product of its position vector  $r$  and the linear momentum  $p$ ,

$$L = r \times p \rightarrow (1)$$

The three rectangular components of  $L$  are

$$\left. \begin{aligned} L_x &= yp_z - zp_y \\ L_y &= zp_x - xp_z \\ L_z &= xp_y - yp_x \end{aligned} \right\} \rightarrow (2)$$

Where  $x, y, z$  are the components of  $r$  and  $p_x, p_y, p_z$  are the components of  $p$  and can be replaced by their quantum mechanical equivalents

$$p_x = -i\hbar \frac{\partial}{\partial x}, p_y = -i\hbar \frac{\partial}{\partial y}, p_z = -i\hbar \frac{\partial}{\partial z} \rightarrow (3)$$

$$\left. \begin{aligned} \therefore L_x &= -i\hbar \left[ y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right] \\ L_y &= -i\hbar \left[ z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right] \\ L_z &= -i\hbar \left[ x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right] \end{aligned} \right\} \text{ and } \rightarrow (4)$$

## NOTES

In terms of spherical coordinates, the operator for the components of angular momentum and  $L^2$  are given by,

$$\left. \begin{aligned} L_x &= i\hbar \left( \sin\theta \frac{\partial}{\partial\theta} + \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right) \\ L_y &= i\hbar \left( -\cos\theta \frac{\partial}{\partial\theta} + \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right) \\ L_z &= -i\hbar \frac{\partial}{\partial\phi} \text{ and} \end{aligned} \right\} \rightarrow (5)$$

$$L^2 = -\hbar^2 \left[ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left( \sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

## 1.2 COMMUTATION RULES FOR ANGULAR MOMENTUM

The commutation relations of the components of L can be easily be obtained in Cartesian coordinates,

$$[L_x, L_y] = [yp_z - zp_y, zp_x - xp_z]$$

$$[L_x, L_y] = [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z] \rightarrow (6)$$

The values of  $p_x, p_y$  and  $p_z$  follows equation (3). In the II & III term of equation (6), all the variables involved, commute with each other and hence both the term vanishes. Since y and  $p_x$  commute with z and  $p_z$ ,

$$[yp_z, zp_x] = yp_x [p_z, z] = -i \hbar yp_x \rightarrow (7)$$

Based on similar arguments, we get

$$[zp_y, xp_z] = p_y x [z, p_z] = i \hbar xp_y \rightarrow (8)$$

Hence,

$$[L_x, L_y] = i \hbar (xp_y - yp_x) = i \hbar L_z \rightarrow (9)$$

Similarly

$$[L_y, L_z] = i \hbar L_x \text{ and } [L_z, L_x] = i \hbar L_y \rightarrow (10)$$

(i.e.) the components of angular momentum do not commute with one another and therefore they are not measurable simultaneously. In other words, if the system is in an eigenstate of one angular momentum component, it will not be simultaneously in an eigenstate of either of the others

The above commutation relations can be symbolically represented as,

$$\mathbf{L} \times \mathbf{L} = i \hbar \mathbf{L} \rightarrow (11)$$

Let us consider the commutator of  $L^2$ ;

$$\begin{aligned}
 [L^2, L_x] &= [L_x^2, L_x] + [L_y^2, L_x] + [L_z^2, L_x] \\
 &= 0 + L_y[L_y, L_x] + [L_y, L_x]L_y + L_z[L_z, L_x] + [L_z, L_x]L_z \\
 &= L_y(-i\hbar L_z) + (-i\hbar L_z)L_y + i\hbar L_z L_y + i\hbar L_y L_z \\
 &\therefore [L^2, L_x] = 0 \rightarrow (12)
 \end{aligned}$$

Similarly,

$$[L^2, L_y] = [L^2, L_z] = 0 \rightarrow (13)$$

which means the square of angular momentum commutes with its components. (i.e.) the angular momentum can be measured simultaneously with any one component.

The commutation relations (9), (10), (12) & (13) form the foundation for the theory of angular momentum.

Let us consider the operators  $L_+$  and  $L_-$  which are defined by

$$L_+ = L_x + iL_y \text{ and } L_- = L_x - iL_y$$

The operator  $L_+$  is called the raising operator and  $L_-$  is the lowering operator.

These two operators will commute with  $L^2$  from their definition.

$$\therefore [L^2, L_+] = 0 \text{ \& } [L^2, L_-] = 0$$

$$\begin{aligned}
 \text{And } [L_z, L_+] &= [L_z, L_x] + i[L_z, L_y] \\
 &= i\hbar L_y + \hbar L_x \\
 &= \hbar L_+
 \end{aligned}$$

Similarly,

$$\left. \begin{aligned}
 [L_z, L_-] &= -\hbar L_- \\
 [L_x, L_+] &= -\hbar L_z \\
 [L_x, L_-] &= \hbar L_z \\
 [L_y, L_+] &= -i\hbar L_z \\
 [L_y, L_-] &= i\hbar L_z
 \end{aligned} \right\} \rightarrow (14)$$

$$[L_+, L_-] = 2\hbar L_z \rightarrow (15)$$

And

## NOTES

$$\left. \begin{aligned} L_+L_- &= L^2 - L_z^2 + \hbar L_z \\ L_-L_+ &= L^2 - L_z^2 - \hbar L_z \end{aligned} \right\} \rightarrow (16)$$

### 1.2.1 Allowed values of j and m

It is possible to find simultaneously the eigen values of  $J^2$  and one of the components say  $J_z$ , of the angular momentum operator. Denoting the eigen functions by  $\varphi_{jm}$ , where j and m are the two quantum numbers which define their eigen values, we can write

$$J^2\varphi_{jm} = n_j\hbar^2\varphi_{jm}; J_z\varphi_{jm} = m\hbar\varphi_{jm} \rightarrow (1)$$

The quantum numbers j and m are known as the angular momentum quantum number and magnetic quantum number. Since,  $J_z$  does not commute with  $J_x$  and  $J_y$ ,  $\varphi_{jm}$  cannot be an eigen function of  $J_x$  and  $J_y$  operators.

Since the ladder operator steps up or steps down m by unity, it follows that m can take a spectrum of values in steps of unity.

Further,

$$(J_x^2 + J_y^2)\varphi_{jm} = (J^2 - J_z^2)\varphi_{jm} = (n_j - m^2)\hbar^2\varphi_{jm} \rightarrow (2)$$

$\because J_x$  and  $J_y$  are hermitian operators, the eigen value of the sum of the squares of hermitian operators should be a positive quantity,

$$n_j^2 - m^2 \geq 0$$

This means that the values that m can take for a given value of j are bounded. If  $m_1$  and  $m_2$  are the lowest and highest values of m respectively then,

$$m = m_1, m_1+1, m_1+2, \dots, m_2-1, m_2.$$

It follows that,

$$J_-\varphi_{jm_1} = 0 \rightarrow (3a) \quad J_+\varphi_{jm_2} = 0 \rightarrow (3b)$$

Since there cannot be a m value less than  $m_1$  or greater than  $m_2$ . Multiplying (3a) by  $J_+$  on the left and (3b) by  $J_-$  on the left we get

$$\left. \begin{aligned} J_+J_-\varphi_{jm_1} &= 0 \\ J_-J_+\varphi_{jm_2} &= 0 \end{aligned} \right\} \rightarrow (4)$$

$$\begin{aligned} \because J_+J_- &= (J_x + iJ_y)(J_x - iJ_y) = J_x^2 + J_y^2 - i[J_x, J_y] \\ &= J^2 - J_z^2 + \hbar J_z = J^2 - J_z(J_z - \hbar) \rightarrow (5) \end{aligned}$$

$$\& J_-J_+ = (J_x - iJ_y)(J_x + iJ_y) = J_x^2 + J_y^2 + i[J_x, J_y]$$

$$= J^2 - J_z^2 - \hbar J_z = J^2 - J_z(J_z + \hbar) \rightarrow (6)$$

Equation (4) becomes [using (1)]

$$\left. \begin{aligned} \{n_j - m_1(m_1 - 1)\}\hbar^2 = 0 \\ \{n_j - m_2(m_2 + 1)\}\hbar^2 = 0 \end{aligned} \right\} \rightarrow (7)$$

$\therefore$ , we deduce that

$$m_1(m_1 - 1) = m_2(m_2 + 1)$$

Equivalently  $(m_1 + m_2)(m_2 - m_1 + 1) = 0$

$\therefore m_2$  is the highest value and  $m_1$ , the lowest value that  $m$  can take,  $(m_2 - m_1 + 1)$  should be a positive quantity and so, for the condition to be satisfied; the only possibility is that  $(m_1 + m_2)$  should be zero,

$$(or) m_1 = -m_2 \rightarrow (8)$$

Equation (7) indicates that  $m_1$  and  $m_2$  should depend upon the quantum number  $j$ . If one chooses  $m_2 = j$ , then the spectrum of values that the quantum number  $m$  can take for a given value of  $j$  is

$$-j, -j+1, -j+2, \dots, j-2, j-1, j \rightarrow (9)$$

The series (9) with the lowest value  $-j$  and the highest value  $+j$  is possible only if  $j$  is an integer or half-integer. For each value of  $j$ , there are  $2j+1$  values for  $m$ .

From equation (7), we obtain

$$n_j = j(j+1) \rightarrow (10)$$

The admissibility of half-integral values for  $j$  validates the spin  $\frac{1}{2}\hbar$  of the electron.

### 1.3 CHECK YOUR PROGRESS

1. List some of the commutation relations of angular momentum.
2. Define the commutator of two operators.
3. What are raising and lowering operators.
4. How does the value of  $m$  depend on that “ $j$ ” values.

#### Let us sum up

In this unit the importance of the interesting property of physical systems in both classical and quantum physics namely angular momentum is explained. Also the allowed values of quantum numbers

$j$  and  $m$  which are used to represent the angular momentum operator in matrix form are clearly explained.

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## 1.4 UNIT-END EXERCISES

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1. Show that  $[L_y, L_z] = i\hbar L_x$
2. Show that  $[L^2, L_+] = 0$ .

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## 1.5 ANSWERS TO CHECK YOUR PROGRESS

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### NOTES

$$1. [L_x, L_y] = i\hbar(xp_y - yp_x) = i\hbar L_z$$

$$[L_y, L_z] = i\hbar L_x \text{ and } [L_z, L_x] = i\hbar L_y$$

$$\therefore [L^2, L_x] = 0$$

$$[L^2, L_y] = [L^2, L_z] = 0$$

$$[L_z, L_-] = -\hbar L_-$$

$$[L_x, L_+] = -\hbar L_z$$

$$[L_x, L_-] = \hbar L_z$$

$$[L_y, L_+] = -i\hbar L_z$$

$$[L_y, L_-] = i\hbar L_z$$

$$[L_+, L_-] = 2\hbar L_z$$

2. If A and B are two operators, the commutation relation is given by  $[A, B] = AB - BA$ .

3.  $L_+ = L_x + iL_y$  and  $L_- = L_x - iL_y$  are the raising and lowering operators respectively.

4. For each value of  $j$ , there are  $2j+1$  values for  $m$ .

### Answers to Unit-End Exercises

$$1. [L_y, L_z] = [(zp_z - xp_z), (xp_y - yp_x)] \\ = [zp_x, xp_y] - [zp_x, yp_x] - [xp_z, xp_y] + [xp_z, yp_x]$$

$$\text{Now } [zp_x, xp_y] = zp_y[p_x, x] = -i\hbar zp_y$$

$$\text{Similarly, } [xp_z, yp_x] = p_z y[x, p_z] = i\hbar yp_z$$

$$\therefore [L_y, L_z] = -i\hbar zp_y - 0 - 0 + i\hbar yp_z \\ = i\hbar(yp_z - zp_y) = i\hbar L_x$$

$$2. [L^2, L_+] = [L_x^2 + L_y^2 + L_z^2, L_+] \\ = [L_x^2, L_+] + [L_y^2, L_+] + [L_z^2, L_+]$$



$$\begin{aligned}
&=L_x[L_x,L_z]+[L_x,L_z]L_x+L_y[L_y,L_z]+[L_y,L_z]L_y \\
&=L_x(-i\hbar L_y)+(-i\hbar L_y)L_x+L_y(i\hbar L_x)+(i\hbar L_x)L_y \\
&=-i\hbar L_xL_y+i\hbar L_xL_y+i\hbar L_yL_x-i\hbar L_yL_x \\
&=0.
\end{aligned}$$

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## 1.6 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, II<sup>nd</sup> edition McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldas- PHI learning Private limited, New Delhi 2008.
3. Foundation of Quantum Mechanics – A.B. Gupta, Books and Allied (P) Ltd., Kolkata, 2015.
4. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.

## NOTES

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# UNIT-II MATRIX REPRESENTATION OF ANGULAR MOMENTUM

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## NOTES

### Structure

#### 2.1 Angular momentum matrices

##### 2.1.1 Matrix for $J^2$

##### 2.1.2 Matrix for $J_z$

##### 2.1.3 Matrices for $J_x, J_y, J_x$ and $J_y$

#### 2.2 Spin angular momentum

#### 2.3 Check your progress

#### 2.4 Unit – End Exercises

#### 2.5 Answer to Check your progress

#### 2.6 Suggested Readings

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### 2.1 ANGULAR MOMENTUM MATRICES

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The states  $|jm\rangle$  form a complete orthonormal set and they can be used as a basis for the matrix representation of an angular momentum. In this representation a function  $F$  of the angular momentum components can be represented by a matrix with elements  $\langle j'm'|F|jm\rangle$ . The rows of the matrix will be labelled by the  $j'$  and  $m'$  values and the column by the  $j$  and  $m$  values.

$$\text{We know that, } J_z = m\hbar \rightarrow (1)$$

$$J^2 = j(j+1)\hbar^2 \rightarrow (2)$$

Where ' $m$ ' varies from  $-j$  to  $+j$  and has  $(2j+1)$  values with  $j=0, 1/2, 3/2, \dots$ . Hence the dimensions of these diagonal matrices will be  $(2j+1)$ . The explicit forms of angular momentum matrices are shown below:

$$J_z = \hbar \begin{bmatrix} j & 0 & \dots & \dots & 0 \\ 0 & j-1 & \dots & \dots & 0 \\ 0 & 0 & j-2 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \dots & -j \end{bmatrix} \rightarrow (3)$$

$$J^2 = \hbar^2 \begin{bmatrix} j(j+1) & \dots & \dots & \dots & 0 \\ 0 & j(j+1) & \dots & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \dots & j(j+1) \end{bmatrix} \rightarrow (4)$$

As  $J^2$  commutes with  $J_z$ , the matrices for  $J^2$  and  $J_z$ , will be diagonal. In that representation,  $J_x$  and  $J_y$  will not be diagonal since,  $J_z$  does not commute with  $J_x$  and  $J_y$ . Denoting the simultaneous eigen vector of  $J^2$  and  $J_z$  by  $|jm\rangle$  we get from (1) and (2);

$$J^2 |jm\rangle = j(j+1)\hbar^2 |jm\rangle \rightarrow (5)$$

$$\text{and } J_z |jm\rangle = m\hbar |jm\rangle$$

Multiplication of the equation(5) from left by  $\langle j'm'|$  gives,

$$\langle j'm'|J^2|jm\rangle = j(j+1)\hbar^2 \delta_{jj'} \delta_{mm'} \rightarrow (6)$$

$$\text{And, } \langle j'm'|J_z|jm\rangle = m\hbar \delta_{jj'} \delta_{mm'} \rightarrow (7)$$

The presence of the factor  $\delta_{jj'}$ , and  $\delta_{mm'}$ , indicates that the matrices are diagonal. The explicit form of  $J^2$  and  $J_z$  with infinite dimension is given below;

### 2.1.1 Matrix for $J^2$

|                     |     |  |  |       |
|---------------------|-----|--|--|-------|
| J<br>m<br>j'<br>m'  | 0   | 1/2  | 1  | ..... |
|                     | 0   | 1/2    -1/2  | 1    0    -1   | ..... |
| 0    0              | 0   | (0)  | (0)  | ..... |
| 1/2 {<br>1/2<br>1/2 | (0) | $\begin{bmatrix} 3\hbar^2/4 & 0 \\ 0 & 3\hbar^2/4 \end{bmatrix}$ | (0)  | ..... |
| 1 {<br>0<br>-1      | (0) | (0)  | $\begin{bmatrix} 2\hbar^2 & 0 & 0 \\ 0 & 2\hbar^2 & 0 \\ 0 & 0 & 2\hbar^2 \end{bmatrix}$ | ..... |
| ⋮                   | ⋮   | ⋮  | ⋮  | ⋮     |

(9)

For  $j=0$ ,  $J^2$  and  $J_z$  are represented by null matrices of unit rank (0).

For  $j=1/2$ ,  $m=1/2, -1/2$  and dimension of  $J^2$  and  $J_z$  matrices  $=2j + 1 = 2$

$$J^2 = \hbar^2 j(j+1) = \frac{3\hbar^2}{4}, \text{ Then } J^2 = \begin{bmatrix} \frac{3\hbar^2}{4} & 0 \\ 0 & \frac{3\hbar^2}{4} \end{bmatrix}$$

$$\text{Similarly, } J_z = \begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix}$$

### 2.1.2 Matrix for $J_z$

|                      |     |   |  |       |
|----------------------|-----|---|--|-------|
| j<br>m               | 0   | 1/2   | 1  | ..... |
| j'<br>m'             | 0   | 1/2    -1/2   | 1    0    -1   | ..... |
| 0    0               | (0) | (0)   | (0)  | ..... |
| 1/2 {<br>1/2<br>-1/2 | (0) | $\begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix}$ | (0)  | ..... |
| 1 {<br>1<br>0<br>-1  | (0) | (0)   | $\begin{bmatrix} 1\hbar & 0 & 0 \\ 0 & \hbar & 0 \\ 0 & 0 & -1\hbar \end{bmatrix}$ | ..... |
| ⋮                    | ⋮   | ⋮   | ⋮  | ⋮     |

→(10)

### NOTES

This shows that  $J^2$  and  $J_z$  matrices contain only principal diagonal.

### 2.1.3 Matrices for $J_+, J_-, J_x$ and $J_y$

$$J_+ = \hbar\sqrt{(j-m)(j+m+1)} \rightarrow (11) \text{ and}$$

$$J_- = \hbar\sqrt{(j+m)(j-m+1)} \rightarrow (12)$$

$$\text{Also, } J_x = 1/2(J_+ + J_-) \rightarrow (13)$$

$$\text{and } J_y = 1/2i(J_+ - J_-) \rightarrow (14)$$

For  $j=0$ ,

$$J_+ = 0, J_- = 0, J_x = 0, J_y = 0 \rightarrow (15)$$

For  $j=1/2$ ,

$$J_+ = \hbar \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, J_- = \hbar \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \rightarrow (16)$$

$$J_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, J_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\text{For } j=1, J_+ = \hbar \begin{bmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix}, J_- = \hbar \begin{bmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{bmatrix} \rightarrow (17)$$

$$J_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, J_y = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix} \rightarrow (18)$$

Matrix for  $\frac{2J_x}{\hbar}$

|   |          |   |   |          |
|---|----------|---|---|----------|
| $j \backslash m$  | 0        | $\begin{matrix} 1/2 \\ \hline 1/2 & -1/2 \end{matrix}$        | $\begin{matrix} 1 \\ \hline 1 & 0 & -1 \end{matrix}$  | .....    |
| $j' \backslash m'$  | 0        | $\begin{matrix} 1/2 & -1/2 \\ \hline 1/2 & -1/2 \end{matrix}$ | $\begin{matrix} 1 & 0 & -1 \\ \hline 1 & 0 & -1 \end{matrix}$                                   | .....    |
| 0 0   | (0)      | (0)   | (0)   | .....    |
| $1/2 \left\{ \begin{matrix} 1/2 \\ -1/2 \end{matrix} \right.$ | (0)      | $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$                | (0)   | .....    |
| $1 \left\{ \begin{matrix} 1 \\ 0 \\ -1 \end{matrix} \right.$  | (0)      | (0)   | $\begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix}$ | .....    |
| $\vdots$  | $\vdots$ | $\vdots$  | $\vdots$  | $\vdots$ |

NOTES

Matrix for  $\frac{2J_y}{\hbar}$

|   |          |   |   |          |
|---|----------|---|---|----------|
| $j \backslash m$  | 0        | $\begin{matrix} 1/2 \\ \hline 1/2 & -1/2 \end{matrix}$        | $\begin{matrix} 1 \\ \hline 1 & 0 & -1 \end{matrix}$  | .....    |
| $j' \backslash m'$  | 0        | $\begin{matrix} 1/2 & -1/2 \\ \hline 1/2 & -1/2 \end{matrix}$ | $\begin{matrix} 1 & 0 & -1 \\ \hline 1 & 0 & -1 \end{matrix}$   | .....    |
| 0 0   | (0)      | (0)   | (0)   | .....    |
| $1/2 \left\{ \begin{matrix} 1/2 \\ -1/2 \end{matrix} \right.$ | (0)      | $\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$               | (0)   | .....    |
| $1 \left\{ \begin{matrix} 1 \\ 0 \\ -1 \end{matrix} \right.$  | (0)      | (0)   | $\begin{bmatrix} 0 & -i\sqrt{2} & 0 \\ i\sqrt{2} & 0 & -i\sqrt{2} \\ 0 & i\sqrt{2} & 0 \end{bmatrix}$ | .....    |
| $\vdots$  | $\vdots$ | $\vdots$  | $\vdots$  | $\vdots$ |

## 2.2 SPIN ANGULAR MOMENTUM

Accounting for the multiplicity of the atomic states it is understood that an electron possesses an intrinsic angular momentum called spin angular momentum (S) whose projection on Z-axis can have the values.

$$S_z = m_s \hbar, m_s = \pm 1/2$$

Assuming that all the stable and unstable particles to have spin angular momentum S, the components  $S_x, S_y$  and  $S_z$  are expected to obey commutation relations of  $J_x, J_y$  and  $J_z$  and  $S^2$  and  $S_z$  to have the

NOTES

eigen values  $s(s + 1)\hbar^2$  and  $m_s\hbar$ ,  $m_s = -s, -s + 1, \dots, s$  respectively.

Therefore, the matrices representing  $S_x, S_y$  and  $S_z$  can be obtained from  $J_x, J_y$  and  $J_z$  corresponding to  $j=1/2$ ,

$$\text{That is, } S_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; S_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, S_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

A matrix  $\sigma$  is defined as

$$S = \frac{1}{2}\sigma \text{ Where,}$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

and are called as Pauli's spin matrices. From the definition it is obvious that their eigen values are  $\pm 1$ .

The matrices satisfy the following relations;

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$$

$$\sigma_x\sigma_y = i\sigma_z$$

$$\sigma_y\sigma_z = i\sigma_x$$

$$\sigma_z\sigma_x = i\sigma_y$$

$$\sigma_x\sigma_y + \sigma_y\sigma_x = \sigma_y\sigma_z + \sigma_z\sigma_y = \sigma_z\sigma_x + \sigma_x\sigma_z = 0$$

Including spin, the system has now four degrees of freedom; three position co-ordinates and one corresponds to the spin. Therefore, the electron waveform can be written as  $\Psi(r, m_s)$  or  $\Psi(r, S_z)$ .

When the interaction between the spin and space parts is negligible.

$$\Psi(r, m_s) = \Phi(r)\chi(m_s)$$

Where  $\Phi(r)$  represents the part that depends on the position coordinates and  $\chi(m_s)$ , the part that depends on the spin coordinates. Since the matrices  $S_x, S_y$  and  $S_z$  are  $2 \times 2$ , the eigenvectors must be column vectors with two components.

The eigenvalue equation for  $S_z$  with eigen value  $\frac{\hbar}{2}$  is

$$\frac{1}{2}\hbar \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

(or)

$$\begin{bmatrix} a_1 \\ -a_2 \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

i.e.,  $a_2 = 0$ . The normalization condition gives

$$|a_1|^2 = 1 \quad (\text{or}) \quad a_1 = 1$$

The eigen vector of the matrix  $S_z$  corresponding to the eigen value  $\hbar/2$  is then

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and similarly for  $-\hbar/2$  it is  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

These eigen vectors are denoted by  $\alpha$  and  $\beta$ , they are usually called spin-up and spin-down states respectively.

$$\alpha = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \beta = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

The two components Eigen vectors are also called spinors. Eigen vectors of  $S_x$  and  $S_y$  can also be found in the same way.

## NOTES

**NOTES**

| Spin components | Spin matrix   | Eigen value   | Eigen vectors   |
|-----------------|---|---|---|
| $S_x$           | $\frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$  | $\begin{cases} \frac{\hbar}{2} \\ -\frac{\hbar}{2} \end{cases}$ | $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$<br>$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ |
| $S_y$           | $\frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ | $\begin{cases} \frac{\hbar}{2} \\ -\frac{\hbar}{2} \end{cases}$ | $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}$<br>$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix}$ |
| $S_z$           | $\frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ | $\begin{cases} \frac{\hbar}{2} \\ -\frac{\hbar}{2} \end{cases}$ | $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$<br>$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$  |

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**2.3 CHECK YOUR PROGRESS**

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1. What are spinors?
2. Write down Pauli's spin matrices.
3. Write the matrix form of angular momentum operator.

**Let us sum up**

The angular momentum operators are designed based on their eigen value equations. The contributions of intrinsic angular momentum namely spin to the orbital angular momentum and Pauli's matrices are clearly explained. Some properties of spin matrices are also listed.

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**2.4 UNIT-END EXERCISES**

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1. List some properties of Pauli matrices.
2. Show that the eigen values of  $L_2$  are  $m\hbar$ .

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**2.5 ANSWERS TO CHECK YOUR PROGRESS**

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1.  $\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ ,  $\beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ . These two component eigen vector are called spinors.

2.  $S_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ ;  $S_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ ,  $S_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$



$$3. J_z = \hbar \begin{bmatrix} j & 0 & \dots & \dots & 0 \\ 0 & j-1 & \dots & \dots & 0 \\ 0 & 0 & j-2 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \dots & -j \end{bmatrix}$$

$$J^2 = \hbar^2 \begin{bmatrix} j(j+1) & \dots & \dots & \dots & 0 \\ 0 & j(j+1) & \dots & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \dots & j(j+1) \end{bmatrix}$$

## NOTES

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### 2.6 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, II<sup>nd</sup> edition McGraw hill, New Delhi 2010.
2. Quantum Mechanics - G. Aruldas- PHI learning Private limited, New Delhi 2008.
3. Foundation of Quantum Mechanics – A.B. Gupta, Books and Allied (P) Ltd., Kolkata, 2015.
4. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.

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## UNIT-III ADDITION OF ANGULAR MOMENTUM

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### Structure

3.1 Addition of angular momenta of two non- interacting Systems

3.2 Clebsch - Gordan coefficients

3.2.1 Recursion relations

3.2.2 CG coefficients for a system having  $j_1=1/2$  and  $j_2=1/2$

3.3 Check your progress

3.4 Unit – End Exercises

3.5 Answer to Check your progress

3.6 Suggested Readings

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### 3.1 ADDITION OF ANGULAR MOMENTA OF TWO NON- INTERACTING SYSTEMS

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Consider two non-interacting systems having angular momenta  $J_1$  and  $J_2$  and eigenkets  $|j_1 m_1 \rangle$  and  $|j_2 m_2 \rangle$  respectively. (ie)

$$J_1^2 |j_1 m_1 \rangle = j_1(j_1 + 1)\hbar^2 |j_1 m_1 \rangle \rightarrow (1) \text{ (a)}$$

$$J_{1z} |j_1 m_1 \rangle = m_1 \hbar |j_1 m_1 \rangle \rightarrow (1) \text{ (b)}$$

and

$$J_2^2 |j_2 m_2 \rangle = j_2(j_2 + 1)\hbar^2 |j_2 m_2 \rangle \rightarrow (2) \text{ (a)}$$

$$J_{2z} |j_2 m_2 \rangle = m_2 \hbar |j_2 m_2 \rangle \rightarrow (2) \text{ (b)}$$

Where,  $m_1 = j_1, j_1 - 1, \dots, -j_1$  and  $m_2 = j_2, j_2 - 1, \dots, -j_2$

Since the two systems are non-interacting,

$$[J_1, J_2] = 0 \text{ and } [J_1^2, J_2^2] = 0$$

and therefore the operators  $J_1^2, J_{1z}, J_2^2,$  and  $J_{2z}$  form a complete set with simultaneous eigenkets  $|j_1 m_1, j_2 m_2 \rangle$  which is a product of  $|j_1 m_1 \rangle$  and  $|j_2 m_2 \rangle$ . For a given values of  $j_1$  and  $j_2$

$$|j_1 m_1, j_2 m_2 \rangle = |j_1 m_1 \rangle |j_2 m_2 \rangle = |m_1 m_2 \rangle.$$

Since  $m_1$  and  $m_2$  can have  $(2j_1 + 1)$  and  $(2j_2 + 1)$  orientations, the subspace with definite values of  $j_1$  and  $j_2$  will have  $(2j_1 + 1)(2j_2 + 1)$  dimensions.

### 3.2 CLEBSCH - GORDAN COEFFICIENTS

For the total angular momentum vector

$$J = J_1 + J_2, J \times J = i\hbar j \rightarrow (1)$$

Also, it follows that

$$[J^2, J_z] = 0, [J^2, J_1^2] = [J^2, J_2^2] = 0 \rightarrow (2)$$

The orthogonal eigenkets of  $J^2$  and  $J_z$  be  $|jm\rangle$ . Since  $J^2$  commutes with  $J_z, J_1^2$  and  $J_2^2$  they form another complete set and their simultaneous eigenkets will be  $|j_1 j_2 j m\rangle$

We can express the unknown kets  $|jm\rangle$  in terms of known kets  $|m_1 m_2\rangle$  as a linear combination of  $|m_1 m_2\rangle$ .

$$(ie) |jm\rangle = \sum_{m_1 m_2} C_{j m m_1 m_2} |m_1 m_2\rangle \rightarrow (3)$$

The coefficients of this linear combination are called Clebsch-Gordan coefficients

Multiplying eqn(3) with the bra  $\langle m_1 m_2 |$  we get

$$\langle m_1 m_2 | jm \rangle = C_{j m m_1 m_2} \rightarrow (4)$$

Sub (4) in (3),

$$|jm\rangle = \sum_{m_1, m_2} |m_1 m_2\rangle \langle m_1 m_2 | jm \rangle \rightarrow (5)$$

As the coefficients  $\langle m_1 m_2 | jm \rangle$  relates two orthonormal bases, they form a unitary matrix.  $m_1 m_2$  label the rows of the matrix and  $jm$  label the columns.

The inverse of eqn(5) will be,

$$|m_1 m_2\rangle = \langle jm | m_1 m_2 \rangle |jm\rangle \rightarrow (6)$$

Where the summation over  $m$  is from  $-j$  to  $+j$  and  $j$  is from  $|j_1 - j_2|$  to  $j_1 + j_2$ . The unitary character of CG coefficients is expressed by the equation

$$\sum_{jm} \langle m_1 m_2 | jm \rangle \langle jm | m_1' m_2' \rangle = \langle m_1 m_2 | m_1' m_2' \rangle$$

$$= \delta_{m_1 m_1'} \delta_{m_2 m_2'} \rightarrow (7)(a) \text{ and}$$

### NOTES

$$\sum_{m_1, m_2} \langle jm | m_1 m_2 \rangle \langle m_1 m_2 | j' m' \rangle = \langle jm | j' m' \rangle$$

$$= \delta_{jj'} \delta_{mm'} \rightarrow (7)(b)$$

Where  $\langle jm | m_1 m_2 \rangle = \langle m_1 m_2 | jm \rangle^*$

Operating eqn(5) from left by  $J_z$  we have,

**NOTES**

$$J_z |jm \rangle = \sum_{m_1, m_2} (J_{1z} + J_{2z}) |m_1 m_2 \rangle \langle m_1 m_2 | jm \rangle$$

$$(or) m\hbar |jm \rangle = \sum_{m_1, m_2} (m_1 + m_2) \hbar |m_1 m_2 \rangle \langle m_1 m_2 | jm \rangle$$

Replacing  $|jm \rangle$  using eqn (5) and rearranging, we get,

$$\sum_{m_1, m_2} (m - m_1 - m_2) |m_1 m_2 \rangle \langle m_1 m_2 | jm \rangle = 0 \rightarrow (8)$$

Which is valid only if the coefficient of each term vanishes separately. This leads to one of the rules of vector atom model, (ie)

$$m = m_1 + m_2 \rightarrow (9)$$

| $m_1$  | $m_2$  | $m$             | $j$   |
|--|--|-----------------|---|
| $j_1$  | $j_2$  | $j_1 + j_2$     | $j_1 + j_2$   |
| $j_1$<br>$j_1 - 1$                                       | $j_2 - 1$<br>$j_2$   | $j_1 + j_2 - 1$ | $\left\{ \begin{array}{l} j_1 + j_2 \\ j_1 + j_2 - 1 \end{array} \right.$   |
| $j_1$<br>$j_1 - 1$<br>$j_1 - 2$                          | $j_2 - 2$<br>$j_2 - 1$<br>$j_2$                                  | $j_1 + j_2 - 2$ | $\left\{ \begin{array}{l} j_1 + j_2 \\ j_1 + j_2 - 1 \\ j_1 + j_2 - 2 \end{array} \right.$                            |
| $\vdots$   | $\vdots$   | $\vdots$        | $\vdots$  |
| $j_1$<br>$j_1 - 1$<br>$j_1 - 2$<br>$\vdots$<br>$j_1 - k$ | $j_2 - k$<br>$j_2 - k + 1$<br>$j_2 - k + 2$<br>$\vdots$<br>$j_2$ | $j_1 + j_2 - k$ | $\left\{ \begin{array}{l} j_1 + j_2 \\ j_1 + j_2 - 1 \\ j_1 + j_2 - 2 \\ \vdots \\ j_1 + j_2 - k \end{array} \right.$ |
| $\vdots$   | $\vdots$   | $\vdots$        | $\vdots$  |

The smallest value of  $j$  occurs for  $j_1 - k = -j_1$  (or)  $j_2 - k = -j_2$

$$(ie) \text{ when } k = 2j_1 \text{ (or) } k = 2j_2$$

The smallest value of  $j$  is then,

$$j_1 + j_2 - 2j_1 = j_2 - j_1 \text{ (or)} j_1 + j_2 - 2j_2 = j_1 - j_2$$

In other words, the permitted values of  $j$  are

$$(j_1 + j_2), (j_1 + j_2 - 1), (j_1 + j_2 - 2), \dots, |j_1 - j_2|$$

Which is the triangle rule of the vector atom model.

### 3.2.1 Recursion relations

These relations are used to evaluate explicit expressions for CG Coefficients.

Operating eqn(5) from left by  $J_-$  and replacing  $J_-$  by  $J_{1-} + J_{2-}$  on the R.H.S we get,

$$J_- |jm\rangle = \sum_{m_1', m_2'} (J_{1-} + J_{2-}) |m_1' m_2'\rangle \langle m_1', m_2' | jm \rangle \rightarrow \text{(10)}$$

We know that,

$$\langle j' m' | J_- | jm \rangle = [j(j+1) - m(m-1)]^{1/2} \hbar |j, m-1\rangle$$

Now eqn(10) becomes,

$$\begin{aligned} & [j(j+1) - m(m-1)]^{1/2} \hbar |j, m-1\rangle \\ &= \sum_{m_1', m_2'} [j_1(j_1+1) - m_1'(m_1'-1)]^{1/2} \hbar |m_1' \\ & \quad -1, m_2'\rangle \langle m_1' m_2' \\ & > + \sum_{m_1', m_2'} [j_2(j_2+1) - m_2'(m_2'-1)]^{1/2} \hbar |m_1', m_2' \\ & \quad -1\rangle \langle m_1' m_2' | jm \rangle \rightarrow \text{(11)} \end{aligned}$$

Multiplying both sides by  $\langle m_1 m_2 |$ , we get

$$\begin{aligned} & [j(j+1) - m(m-1)]^{1/2} \\ & \quad \langle m_1 m_2 | j, m-1 \rangle = [j_1(j_1+1) - m_1(m_1+1)]^{1/2} \\ & \quad \langle m_1+1, m_2 | jm \rangle + [j_2(j_2+1) - m_2(m_2+1)]^{1/2} \\ & \quad \langle m_1, m_2+1 | jm \rangle \rightarrow \text{(12)} \end{aligned}$$

Similarly for  $J_+$ , we get,

$$\begin{aligned} & [j(j+1) - m(m-1)]^{1/2} \langle m_1 m_2 | j, m+1 \rangle = [j_1(j_1+1) - \\ & \quad m_1 m_1 - 1]^{1/2} \langle m_1-1, m_2 | jm \rangle + \\ & \quad [j_2(j_2+1) - m_2(m_2-1)]^{1/2} \langle m_1, m_2-1 | jm \rangle \rightarrow \text{(13)} \end{aligned}$$

## NOTES

**NOTES**

Eqns (12) and (13) are the recursion relations required for the computation of CGCoefficients.

The Clebsch-Gordan coefficient matrix  $\langle m_1 m_2 | j m \rangle$  has  $(2j+1)$   $(2j+2)$  rows and columns.

For convenience, the first  $|1 \times 1|$  submatrix is selected as +1.

$$(ie) \langle j_1, j_2, |j_1 + j_2, j_1 + j_2 \rangle = +1 \rightarrow (14)$$

To compute the next  $2 \times 2$  matrix set  $m_1 = j_1, m_2 = j_2 - 1, j = j_1 + j_2$  and  $m = j_1 + j_2$  in eqn (12)

On simplification we get,

$$(j_1 + j_2)^{1/2} \langle j_1, j_2 - 1 | (j_1 + j_2), j_1 + j_2 - 1 \rangle = j_2^{1/2} \langle j_1, j_2 | (j_1 + j_2), (j_1 + j_2) \rangle$$

Using (14) eqn, this eqn becomes,

$$\langle j_1, j_2 - 1 | (j_1 + j_2), j_1 + j_2 - 1 \rangle = \left( \frac{j_2}{j_1 + j_2} \right)^{1/2} \rightarrow (15)$$

Proceeding on similar lines the other equations required to compute CG Coefficients are

$$\langle j_1 - 1, j_2 | (j_1 + j_2), j_1 + j_2 - 1 \rangle = \left( \frac{j_1}{j_1 + j_2} \right)^{1/2} \rightarrow (16)$$

$$\langle j_1, j_2 - 1 | (j_1 + j_2 - 1), j_1 + j_2 - 1 \rangle = \left( \frac{j_1}{j_1 + j_2} \right)^{1/2} \rightarrow (17)$$

$$\langle j_1 - 1, j_2 | (j_1 + j_2 - 1), j_1 + j_2 - 1 \rangle = - \left( \frac{j_2}{j_1 + j_2} \right)^{1/2} \rightarrow (18)$$

**3.2.2 CG coefficients for a system having  $j_1=1/2$  and  $j_2=1/2$**

The system has two angular momenta with  $j_1=1/2$  and  $j_2=1/2$ . The allowed values of  $j$  are 1 and 0.

For  $j=1$ ,  $m=1, 0, -1$  and for  $j=0$ ,  $m=0$ .

The number of  $|j m \rangle$  eigen states is thus four.

The elements  $\langle 1/2, 1/2 | 1, 1 \rangle, \langle 1/2, -1/2 | 1, 0 \rangle, \langle -1/2, 1/2 | 1, 0 \rangle, \langle 1/2, -1/2 | 0, 0 \rangle,$

$\langle -1/2, 1/2 | 0, 0 \rangle$  are easily evaluated with the help of equations (14)  $\rightarrow$  (18) and are listed in the table. The remaining element can be calculated as follows

$\langle -1/2, -1/2 | 1, -1 \rangle$  can be evaluated by setting  $j=1, m=0, m_1=-1/2, m_2=-1/2$

Eqn (12) becomes,

$$\begin{aligned}\sqrt{2}\langle -1/2, -1/2 | 1, -1 \rangle &= \sqrt{1}\langle 1/2, -1/2 | 1, 0 \rangle + \sqrt{1}\langle -1/2, 1/2 | 1, 0 \rangle \\ &= 1/\sqrt{2} + 1/\sqrt{2} \\ &= 2/\sqrt{2} \\ &\text{(or)} \\ \langle -1/2, -1/2 | 1, -1 \rangle &= 1\end{aligned}$$

Central Field  
Approximation

NOTES

| $m_1$ | $m_2$ | $ jm\rangle$  |               |               |                |
|-------|-------|---------------|---------------|---------------|----------------|
|       |       | $ 1,1\rangle$ | $ 1,0\rangle$ | $ 0,0\rangle$ | $ 1,-1\rangle$ |
| 1/2   | 1/2   | 1             | 0             | 0             | 0              |
| 1/2   | -1/2  | 0             | $1/\sqrt{2}$  | $1/\sqrt{2}$  | 0              |
| -1/2  | 1/2   | 0             | $1/\sqrt{2}$  | $-1/\sqrt{2}$ | 0              |
| -1/2  | -1/2  | 0             | 0             | 0             | 1              |

Table 1:CG Coefficients for  $j_1=1/2$  and  $j_2=1/2$

### 3.3 CHECK YOUR PROGRESS

1. What are CG coefficients?
2. Write down the recursion relations.

#### Let us sum up

In this unit, steps involved in combining the angular momenta associated with two parts of a system such as the orbital momenta of two electrons or the spin orbital angular momenta of the same electron to form the angular momentum of the whole system are explained clearly.

### 3.4 UNIT-END EXERCISES

1. Obtain CG coefficients for  $j_1=j_2=1/2$ .
2. Show that the possible values of  $j$ , resulting from the addition of two angular momenta  $j_1, j_2$  are  $(j_1+j_2), (j_1+j_2-1), \dots, |j_1 - j_2|$ .

### 3.5 ANSWERS TO CHECK YOUR PROGRESS

1.  $|jm\rangle = \sum_{m_1 m_2} C_{j m m_1 m_2} |m_1 m_2\rangle$  The coefficients of this linear combination are called Clebsch-Gordan coefficients.

NOTES

$$2. \quad [j(j+1) - m(m-1)]^{1/2} \langle m_1 m_2 | j, m-1 \rangle = [j_1(j_1 + 1 - m_1 m_1 + 1) \langle m_1 + 1, m_2 | j m \rangle + [j_2(j_2 + 1) - m_2(m_2 + 1)]^{1/2} \langle m_1, m_2 + 1 | j m \rangle$$

$$[j(j+1) - m(m-1)]^{1/2} \langle m_1 m_2 | j, m+1 \rangle = [j_1(j_1 + 1) - m_1(m_1 - 1)]^{1/2} \langle m_1 - 1, m_2 | j m \rangle + [j_2(j_2 + 1) - m_2(m_2 - 1)]^{1/2} \langle m_1, m_2 - 1 | j m \rangle$$

$$(ie) \langle j_1, j_2, |j_1 + j_2, j_1 + j_2 \rangle = +1$$

$$\langle j_1, j_2 - 1 | (j_1 + j_2), j_1 + j_2 - 1 \rangle = \left( \frac{j_2}{j_1 + j_2} \right)^{1/2}$$

$$\langle j_1 - 1, j_2 | (j_1 + j_2), j_1 + j_2 - 1 \rangle = \left( \frac{j_1}{j_1 + j_2} \right)^{1/2}$$

$$\langle j_1, j_2 - 1 | (j_1 + j_2 - 1), j_1 + j_2 - 1 \rangle = \left( \frac{j_1}{j_1 + j_2} \right)^{1/2}$$

$$\langle j_1 - 1, j_2 | (j_1 + j_2 - 1), j_1 + j_2 - 1 \rangle = - \left( \frac{j_2}{j_1 + j_2} \right)^{1/2}$$

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### 3.6 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldas- PHI learning Private limited, New Delhi 2008.
3. Foundation of Quantum Mechanics – A.B. Gupta, Books and Allied (P) Ltd., Kolkata, 2015.
4. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.



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## BLOCK II: SELF CONSISTENT FIELD

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### NOTES

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### UNIT-IV CENTRAL FIELD APPROXIMATION

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#### Structure

- 4.1 Field
- 4.2 Central field approximation
- 4.3 Thomas Fermi model
- 4.4 Check your progress
- 4.5 Unit – End Exercises
- 4.6 Answer to Check your progress
- 4.7 Suggested Readings

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#### 4.1 FIELD

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The fields are continuous mechanical systems with non-denumerable infinite no of degrees of freedom. The degree of freedom of the field is called the field functions and these assume the role of the generalized co-ordinates of a mechanical system with a finite no of degree of freedom.

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#### 4.2 CENTRAL FIELD APPROXIMATION

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In the central field approximation each electron moves in a spherically symmetric potential  $V(r)$  which is produced by the nucleus and all the other (N-1) electrons. Spherically symmetric systems are those in which the potential energy of the particle does not depend upon  $\theta$  and  $\phi$  and is only the function of radial distance  $r$  and hence the wave equation can be separated in spherical coordinates.

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### 4.3 THOMAS FERMI MODEL

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The Thomas- Fermi model assumes that potential energy,  $V(r)$  varies slowly so that many electrons can be found in a volume element over which the potential energy is sensibly constant. The electron can now be regarded as a system of particles that obey Fermi-Dirac statistics. The electron states are filled in order of increasing energy. As electrons are treated as a gas of fermions, one can apply the concept of cells in phase space to the states of individual electrons.

The volume of phase space occupied by electrons is

$$\frac{4}{3}\pi p^3 dv$$

This is multiplied by 2 to account for the two possible spin states.

Therefore the number of cells (states) corresponding to this volume is

$$2\left(\frac{4}{3}\right)\pi p^3 dv/\hbar^3$$

Now the number of electrons per unit volume  $n(r)$  whose K.E. does not exceed  $p^2/2m$  is given by

$$n(r) = \frac{8\pi p^3}{3h^3} = \frac{p^3}{3\pi^2\hbar^3} \rightarrow (1)$$

For the electrons not to escape from the nucleus, the maximum allowed K.E. at any distance  $r$  from the nucleus is  $-V(r)$

$$(ie) \frac{p^2}{2m} = -V(r) \rightarrow (2)$$

From (1) and (2)

$$n(r) = \frac{[-2mV(r)]^{3/2}}{3\pi^2\hbar^3} \rightarrow (3)$$

The electrostatic potential and the charge density obey the Poisson equation

$$\frac{1}{e}\nabla^2 V(r) = -4\pi n(r) \rightarrow (4)$$

Since the potential is spherically symmetric,

$$\nabla^2 V(r) = \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dV}{dr} \right) \rightarrow (5)$$

with the value of equation (5), (4) becomes

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dv}{dr} \right) = -4\pi e^2 n(r) \rightarrow (6)$$

Sub equation (3) in (6)

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dv}{dr} \right) = \frac{4e^2}{3\pi\hbar^3} [-2m V(r)]^{3/2} \rightarrow (7)$$

Which is Thomas-Fermi equation

When  $r \rightarrow 0$  (ie) near the nucleus, the leading term in the potential is due to the nucleus, so that

$$V(r) \rightarrow -Ze^2/r$$

When  $r \rightarrow \infty$ , there can be no net charge inside the sphere of radius 'r' for a neutral atom, so that V falls off more rapidly than  $1/r$  (ie)  $r V(r) \rightarrow 0$ .

The non-linear equation (7) cannot be solved exactly.

$$\therefore \text{put } V(r) = -\frac{Ze^2\chi(r)}{r} \rightarrow (8)$$

Substituting this value of  $V(r)$  in equation (7) we have

$$\frac{d^2\chi}{dr^2} = \frac{4e^3(2m)^{3/2} Z^{1/2} \chi^{3/2}}{3\pi\hbar^3 r^{1/2}} \rightarrow (9)$$

To write equation (9) in dimensionless form we take  $r = bx$

Now (9) becomes,

$$\frac{d^2\chi}{dx^2} = b^{3/2} \frac{4e^3(2m)^{3/2} Z^{1/2} \chi^{3/2}}{3\pi\hbar^3 x^{1/2}} \rightarrow (10)$$

'b' is selected such that the coefficient of  $\chi^{3/2}/x^{1/2}$  is unity.

$$b^{3/2} \frac{4e^3(2m)^{3/2} Z^{1/2}}{3\pi\hbar^3} = 1$$

(or)

$$b^{3/2} = \frac{3\pi\hbar^3}{4e^3(2m)^{3/2} Z^{1/2}}$$

$$b = \left(\frac{3\pi}{4}\right)^{2/3} \cdot \frac{1}{2m} \cdot \frac{\hbar^2}{e^2} \cdot \frac{1}{Z^{1/3}}$$

## NOTES

$$b = \frac{1}{2} \left( \frac{3\pi}{4} \right)^{2/3} \cdot \frac{\hbar^2}{me^2} \frac{1}{Z^{1/3}}$$
$$= \frac{0.8853 a_0}{Z^{1/3}} \rightarrow (11)$$

Putting (11) in (10) we have

## NOTES

$$\frac{d^2 \chi}{dx^2} = \frac{\chi^{3/2}}{x^{1/2}}$$

which is called as dimensionless Thomas- Fermi equation.

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## 4.4 CHECK YOUR PROGRESS

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1. Define self consistent field method.
2. Differentiate field and system.

### Let us sum up

This unit describes how the approach of a screened nucleus with an effective nuclear charge can be extended to many electron systems. An equation for Thomas Fermi model has been derived for many electron systems.

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## 4.5 UNIT-END EXERCISES

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1. Deduce Thomas Fermi model.

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## 4.6 ANSWERS TO CHECK YOUR PROGRESS

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1. Self-consistent field method is an iterative method which involves selecting an appropriate Hamiltonian and solving the Schrodinger equation to obtain a more accurate set of orbitals. The procedure is repeated until the result converges.
2. Field has infinite no. of degrees of freedom whereas any mechanical system has finite degrees of freedom.

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## 4.7 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldas- PHI learning Private limited, New Delhi 2008.
3. Quantum Mechanics – Theory and Application – Ajoy Ghatak and S. Lokanathan – 5<sup>th</sup> edition – Trinity Press, 2012.

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# UNIT-V IDENTICAL PARTICLES

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## Structure

5.1 Identical particles

5.2 Bosons and fermions

5.3 Symmetric and anti-symmetric wave functions

5.3.1 Construction of symmetric and anti-symmetric wave functions

5.3.2 Pauli principle

5.4 Check your progress

5.5 Unit – End Exercises

5.6 Answer to Check your progress

5.7 Suggested Readings

## NOTES

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### 5.1 IDENTICAL PARTICLES

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There are many systems in nature that are made of several particles of the same species. These particles all have the same mass, charge and spin. For example, the electrons in an atom are identical particles. Particles that can be substituted for each other with no change in the physical situation are said to be indistinguishable particles. Therefore interchanging the co-ordinates of two electrons does not change the Hamiltonian. Hence Hamiltonian is symmetric in the co-ordinates of the particles.

$$(i.e) H(1, 2, 3 \dots n) = H(2, 1, 3 \dots n) \rightarrow (1)$$

where each number represents all the co-ordinates both position and spin of the particles.

The energy eigen value equation of a two particle system is,

$$H(1,2)\psi(1,2) = E \psi(1,2) \rightarrow (2)$$

Interchanging 1, 2 does not affect eqn. (2)

$$H(2,1)\psi(2,1) = E \psi(2,1) \rightarrow (3)$$

From (1),

$$H(1,2)\psi(2,1) = E \psi(2,1) \rightarrow(4)$$

Particle exchange operator  $P_{12}$  is defined such that when it operates on a state, it interchanges all the co-ordinates of particles 1 and 2. Thus,

$$P_{12}\psi(1,2) = \psi(2,1) \rightarrow(5)$$

Now (4) becomes,

**NOTES**

$$\begin{aligned} H(1,2) P_{12} \psi(1,2) &= E P_{12} \psi(1,2) \\ &= P_{12} E \psi(1,2) \\ &= P_{12} H(1,2) \psi(1,2) \end{aligned}$$

It follows that

$$\begin{aligned} H(1,2) P_{12} &= P_{12} H(1,2) \\ [P_{12}, H(1,2)] &= 0 \end{aligned}$$

That is  $P_{12}$  is a constant of motion and therefore any operator representing a physical property must commute with  $P_{12}$ .

Let us consider the function  $\psi(1,2)$  which is an eigen function of  $P_{12}$  and has eigen value  $p$

$$\therefore P_{12}\psi(1,2) = p \psi(1,2) \rightarrow(6)$$

$$\psi(2,1) = p \psi(1,2) \rightarrow(7)$$

Operating on both sides by  $P_{12}$ , we get

$$\psi(1,2) = p P_{12} \psi(1,2) = p^2 \psi(1,2)$$

$$\text{Hence } p^2 = 1 \text{ or } p = \pm 1$$

$\therefore$  The eigen value of  $P_{12}$  is  $\pm 1$ .

It follows from eqn. (7) that

$$\psi(2,1) = \pm \psi(1,2) \rightarrow(8)$$

In case of indistinguishable particles, even in the absence of mutual interactions they still have a profound influence on each other, since the number of ways in which the same quantum state can be occupied by two or more is severely restricted. This is a consequence of so called spin-statistics theorem.

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## 5.2 BOSONS AND FERMIONS

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Spin and statistics are related at the level of quantum field theory. System of identical particles with integer spin ( $s = 0, 1, 2, \dots$ ) known as bosons have wave functions which are symmetric under interchange of any pair of particle labels. The wave function is said to obey Bose-Einstein statistics.

System of identical particles with half odd integer spin ( $s = \frac{1}{2}, \frac{3}{2}, \dots$ ) known as fermions have wave functions which are antisymmetric under interchange of any pair of particle labels. The wave function is said to obey Fermi-Dirac statistics. The antisymmetric wave function vanishes when two identical particles have the same set of co-ordinates. In other words, two identical fermions cannot occupy the same state. This is one form of Pauli's exclusion principle.

Whereas two identical bosons can occupy the same quantum state. Hence Bosons do not obey Pauli's exclusion principle.

### NOTES

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## 5.3 Symmetric and anti-symmetric wave functions

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If the interchange of any pair of particles does not change the sign of  $\psi$ , then it is said to be symmetric wave function.

If the interchange of any pair of particle changes the sign of  $\psi$ , then it is said to be antisymmetric wave function.

We know that,

$$\psi(2,1) = \pm\psi(1,2) \text{ [ from (8) ]}$$

which means that any physically acceptable wave function representing two identical particles must be symmetric or antisymmetric with respect to an interchange of the particles.

Also the symmetry character of a wave function does not change with time. Let the wave function  $\psi(1, 2, \dots n, t)$  is symmetric at a particular time  $t$ .  $H\psi$  is then symmetric since  $H$  is symmetric in its arguments. The Schrodinger equation states that,

$$i\hbar\frac{\partial\psi}{\partial t}(1, 2, \dots n, t) = H(1, 2, \dots n) \psi(1, 2, \dots n, t) \rightarrow \mathbf{(1)}$$

Since  $H\psi$  is symmetric,  $\frac{\partial\psi}{\partial t}$  is also symmetric. The same arguments can be extended for an infinitesimally latter time  $t + dt$  and also can be continued to cover large time intervals.

In similar way, if  $\psi$  is antisymmetric at any time, it is always antisymmetric. Thus a wave function which is symmetric continues to

NOTES

be symmetric and a wave function which is antisymmetric continues to be antisymmetric.

**5.3.1 Construction of symmetric and anti-symmetric wave functions**

It is known that the Hamiltonian does not depend on time and hence if E is the energy eigen value, then the possible stationary solutions are,

$$\psi(1, 2, \dots n, t) = \psi(1, 2, \dots n) \exp\left(\frac{-iEt}{\hbar}\right)$$

If the two particles are interchanged, it remains the same as it simply corresponds to relabeling of the particles. Hence we can get n! solutions from one solution and also these solutions correspond to the same energy. The degeneracy arising due to the interchange of identical particles is called exchange degeneracy.

Any linear combination of these solutions is also a solution of the wave equation. The sum of all these functions is a symmetrical unnormalized wave function  $\psi_s$ . An antisymmetric unnormalized wave function  $\psi_{as}$  can be constructed by adding together all permuted functions obtained from the original solution by an even number of interchanges of pair of particles and subtracting the sum of all permuted functions obtained by odd number of interchanges of a pair of particles.

For a two particle system,

$$\psi_s = \psi(1,2) + \psi(2,1)$$

and

$$\psi_{as} = \psi(1,2) - \psi(2,1)$$

For a three particle system,

$$\psi_s = \psi(1, 2, 3) + \psi(1, 3, 2) + \psi(3, 2, 1) + \psi(2, 1, 3) + \psi(2, 3, 1) + \psi(3, 1, 2)$$

and

$$\psi_{as} = [\psi(1, 2, 3) + \psi(2, 3, 1) + \psi(3, 1, 2)] - [\psi(2, 1, 3) + \psi(1, 3, 2) + \psi(3, 2, 1)]$$

**5.3.2 Pauli principle**

The Hamiltonian H of 'n' noninteracting indistinguishable particles are

$$H(1,2,\dots,n) = H(1) + H(2) + \dots + H(n) \rightarrow (1)$$



If  $u_a(1), u_b(2), \dots, u_n(n)$  are the  $n$  one-particle eigen functions, then the energy eigen function,

$$\psi(1, 2, \dots, n) = u_a(1), u_b(2), \dots, u_n(n) \rightarrow (2)$$

$$\text{And } E = E_a + E_b + E_c + \dots + E_n \rightarrow (3)$$

Eqn (2) does not mean that state  $u_a$  is occupied by particle 1,  $u_b$  by particle 2 and so on. whereas we can say that one particle is in state  $u_a$ , a second in in  $u_b$  and so on.

The symmetric and asymmetric combinations are:

$$\psi_s = u_a(1)u_b(2) + u_a(2)u_b(1) \rightarrow (4)$$

$$\& \psi_{as} = u_a(1)u_b(2) - u_a(2)u_b(1) = \begin{vmatrix} u_a(1) & u_a(2) \\ u_b(1) & u_b(2) \end{vmatrix} \rightarrow (5)$$

If both the particles are put in the same state then,

$$\psi_s = u_a(1)u_a(2) + u_a(2)u_a(1) = 2u_a(1)u_a(2)$$

$$\text{and } \psi_{as} = u_a(1)u_a(2) - u_a(2)u_a(1) = 0$$

Which means  $\psi_{as}$  vanishes when two identical particles have the same set of co ordinates. In other words, two identical fermions cannot occupy the same state and hence obeys paulis exclusion principle.

For  $n$  particle system, the normalized asymmetric combinations can be written as,

$$\psi_{as}(1, 2, \dots, n) = \frac{1}{\sqrt{n!}} \begin{vmatrix} u_a(1) & u_a(2) & \dots & u_a(n) \\ u_b(1) & u_b(2) & \dots & u_b(n) \\ \vdots & \vdots & \dots & \vdots \\ u_n(1) & u_n(2) & \dots & u_n(n) \end{vmatrix}$$

The factor  $1/\sqrt{n!}$  is the normalization constant and the determinant is called the slater determinant.

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## 5.4 CHECK YOUR PROGRESS

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1. What are symmetric and antisymmetric wave functions.
2. Identical particles and particle exchange operator.

### Let us sum up

A thorough introduction of indistinguishable particles is presented in this unit. Also the symmetric and anti-symmetric nature of wavefunctions with respect to interchanging particle labels are discussed.

## NOTES

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## 5.6 UNIT-END EXERCISES

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1. Differentiate bosons and fermions.

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## 5.7 ANSWERS TO CHECK YOUR PROGRESS

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1. If the interchange of any pair of particles does not change the sign of  $\psi$ , then it is said to be symmetric wave function. If the interchange of any pair of particle changes the sign of  $\psi$ , then it is said to be antisymmetric wave function. (ie),  $\psi(2,1) = \pm\psi(1,2)$ .

2. Particles that can be substituted for each other with no change in the physical situation are said to be indistinguishable particles. Particle exchange operator  $P_{12}$  is defined such that when it operates on a state, it interchanges all the co-ordinates of particles 1 and 2. Thus,  $P_{12}\psi(1,2) = \psi(2,1)$ .

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## 5.7 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldhas- PHI learning Private limited, New Delhi 2008.
3. Quantum Mechanics – Theory and Application – Ajoy Ghatak and S. Lokanathan – 5<sup>th</sup> edition – Trinity Press, 2012.
4. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.

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# UNIT-VI HARTREE EQUATION

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Hartree Equation

## Structure

6.1 Hartree equation

6.2 Hartree -Fock equation

6.3 Central field approximation & periodic system of the elements

6.4 The alkali atoms

6.4.1 Features of alkali spectra

6.4.2 Doublet separation

6.4.3 Doublet intensity

6.5 Check your progress

6.6 Unit – End Exercises

6.7 Answer to Check your progress

6.8 Suggested Readings

NOTES

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## 6.1 HARTREE EQUATION

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Consider an atom with Z electrons. Its Hamiltonian is

$$H = \sum_{i=1}^Z \left[ \frac{(-h/2\pi)^2}{2m} \nabla_i^2 + V(r_i) \right] + \frac{1}{2} \sum_{i,j \neq 1} \frac{e^2}{r_{ij}} \rightarrow (1)$$

The second term on the right represents the interaction between the electrons.

$$H_i = \frac{(-h/2\pi)^2}{2m} \nabla_i^2 + V(r_i)$$

and

$$V_{ij} = \frac{e^2}{r_{ij}} \rightarrow (2)$$

We get,

$$H = \sum_i H_i + \frac{1}{2} \sum_{i,j \neq 1} V_{ij} \rightarrow (3)$$

## NOTES

The Schrodinger wave equation to be solved is,

$$H\Psi(r_1, r_2, \dots, r_z) = E\Psi(r_1, r_2, \dots, r_z) \rightarrow (4)$$

which is a partial differential equation in 3z dimensions.

In the variation method, the procedure followed is to assume a trial wave function with variable parameters, calculate  $\langle H \rangle$  and then minimize  $\langle H \rangle$  with respect to the parameters. However, Hartree followed a different procedure in which the variational method itself is used to select the trial wave function.

Let us assume the trial wave function to be of the form,

$$\Psi(r_1, r_2, \dots, r_z) = u_1(r_1), u_2(r_2), \dots, u_z(r_z) \rightarrow (5)$$

Where  $u_1(r_1), u_2(r_2), \dots$  are normalized single particle functions. That is

$$\int u_i^* u_i d\tau_i = 1 \quad i = 1, 2, 3, \dots, z \rightarrow (6)$$

With the trial function in equation(5),  $\langle H \rangle$  can be written as

$$\langle H \rangle = \int u_1^* u_2^* \dots u_z^* (\sum_i H_i + \frac{1}{2} \sum_{i,j \neq i} V_{ij}) u_1, u_2 \dots u_z d\tau \rightarrow (7)$$

Where  $d\tau = d\tau_1, d\tau_2, \dots, d\tau_z$

In equation (7)  $H_i$  operates on only the coordinates of  $i^{\text{th}}$  electron and  $V_{ij}$  operates on the coordinates of electrons  $i$  and  $j$ , we have

$$\langle H \rangle = \sum_i \int u_i^* (H_i + \frac{1}{2} \sum_{j \neq i} \int u_j^* V_{ij} u_j d\tau_j) u_i d\tau_i \rightarrow (8)$$

The next step is to minimize  $\langle H \rangle$  with respect to  $u_1^*, u_2^*, \dots$  which gives

$$\delta \langle H \rangle = \sum_i \int \delta u_i^* (H_i + \sum_{j \neq i} \int u_j^* V_{ij} u_j d\tau_j) u_i d\tau_i = 0 \rightarrow (9)$$

Neglecting  $\frac{1}{2}$  leads to double counting of repulsive electronic form. This will be taken care in the end.

In equation (9)  $\delta u_i^*$  satisfies the equation

$$\int \delta u_i^* u_i d\tau_i = 0 \quad i=1, 2, \dots, Z \rightarrow (10)$$

Solution of (9) is subject to these Z equations of constraints

Multiplying equation (10) by a multiplier  $\epsilon_i$ , we have

$$\int \delta u_i^* \epsilon_i u_i d\tau_i = 0 \rightarrow (11)$$

Subtracting (11) from (9) we have

$$\sum_i \int \delta u_i^* (H_i + \sum_{j \neq i} \int u_j^* V_{ij} u_j d\tau_j - \epsilon_i) u_i d\tau_i = 0 \rightarrow (12)$$

As the variations  $\delta u_i^*$  are independent, the coefficient of each  $\delta u_i^*$  in (12) vanishes.

$$(H_i + \sum_{j \neq i} \int u_j^* V_{ij} u_j d\tau_j - \epsilon_i) u_i = 0$$

$$(i.e) (H_i + \sum_{j \neq i} \int u_j^* V_{ij} u_j d\tau_j) u_i = \epsilon_i u_i \rightarrow (13)$$

Substituting the values of  $H_i$  and  $V_{ij}$  from (2) in (13) we get,

$$\left[ -\frac{(\hbar/2\pi)^2}{2m} \nabla_i^2 - \frac{z_e^2}{r_i} + e^2 \sum_{j \neq i} \int \frac{1}{r_{ij}} |u_j(r_j)|^2 d\tau_j \right] u_i(r_i) = \epsilon_i u_i(r_i) \rightarrow (14)$$

This is Hartree's equation of self consistent field.

It is an eigen value equation for electron  $i$  located at  $r_i$ , moving in a potential

$$V_i(r_i) = -\frac{z_e^2}{r_i} + e^2 \sum_{j \neq i} \int \frac{1}{r_{ij}} |u_j(r_j)|^2 d\tau_j$$

The first term is the attractive coulomb potential due to the nuclear charge  $Ze$  and the second term is a repulsive contribution due to the charge density of all the other electrons.

The charge density associated with the  $j^{\text{th}}$  electron  $e |u_j(r_j)|^2$  will be known only when we solve equation (14), therefore one has to go in for an iterative procedure assuming an appropriate form for the  $u_i$ 's. The insertion of the refined wave function back in to the equation leads to a better one. This process is continued until the wave functions are self consistent to a high degree of accuracy. The potential thus obtained is called the self consistent potential. The expression for energy is

$$E = \sum_i \epsilon_i - \frac{1}{2} \sum_{i, j \neq i} \int u_i^* \frac{1}{r_{ij}} |u_j(r_j)|^2 u_i d\tau_i d\tau_j$$

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## 6.2 HARTREE-FOCK EQUATION

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In the Hartree method, the many electron wave function is simply a product of one electron wave functions which is not applicable for indistinguishable particles. Whereas, in this method, Fock used an antisymmetrized wave function for the variational calculations. The wave function including the spin is assumed to take the form of a Slater determinant of one electron wave functions.

### NOTES

$$\Psi(x_1, x_2, x_3, \dots, x_z) = \frac{1}{\sqrt{z!}} \begin{vmatrix} u_1(x_1) & u_1(x_2) & \dots & u_1(x_z) \\ u_2(x_1) & u_2(x_2) & \dots & u_2(x_z) \\ \vdots & \vdots & \ddots & \vdots \\ u_z(x_1) & u_z(x_2) & \dots & u_z(x_z) \end{vmatrix} \rightarrow (1)$$

Where  $x_1, x_2, \dots$  represent the coordinates including both space and spin.

## NOTES

The Hamiltonian of a system having  $z$  interacting electrons is given by

$$H = \sum_{i=1}^z \left[ -\frac{(\hbar/2\pi)^2}{2m} \nabla_i^2 + V(r_i) \right] + \frac{1}{2} \sum_{i,j \neq i} \frac{e^2}{r_{ij}}$$

Which can be written as

$$H = \sum_i H_i(r_i) + \frac{1}{2} \sum_{i,j \neq i} V(r_i, r_j) \rightarrow (2)$$

The Schrodinger equation to be solved is

$$H\Psi(x_1, x_2, \dots, x_z) = E\Psi(x_1, x_2, \dots, x_z) \rightarrow (3)$$

As this equation is not separable, we can express the eigen functions of  $H$  as a linear combination of determinantal eigen functions of  $\sum_i H_i(r_i)$ . Therefore the Hamiltonian can be written as

$$H = \sum_i [H_i(r_i)F(r_i)] + \left[ \frac{1}{2} \sum_{i,j \neq 0} V(r_i r_j) - \sum_i F(r_i) \right] \rightarrow (4)$$

The second term on the right side is the modified interaction term.

This modified single  $Z^{\text{th}}$  order determinant has the orbital factors which are eigen functions of the equation

$$\left[ -\frac{(\hbar/2\pi)^2}{2m} \nabla^2 + V(r) + F(r) \right] \phi(r) = \epsilon \phi(r) \rightarrow (5)$$

The operator  $F$  has to be selected such that it minimizes the total energy and does not affect the Hamiltonian.

Use of a single determinant with these functions as the ground state wave function is known as the Hartree-fock method. The choice of  $F$  in accordance with the variational principle is given by

$$\langle n|F|m \rangle = \sum_i [ \langle in|v|im \rangle - \langle ni|v|im \rangle ] \rightarrow (6)$$

Writing the above equation in integral form we have,

$$\int u_n^*(x) F(r) u_m(x) dx = \sum_i \iint u_i^*(x_1) u_n^*(x_2) v(r_1, r_2) u_i(x_1) u_m(x_2) dx_1 dx_2 - \sum_i \iint u_n^*(x_i) u_i^*(x_2) v(r_1, r_2) u_i(x_1) u_m(x_2) dx_1 dx_2$$

$$\begin{aligned}
&= \sum_i \int u_n^*(x_2) \left[ \int |u_i(x_1)|^2 v(r_1, r_2) dx_1 \right] u_m(x_2) dx_2 \\
&- \sum_i \int u_n^*(x_2) \left[ \int u_i^*(x_1) u_m(x_1) v(r_1, r_2) dx_1 \right] u_i(x_2) dx_2 \rightarrow (7)
\end{aligned}$$

Equation(7) is obtained by interchanging  $x_1$  and  $x_2$  in the second integral, since the value of definite integral does not depend on the variable of integration.

Now replacing  $x_2$  by  $x$ , we get,

$$\begin{aligned}
\int u_n^*(x) F(r) u_m(x) dx &= \int u_n^*(x) \sum_i \left[ \int |u_i(x_1)|^2 v(r_1, r_2) u_m(x) dx_1 \right. \\
&\quad \left. - \int u_i^*(x_1) u_m(x_1) v(r_1, r_2) u_i(x) dx_1 \right] dx \rightarrow (8)
\end{aligned}$$

Removing  $\int u_n^*(x)$ , 8 becomes

$$\begin{aligned}
F(r) u_m(r) &= \sum_i \int |u_i(x_1)|^2 v(r_1, r) u_m(x) dx_1 - \sum_i u_i^* \\
&\quad (x_1) u_m(x_1) v(r_1, r) u_i(x) dx_1
\end{aligned}$$

As  $u(x)$  is the product of orbital part  $\phi(r)$  and a spin function, by carrying out the sum over the spin variable, we have

$$\begin{aligned}
F(r) \phi_m(r) &= \sum_i \int |\phi_i(r_1)|^2 v(r_1, r) \phi_m(r) dr_1 \\
&- \sum_{spin\ i=spin\ m} i \int \phi_i^*(r_1) \Psi_m(r_1) v(r_1, r) \phi_i(r) dr_1
\end{aligned}$$

The second term on the right vanishes if  $u_i$  and  $u_m$  have different spin factors.

In non ferromagnetic systems, the numbers of electron with opposite spin are equal.

$$\begin{aligned}
F(r) \phi_m(r) &= 2 \sum_{i=1}^{z/2} \int |\phi_i(r_1)|^2 v(r_1, r) \phi_m(r) \\
&\quad dr_1 - \sum_{i=1}^{z/2} \int \phi_i^*(r_1) \phi_m(r_1) v(r_1, r) \phi_i(r) dr_1
\end{aligned}$$

The Hartree fock eqn .(4) for the function  $\phi_m(r)$  now becomes

$$\begin{aligned}
\left[ -\frac{(\hbar^2)}{2m} \nabla^2 + V(r) \right] \phi_m(r) &+ 2 \sum_{i=1}^{z/2} \int |\phi_i(r_1)|^2 v(r_1, r) dr_1 \phi_m(r) \\
&- \sum_{i=1}^{z/2} \phi_i(r) \int \phi_i^*(r_1) \phi_m(r_1) v(r_1, r) dr_1 = \varepsilon_m \phi_m(r)
\end{aligned}$$

The operator  $F(r)$  depends on all these functions. Hence the set of  $z/2$  equations have to be solved by an iterative procedure until a sufficient degree of self consistency is reached. The third term on L.H.S is called the exchange term. Without this term the equation reduces to Hartree equation.

## NOTES

### 6.3 CENTRAL FIELD APPROXIMATION & PERIODIC SYSTEM OF THE ELEMENTS

#### NOTES

In the central field approximation each electron is supposed to move in a field being taken to spherically symmetric. The Hamiltonian in this approximation evidently commutes with the angular momentum operator  $L$  of each electron. So the state of each individual electron can be characterized by the quantum numbers  $n$ ,  $l$ , and  $m_l$ . To this set  $m_s$  ( $=+1/2$  or  $-1/2$ ) must be added which specifies the spin orientations. Here  $n$  uniquely determines the energy in hydrogen. In complex atoms neglecting the spin-orbit interaction, the energy depends on  $n$  and  $l$ . for example the  $2s$  and  $2p$  orbitals have different energies.

The electrons that have smaller angular momentum penetrate closer to the nucleus and  $V(r)$  is stronger than  $-e^2/r$  there, since the nucleus is less completely screened by the other electrons. Thus, for given  $n$ , the states of lowest  $l$  have the lowest energy. The degeneracy with respect to  $m$  is not affected in case of spherically symmetric potential.

No two electrons can have the same set of four quantum numbers (Pauli principle). Thus  $n$ ,  $l$ ,  $m_l$  and  $m_s$  uniquely identify a spin orbital.

The electrons with the same  $n$  form a shell (or energy level). Electrons with the same values of  $n$  and  $l$  are called equivalent electrons, and occupy the same subshell (or sub level). The maximum number of equivalent electrons is  $2(2l+1)$  as  $-l \leq m_l \leq l$  and  $m_s$  have two possible values.

A closed subshell contains the maximum number of equivalent electrons. In a closed shell, all its subshells are closed. The number of electrons in a closed shell is

$$\sum_{l=0}^{n-1} 2(2l+1) = 2 [1 + 3 + \dots + (2n-1)] = 2n \frac{l+2n-1}{2} = 2n^2 \rightarrow (1)$$

The order in which the electron energy states usually occur in atoms, in order of increasing energy is given in the below table

| No of shells | Electron states | Total no of states in shell |
|--------------|-----------------|-----------------------------|
| 1.           | 1s              | 2                           |
| 2.           | 2s, 2p          | 8                           |



|    |                |    |
|----|----------------|----|
| 3. | 3s,3p          | 8  |
| 4. | 4s,3d,4p       | 18 |
| 5. | 5s,4d,5p       | 18 |
| 6. | 6s, 4f, 5d, 6p | 32 |
| 7. | 7s, 6d, 5f,    |    |

**NOTES**

The self consistent field provides a simple explanation for the order given.

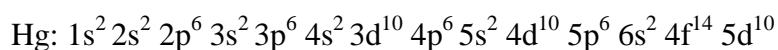
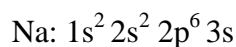
The chemical properties of atoms are determined by the least tightly bound or valence electrons which are in the shell of highest energy. The most important factors are the number of occupied and unoccupied electron states in this shell, and the energy interval between this and the next higher (empty) shell. For example an atom tends to be chemically inert if its highest shell is full and there is an appreciable energy gap to the next higher level, since then electrons are not readily shared with other atoms to form a molecule. The quasi periodic recurrence of similar highest shell structures as  $Z$  increases is responsible for the periodic system of the chemical elements.

In the first approximation, one can use the hydrogen like wave functions  $R_{nl}(r) \sim r^l$  as  $r \rightarrow 0$ ,

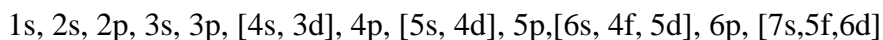
because of the centrifugal potential  $\hbar^2 l(l+1)/2mr^2$ . This means that the s-state electrons can penetrate closer to the nucleus than d or f state electrons. As a result of the s-state electrons feel the full attraction of the nucleus than d or f state electrons. This explains the lower energy of the 4-s state as compared to the 3d state. The screening effect can become so large that the 4-f state is higher than the 6-s state.

Due to the Pauli principle, in a closed sub shell and hence in a closed shell, the sum of  $m_l$  and  $m_s$  is equal to zero. This principle imposes severe restrictions on the distribution of electrons in the levels. It leads to the building-up principle (aufbau principle). In the ground state of an atom, the electrons occupy those orbitals that are allowed by the Pauli principle and which yield the lowest energy.

The ground state configurations of sodium ( $Z=11$ ) and of mercury ( $Z=80$ ) are



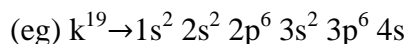
The list defining electron configuration is in the order of increasing electron energy from left to right.



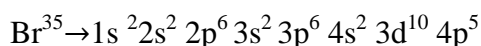
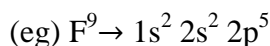
There are two groups of atoms that have a partially full f shell in their ground state configurations fit in at rare earths and at heaviest elements.

## NOTES

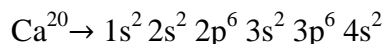
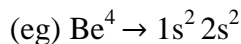
The ground state configuration of (i) an alkali atom consists of a series of full shells followed by a single s electron.



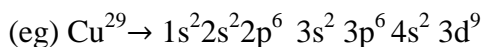
(ii) a halogen atom has one electron short of a full p shell



(iii) an alkaline earth metal atoms have a full s shell followed by p shells in case of Be and Mg and followed by d or f shells in other cases



(iv) noble metals have an s electron missing in the full bracketed shells.




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## 6.4 THE ALKALI ATOMS

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The ground state configuration of an alkali atom consists of a series of full shells followed by a single s electron. Excitation of single valence electrons of alkali atoms produces optical spectra similar to that of single electron system ( $H_2$  atom).

### 6.4.1 Features of alkali spectra

The set of rules for arranging the observed spectral lines of alkali atoms are as follows:

- (1) The structure and multiplicity of the lines
- (2) The case with which they appear
- (3) Their dependence on temperature
- (4) Their sharpness
- (5) Their behavior under electric and magnetic fields

### 6.4.2 Doublet separation

In the spectra of alkali atoms, the prominent lines can be separated into four separate series with the following description:

| Series nomenclature | Series expansion |
|---------------------|------------------|
| Principal series    | 1S-mP m=2,3,4    |
| Diffuse series      | 2P-mD m=3,4,5    |
| Sharp series        | 2P-mS m=3,4      |
| Fundamental series  | 3D-mF m=4,5,6    |

### NOTES

The first line (s) of the principal series (s-p) are called resonance lines since it involves the ground level. Each line of the diffuse and sharp series is a close doublet and this doublet separation is constant for all the lines belonging to the two series. Each line of the principal series is a close doublet and the doublet interval decreases as the wave number of the line increases. Ingoing from an alkali atom of lower atomic number to one of higher atomic number, the doublet separation of the first member of the principal series increases. Doublet separations in the ionized alkaline earths are larger than those for the corresponding doublets in the alkalis. In a spectrum of each atom P doublets are wider than D doublets and D doublets are wider than F doublets of the same m.

Doublet separation (in  $cm^{-1}$ ) of alkali atoms and singly ionized alkaline earth atoms is given below,

| Li    | Na   | K    | Rb    | Cs    | Be <sup>+</sup> | Mg <sup>+</sup> | Ca <sup>+</sup> | Sr <sup>+</sup> | Ba <sup>+</sup> |
|-------|------|------|-------|-------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0.338 | 17.2 | 57.9 | 237.7 | 554.0 | 6.61            | 91.5            | 223.0           | 800.0           | 1691.0          |

The doublet fine structure in alkali atoms can be explained as a result of interaction between two types of angular momenta possessed by the valence electron (orbital angular momentum + spin angular momentum). The interaction energy can be obtained by considering the quantum mechanical properties of the operator for the total angular momentum and is given by

$$\Delta T_{LS} = - \frac{R\alpha^2 z^4}{\pi^3 L \left(L + \frac{1}{2}\right) (L + 1)} \frac{J(J + 1) - L(L + 1) - S(S + 1)}{2}$$

Where  $R = \frac{2\pi^2 m e^4}{ch^3}$  is the Rydberg constant.

and  $\alpha^2 = \frac{4\pi^2 e^4}{c^2 h^2}$  is the fine structure constant and  $\sqrt{L(L+1)}$ ,  $\sqrt{S(S+1)}$ ,  $\sqrt{J(J+1)}$  represent the orbital, spin and total angular momenta respectively of the atom in units of  $\frac{h}{2\pi}$ .

The features of doublet separation are:

## NOTES

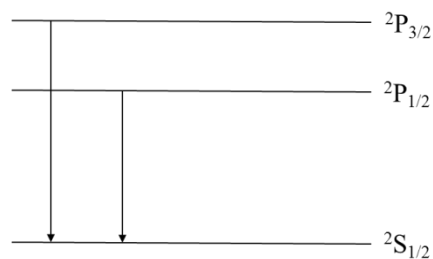
- (1)  $\Delta T_{L,S} = 0$  for  $L = 0$
- (2) For a given atom and a principal quantum number,  $Z$  and  $n$  are constant and  $\Delta T_{L,S}$  is inversely proportional to  $L^3$ .
- (3) For a given atom and a given  $L$  value  $\Delta T_{L,S}$  decreases with increase in principal quantum number.
- (4) For a given  $n$  and  $L$ ,  $\Delta T_{L,S}$  increases with  $Z$  which is in good agreement with the observed features.

### 6.4.3 Doublet Intensity

From the observations of the line intensities in the doublets certain rules have been stated in terms of quantum numbers of electron in the initial and final energy states involved. The rules are:

- (1) The strongest lines in any doublet arise from transitions in which quantum numbers of  $J$  and  $L$  change in the same directions
- (2) When there is more than one line satisfying rule 1 in the same doublet the line involving the largest  $J$  values is the strongest.
- (3) The sum of intensities of those lines of a doublet which come from a common initial level is proportional to the quantum weight  $(2J+1)$  of that level.
- (4) The sum of intensities of those lines of a doublet which end on common level is proportional to the quantum weight  $(2S+1)$  of that level.

As an example we may consider the first principal series doublet. The line  $2P_{3/2} \rightarrow 2S_{1/2}$  is stronger than  $2P_{1/2} \rightarrow 2S_{1/2}$  because in the former  $\Delta L = \Delta J = 1$  while in the latter  $\Delta L = 1$  and  $\Delta J = 0$ .



This is in accordance with rule 1. The two lines starting from upper levels  $2p_{3/2}$  and  $2p_{1/2}$  end on a common lower level  $2s_{1/2}$ . The quantum weights of the upper two levels are  $(2 \times \frac{3}{2} + 1)$  and  $(2 \times \frac{1}{2} + 1)$  giving the intensity ratio of 2:1.

The relative intensities of the two lines of the allowed doublet  $2p_{3/2} \rightarrow 2s_{1/2}$  and  $2p_{1/2} \rightarrow 2s_{1/2}$

can be calculated under the assumption that the radial wave functions are the same for the two excited 2p states. Transitions of this type give rise to the principal series in the alkali spectra. The spontaneous transition probabilities and hence the observed intensities if the two P states are equally likely to be occupied are proportional to the squares of the dipole matrix elements.

The dependence of the two excited 2P states and the ground 2S state on the angular and spin coordinates of the electron is obtained by finding linear combinations of products of the four spherical harmonics

$$Y_{1,1}(\theta, \phi), Y_{1,0}(\theta, \phi), Y_{1,-1}(\theta, \phi) \text{ and } Y_{0,0}(\theta, \phi)$$

and the two spin wave functions (+) and (-).

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## 6.5 CHECK YOUR PROGRESS

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1. What are the shortcomings of Hartree's self-consistent field?
2. When a field is said to be self-consistent?
3. Role of central field approximation in the construction of periodic table.

### Let us sum up

This unit explains the Hartree method of approximation which is used to obtain a self-consistent potential. Also it describes the shortcomings of this method and introduced a modification term using Hartree-Fock method. The role of central field approximation in the construction of periodic table is explained. The typical features of alkali atoms like doublet separation and doublet intensity are also emphasized.

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## 6.6 UNIT-END EXERCISES

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Discuss the Hartree-Fock method of central field approximation.

## NOTES

NOTES

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## 6.7 ANSWERS TO CHECK YOUR PROGRESS

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1. In the Hartree method, the many electron wave function is simply a product of one electron wave functions which is not applicable for indistinguishable particles.
2. The approximate wavefunction of a system of many electrons can be found by an iterative method. Assuming the electrons occupy levels similar to that of hydrogen the electrostatic field in which the electrons exist is guessed and then a new set of energy levels and a new field is calculated. The process is repeated until the system is self-consistent.
3. In the first approximation, one can use the hydrogen like wave functions  $R_{nl}(r) \sim r^l$  as  $r \rightarrow 0$ , because of the centrifugal potential  $\hbar^2 l(l+1)/2mr^2$ . This means that the s-state electrons can penetrate closer to the nucleus than d or f state electrons. As a result of the s-state electrons feel the full attraction of the nucleus than d or f state electrons. This explains the lower energy of the 4-s state as compared to the 3d state. The screening effect can become so large that the 4-f state is higher than the 6-s state.

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## 6.8 SUGGESTED READINGS

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1. Quantum Mechanics-G. Aruldhas- PHI learning Private limited, New Delhi 2008.
2. Quantum Mechanics – Theory and Application – Ajoy Ghatak and S. Lokanathan – 5<sup>th</sup> edition – Trinity Press, 2012.

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# BLOCK III: RELATIVISTIC QUANTUM MECHANICS

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*Klein-Gordon Equation*

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## UNIT-VII KLEIN-GORDON EQUATION

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NOTES

### Structure

#### 7.1 Klein Gordon equation

##### 7.1.1 Plane wave solution

#### 7.2 Interaction with electromagnetic fields – Hydrogen like atom

#### 7.3 Check your progress

#### 7.4 Unit – End Exercises

#### 7.5 Answer to Check your progress

#### 7.6 Suggested Readings

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### 7.1 KLEIN GORDON EQUATION

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The nonrelativistic Schrodinger equation was obtained by replacing  $p$  by  $-i\hbar\nabla$  and  $E$  by  $i\hbar\frac{\partial}{\partial t}$  in the classical energy expression of a free particle  $E = \frac{p^2}{2m}$  where as the relativistic expression for energy was obtained as  $E = (c^2p^2 + m^2c^4)^{1/2}$  and allowing the resulting operator equation to operate on the wavefunction. In order to avoid the difficulties are arising from the square root, the operator replacement of  $p$  and  $E$  be made in the relativistic expression for  $E^2$ .

$$E^2 = c^2p^2 + m^2c^4 \rightarrow (1)$$

Where  $m$  is the rest mass of the particle. Replacing  $E$  and  $p$  by the respective operators,

$$-\hbar^2 \frac{\partial^2}{\partial t^2} = -c^2\hbar^2\nabla^2 + m^2c^4 \rightarrow (2)$$

Operating on a wave function, we have,

$$-\hbar^2 \frac{\partial^2 \psi(r, t)}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \psi(r, t) + m^2 c^4 \psi(r, t) \rightarrow (3)$$

Which is the Klein Gordon equation or Schrodinger relativistic equation.

## NOTES

Rearranging (3) we get,

$$\left( \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \psi(r, t) = \frac{m^2 c^2}{\hbar^2} \psi(r, t) \rightarrow (4)$$

$$(\text{or}) \square \psi(r, t) = \frac{m^2 c^2}{\hbar^2} \psi(r, t) \rightarrow (5)$$

Where  $\square$ , the de Alembertian Operator is given by

$$\square = \left( \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right)$$

### 7.1.1 Plane wave solution

The plane wave represented by

$$\psi(r, t) = \exp[i(k \cdot r - \omega t)] \rightarrow (6)$$

is an eigen function of both energy and momentum operators with eigen values  $\hbar\omega$  and  $\hbar k$  respectively. Substituting (6) in (1), we have

$$(\hbar\omega^2) = c^2 \hbar^2 k^2 + m^2 c^4$$

$$(\text{or}) E = \pm \hbar\omega$$

$$E = \pm (c^2 \hbar^2 k^2 + m^2 c^4)^{1/2} \rightarrow (7)$$

which means that the energy eigen value can have both positive and negative values. The appearance of the negative energy solutions is typical of relativistic wave equation.

In non-relativistic case, the position probability density  $P(r, t)$  and the probability current density  $j(r, t)$  satisfy the equation of continuity

$$\frac{\partial P(r, t)}{\partial t} + \nabla \cdot j(r, t) = 0$$



Which is invariant under Lorentz transformation.

∴ It is reasonable to expect the same continuity relation to be valid in the relativistic case too.

Hence we multiply equation (3) on the left by  $\psi^*$ , its complex conjugate equation by  $\psi$  and subtract one from the other. We get,

$$\psi^* \frac{\partial^2 \psi}{\partial t^2} - \psi \frac{\partial^2 \psi^*}{\partial t^2} = c^2 (\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*)$$

$$\frac{\partial}{\partial t} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) = c^2 \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*)$$

$$\frac{1}{c^2} \frac{\partial}{\partial t} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) - \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) = 0$$

$$\frac{\partial}{\partial t} P(r, t) + \nabla \cdot j(r, t) = 0 \rightarrow \text{(8)}$$

This is a continuity equation with

$$P(r, t) = \frac{i\hbar}{2mc^2} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) \rightarrow \text{(9)}$$

$$j(r, t) = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) \rightarrow \text{(10)}$$

This expression for  $j(r,t)$  is identical with the one in non-relativistic case.

However,  $P$  is quite different.

If  $\psi$  is real,  $P(r,t)$  vanishes. If  $\psi$  is complex, then

$$P(r, t) = \left[ \psi^* i\hbar \frac{\partial \psi}{\partial t} + \psi \left( -i\hbar \frac{\partial}{\partial t} \right) \psi^* \right] \frac{1}{2mc^2}$$

$$P(r, t) = \frac{1}{2mc^2} [\psi^* E \psi + \psi E \psi^*]$$

$$P(r, t) = \frac{E}{mc^2} |\psi|^2 \rightarrow \text{(11)}$$

Hence  $P(r,t)$  is positive when  $E$  is positive and viceversa.  $P$  cannot be a probability density because of its positive and negative values. One

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could multiply  $P$  by a charge  $e$  and then interpret it as a charge density and  $e_j$  as their corresponding electric current density. If the system has a single particle of given charge,  $P$  can have different signs at different points. That means the theory is useful only to a system of particles having both signs of charges. It is known that equation (4) can be used to describe a system of arbitrary numbers of particles and their antiparticles by treating  $\psi$  itself as an operator function instead of a numerical valued function.

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## 7.2 INTERACTION WITH ELECTROMAGNETIC FIELDS – HYDROGEN LIKE ATOM

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The wave equation for a charged particle in the coulomb field  $V(r)$  can be obtained by writing  $E-V(r)$  in equation (1), replacing  $p$  and  $E$  by their operators and allowing the resulting operator equation to operate on  $\psi(r,t)$ .

Therefore, (1) becomes

$$(E - V)^2 = c^2 p^2 + m^2 c^4$$

$$\text{(or)} \left( i\hbar \frac{\partial}{\partial t} - e\varphi \right)^2 \psi - c^2 \left( -i\hbar \nabla - \frac{eA}{c} \right)^2 \psi - m^2 c^4 \psi = 0 \rightarrow \text{(12)}$$

If the potential  $A$  and  $\varphi$  are independent of time 't', solutions will be of the form,

$$\psi(r, t) = u(r) \exp\left(\frac{-iEt}{\hbar}\right) \rightarrow \text{(13)}$$

From (12) and (13) we have

$$\left( E + \frac{Ze^2}{r} \right)^2 u(r) = (-c^2 \hbar^2 \nabla^2 + m^2 c^4) u(r) \rightarrow \text{(14)}$$

Since the potential is spherically symmetric, equation (14) can be separated into radial and angular parts

$$u(r, \theta, \varphi) = R(r) Y_{lm}(\theta, \varphi) \rightarrow \text{(15)}$$

The radial wave equation for  $R(r)$  now becomes

$$\left[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{E^2 - m^2 c^4}{\hbar^2 c^2} + \frac{2EZ e^2}{\hbar^2 c^2 r} - \frac{l(l+1) - \frac{z^2 e^4}{\hbar^2 c^2}}{r^2} \right] R = 0$$

→ (16)

This equation has almost the same form as the radial wave equation for the hydrogen atom. For bound states, E must be less than the rest energy  $mc^2$ , so that the second term in (16) is negative. The last term corresponds to the centrifugal term.

By performing the scale transformation

$$\rho = \alpha r \text{ where } \alpha^2 = \frac{4(m^2 c^4 - E^2)}{c^2 \hbar^2} \quad \gamma = \frac{ze^2}{\hbar e} \quad \lambda = \frac{2E\gamma}{c\hbar\alpha} \rightarrow (17)$$

Equation (16) reduces to

$$\left[ \frac{1}{\rho^2} \frac{d}{d\rho} \left( \rho^2 \frac{d}{d\rho} \right) \alpha^2 - \frac{\alpha^2}{4} + \frac{\lambda \alpha^2}{\rho} - \frac{l(l+1) - \gamma^2}{\rho^2} \alpha^2 \right] R = 0$$

Cancelling  $\alpha^2$  throughout, we have

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left( \rho^2 \frac{dR}{d\rho} \right) + \left[ \frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1) - \gamma^2}{\rho^2} \right] R = 0 \rightarrow (18)$$

If we write  $s(s+1) = l(l+1) - \gamma^2$ , equation (17) becomes,

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left( \rho^2 \frac{dR}{d\rho} \right) + \left[ \frac{\lambda}{\rho} - \frac{1}{4} - \frac{s(s+1)}{\rho^2} \right] R = 0 \rightarrow (19)$$

From the requirement that the wave function be well behaved at infinity, we get the condition

$$\lambda = n' + s + 1 \rightarrow (20) \quad n' = 0, 1, 2, \dots$$

$$\text{With } s = -\frac{1}{2} \pm \left[ \left( l + \frac{1}{2} \right)^2 - \gamma^2 \right]^{\frac{1}{2}} \rightarrow (21)$$

For  $l > 0$ , the positive sign leads to a positive value for s and negative sign to a negative value

For  $l = 0$ , both the value of s are negative.

From equation (17) and (20)

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$$\gamma E (m^2 c^4 - E^2)^{-\frac{1}{2}} = n' + \frac{1}{2} + \left[ \left( l + \frac{1}{2} \right)^2 - \gamma^2 \right]^{\frac{1}{2}} \rightarrow (22)$$

On solving this equation for E, we get the quantized energy levels.

From (22)

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$$\begin{aligned} \frac{E\gamma}{(m^2 c^4 - E^2)^{\frac{1}{2}}} &= n' + \frac{1}{2} + \left[ \left( l + \frac{1}{2} \right)^2 - \gamma^2 \right]^{\frac{1}{2}} \\ &= n' + \frac{1}{2} + \left( l + \frac{1}{2} \right) \left[ 1 - \frac{\gamma^2}{2 \left( l + \frac{1}{2} \right)^2} \right] \rightarrow (23) \end{aligned}$$

Writing  $n' + l + 1 = n$  and putting  $\left[ n - \frac{\gamma^2}{2 \left( l + \frac{1}{2} \right)} \right]^2 = A$  in equation (23),

$$\text{we have } \frac{E^2 \gamma^2}{m^2 c^4 - E^2} = A$$

(or)

$$\frac{E^2 \gamma^2}{A} = m^2 c^4 - E^2$$

$$E = mc^2 \left( 1 + \frac{\gamma^2}{A} \right)^{-\frac{1}{2}}$$

$$E = mc^2 \left( 1 - \frac{\gamma^2}{2A} + \frac{3\gamma^4}{8A^2} \right)$$

$$E = mc^2 \left( 1 - \frac{\gamma^2 A^{-1}}{2} + \frac{3\gamma^4 A^{-2}}{8} \right)$$

Expanding  $A^{-1}$  and  $A^{-2}$  by binomial series and retaining terms up to  $\gamma^4$ ,

$$E = mc^2 \left\{ 1 - \frac{\gamma^2}{2n^2} \left[ 1 + \frac{2\gamma^2}{2n \left( l + \frac{1}{2} \right)} \right] + \frac{3\gamma^4}{8n^4} \right\}$$

$$E = mc^2 \left[ 1 - \frac{\gamma^2}{2n^2} - \frac{\gamma^4}{2n^4} \left( \frac{n}{l + \frac{1}{2}} - \frac{3}{4} \right) \right] \rightarrow (24)$$

The first term in equation (24) is the rest energy and the second term  $\frac{-mc^2\gamma^2}{2n^2} = \frac{-z^2me^4}{2\hbar^2n^2}$  is simply the nonrelativistic energy expression of the hydrogen atom.

The third term is the 'relativistic correction' which removes the  $l$ -degeneracy. This term is often referred to the fine structure energy.

The total spread of a level due to fine structure, (ie) the change in  $E$  as  $l$  goes from 0 to  $(n-1)$  for a given  $n$  is

$$\frac{-mc^2\gamma^4}{2n^4} \left[ \left( \frac{n}{n-1 + \frac{1}{2}} - \frac{3}{4} \right) - \left( \frac{n}{\frac{1}{2}} - \frac{3}{4} \right) \right] = \frac{2mc^2\gamma^4}{n^3} \frac{n-1}{2n-1}$$

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### 7.3 CHECK YOUR PROGRESS

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1. Express De Alembertion operator.
2. How the degeneracy can be removed.

#### Let us sum up

The procedure to derive relativistic wave equation for spin '0' particle is explained. The solution and application of the Klien Gordon equation is also dealt.

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### 7.4 UNIT-END EXERCISES

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1. Differentiate Relativistic and non relativistic fields. Obtain the solution for klein Gordon equation and justify how particles accompany its antiparticles.

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### 7.5 ANSWERS TO CHECK YOUR PROGRESS

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1.  $\square = \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}$
2. The relativistic correction term in the energy equation removes the  $l$  degeneracy.

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### 7.6 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldas- PHI learning Private limited, New Delhi 2008.

3. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.

**NOTES**

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# UNIT-VIII RELATIVISTIC HAMILTONIAN

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## Structure

- 8.1 Dirac's relativistic Hamiltonian
- 8.2 Dirac Matrices
- 8.3 Check your progress
- 8.4 Unit – End Exercises
- 8.5 Answer to Check your progress
- 8.6 Suggested Readings

## NOTES

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### 8.1 DIRAC'S RELATIVISTIC HAMILTONIAN

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The occurrence of negative probability density in Klein Gordon equation is due to the presence of time derivatives in the expression for  $P(r,t)$ . Dirac observed that only a first order equation of this form would be free of difficulties experienced with respect to KG equation. He postulated the existence of a Hamiltonian operator  $H$  for relativistic particles, and ensured that the wave equation would be linear in space differential operators thus preserving the relativistic symmetry between space and time

The basic energy equation is

$$E = \pm(c^2 p^2 + m^2 c^4)^{1/2}$$

Replacing  $E$  and  $p$  by its operators the resulting equation will be

$$i\hbar \frac{\partial \psi(r,t)}{\partial t} = \pm (-c^2 \hbar^2 \nabla^2 + m^2 c^4)^{1/2} \psi(r,t) \rightarrow (1)$$

The Dirac Hamiltonian is

$$E = H = c\alpha p + \beta mc^2 \rightarrow (2)$$

Where  $\beta$  and the coefficient of momentum operators  $\alpha_x, \alpha_y, \alpha_z$  are independent of  $p$  since  $H$  is to be linear in  $p$

Equation (2) can also be written as

$$c^2 p^2 + m^2 c^4 = [c(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z + \beta mc)]^2 \rightarrow (3)$$

NOTES

$\alpha_x, \alpha_y, \alpha_z$  and  $\beta$  are not numbers. If they were so, the square of the energy operator would contain terms proportional to  $p_x, p_y, p_z, mc^2$ . But the relativistic energy equation contains no such terms. Hence Dirac postulated that  $\alpha_x, \alpha_y, \alpha_z$  and  $\beta$  are not only numbers, but also they do not commute among themselves, (ie)  $\alpha$ 's and  $\beta$  anticommute in pairs and their squares are unity therefore for equation (3) to hold true, we have

$$\left. \begin{aligned} \alpha_x^2 = \alpha_y^2 = \alpha_z^2 = 1, \beta^2 = 1 \\ \alpha_x \alpha_y + \alpha_y \alpha_x = \alpha_y \alpha_z + \alpha_z \alpha_y = \alpha_z \alpha_x + \alpha_x \alpha_z = 0 \\ \alpha_x \beta + \beta \alpha_x = \alpha_y \beta + \beta \alpha_y = \alpha_z \beta + \beta \alpha_z = 0 \end{aligned} \right\} \rightarrow (4)$$

The energy can now be written as

$$E = \pm c (\alpha_x p_x + \alpha_y p_y + \alpha_z p_z + \beta mc) \rightarrow (5)$$

The positive or negative sign can be taken since replacement of  $\alpha$  by  $-\alpha$  and  $\beta$  and  $-\beta$  does not change the relationships between  $\alpha$ 's and  $\beta$ .

Now replacing  $E$  and  $p$  by their operators and allowing the resulting operator equation to operate on  $\psi(r,t)$ , we have (from (1) and (2) )

$$i\hbar \frac{\partial \psi(r,t)}{\partial t} = -i\hbar \left( \alpha_x \frac{\partial}{\partial x} + \alpha_y \frac{\partial}{\partial y} + \alpha_z \frac{\partial}{\partial z} \right) \psi(r,t) + \beta mc^2 \psi(r,t) \rightarrow (6)$$

Equation (6) is Dirac's relativistic equation for a free particle.

## 8.2 DIRAC MATRICES

The Hamiltonian in equation (2) has to be Hermitian and therefore the matrices  $\alpha_x, \alpha_y, \alpha_z$  and  $\beta$  must be Hermitian and hence square. The eigenvalues of all the four matrices are  $\pm 1$ , since their squares are unity we have

$$\begin{aligned} \alpha_x = \alpha_x \beta^2 = \alpha_x \beta \beta = -\beta \alpha_x \beta \text{ and} \\ \text{tr} \alpha_x = \text{tr}(-\beta \alpha_x \beta) = -\text{tr}(\alpha_x \beta^2) = -\text{tr} \alpha_x \rightarrow (7) \end{aligned}$$

In the III step the cyclic property of trace of matrices (ie)  $\text{tr}(ABCD) = \text{tr}(BCDA)$  is used. It is evident from equation (1) that  $\text{tr} \alpha_x = 0$ . This is possible only when the number of +1 eigenvalues is equal in number to the -1 eigenvalues. The consequence of this result is that the dimension  $n$  of the matrices has to be even. The same is true for the other three matrices ( $\alpha_y, \alpha_z$  and  $\beta$ )

The three Pauli matrices,

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

do anticommute and the square of each is the unit matrix.



Since a fourth matrix that anticommutes with these three cannot be found, with dimension  $n=4$ , one can find four anticommuting matrices.  $\beta$  matrix is taken to be diagonal with two +1 eigenvalues and two -1 eigenvalues. Then one can easily find the 3 other  $4 \times 4$  matrices anticommuting with  $\beta$  and satisfying the conditions specified by equation (4).

$$a_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} \rightarrow \mathbf{(8a)}$$

$$a_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} \rightarrow \mathbf{(8b)}$$

$$a_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} \rightarrow \mathbf{(8c)}$$

$$\beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \rightarrow \mathbf{(8d)}$$

Obviously these matrices are Hermitian since  $\sigma_x, \sigma_y, \sigma_z$  are Hermitian. The matrices given in equations (8) are the Dirac matrices in the standard representation.

Since  $\alpha$ 's and  $\beta$  are  $4 \times 4$  matrices, like Dirac wave function,  $\psi(r,t)$  must be a four column vector.

$$\Psi(r,t) = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}, \psi^\dagger = (\psi_1^* \quad \psi_2^* \quad \psi_3^* \quad \psi_4^*) \rightarrow \mathbf{(9)}$$

These wave functions do not transform as four vectors. They are sometimes referred to as Dirac spinors.

The counter part of a Schrodinger operator in Diracs theory is a  $4 \times 4$  diagonal matrix. Thus, the Schrodinger operators  $x$  and  $p_x$  are represented as,

$$x = \begin{bmatrix} x & 0 & 0 & 0 \\ 0 & x & 0 & 0 \\ 0 & 0 & x & 0 \\ 0 & 0 & 0 & x \end{bmatrix}, \quad p_x = \begin{bmatrix} p_x & 0 & 0 & 0 \\ 0 & p_x & 0 & 0 \\ 0 & 0 & p_x & 0 \\ 0 & 0 & 0 & p_x \end{bmatrix} \rightarrow \mathbf{(10)}$$

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### 8.3 CHECK YOUR PROGRESS

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1. What is the relativistic equation used for treating spin  $\frac{1}{2}$  particles?
2. Express Dirac relativistic Hamiltonian.

#### Let us sum up

The importance of relativistic Hamiltonian in Dirac equation to obtain relativistic wave equation for spin  $\frac{1}{2}$  particles is explained. Dirac's relativistic equation for a free particle and Dirac matrices were obtained.

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### 8.4 UNIT-END EXERCISES

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1. Explain why the dimension of Dirac matrices has to be even.
2. Properties of Dirac matrices.

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### 8.5 ANSWERS TO CHECK YOUR PROGRESS

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1.  $i\hbar \frac{\partial \psi(r,t)}{\partial t} = -i\hbar \left( \alpha_x \frac{\partial}{\partial x} + \alpha_y \frac{\partial}{\partial y} + \alpha_z \frac{\partial}{\partial z} \right) \psi(r,t) + \beta mc^2 \psi(r,t)$
2.  $H = c\alpha p + \beta mC^2$

#### Answers to Unit-End Exercises

1. The trace of Dirac matrices must be equal to zero which is possible only when the no of +1 eigen values is equal to that of -1 eigenvalues. The consequence of this result is that the dimension 'n' of the matrices has to be even.

2.  $\alpha$  and  $\beta$  matrices are hermitian.

$\alpha$  and  $\beta$  matrices are non-singular.

Their determinant is non-zero.

Dirac's  $\alpha$  and  $\beta$  matrices are traceless.

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### 8.6 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldas- PHI learning Private limited, New Delhi 2008.
3. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.

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# UNIT-IX DIRAC PARTICLE

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## Structure

- 9.1 Negative Energy States
- 9.2 Spin of the particle
- 9.3 Check your progress
- 9.4 Unit – End Exercises
- 9.5 Answer to Check your progress
- 9.6 Suggested Readings

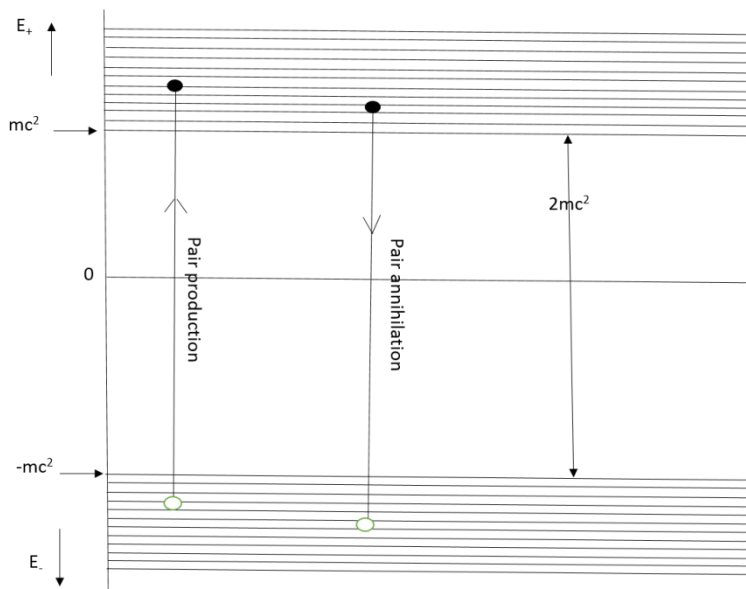
## NOTES

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### 9.1 NEGATIVE ENERGY STATES

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The solutions of Dirac equation consists of four equations. Hence  $E_+$  and  $E_-$  occur twice, when  $p=0$ ,  $E_+=mc^2$  and  $E_-=-mc^2$ . The energy spectrum of a free particle has two branches corresponding to  $E_+$  and  $E_-$ ; one starting from  $mc^2$  and extending to  $\infty$  as  $|p| \rightarrow \infty$  and the other starting at  $-mc^2$  and extending to  $-\infty$  as  $|p| \rightarrow \infty$ . The two branches are separated by a forbidden gap of width  $2mc^2$ . No energy level exists in the forbidden gap.



**Energy levels of a free Dirac particle**

It is very difficult to imagine negative energy states because even a small perturbation could cause transition in an electron in a

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positive energy state to a state of negative energy state thereby releasing an enormous amount of energy. No such things happen in reality. To overcome this problem, Dirac postulated that all negative energy states are normally occupied by electrons and this sea of negative energy electrons have no physically observable effects. Since electrons obey Fermi-Dirac statistics these occupied states cannot accommodate any more electrons. Thus transitions to negative energy states are prevented. It is further assumed that when electron occupying the negative energy state picks up energy and goes to the positive energy state, it takes its place as an ordinary observable electron. The empty space in the midst of the negative energy states behaves as if it is a particle of positive charge. It responds to electric and magnetic fields. The empty space is called a hole. The whole process may, therefore be described as the disappearance of the quantum of energy supplied with a creation of a pair of observable particles; a positive energy electron and another particle differing from the electron only in the sign of its charge. Later, it was named as 'positron' after the discovery of conversion of high energy gamma rays into electron-positron pairs.

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## 9.2 SPIN OF THE DIRAC PARTICLE

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The spin of an electron carries no energy and therefore it can be observed only through its coupling with the orbital motion of the electron. This can be demonstrated through the "conservation of total angular momentum" and through the spin-orbit coupling energy. Hence the existence of spin angular momentum can be proved by Dirac theory.

A dynamical variable that is conserved should commute with the Hamiltonian. The orbital angular momentum  $L = r \times p$ . Let  $L_x$  be the x component of angular momentum and the time rate of change of  $L_x$  for a particle is given by

$$\begin{aligned} i\hbar \frac{dL_x}{dt} &= [L_x, H] \\ &= [y p_z - z p_y, c\alpha_x p_x + \beta m c^2] \\ &= [y p_z, c\alpha_y p_y] - [z p_y, c\alpha_z p_z] \rightarrow (1) \end{aligned}$$

Since  $\alpha$  and  $\beta$  commutes with  $r$  and  $p$ , all the other commutators vanish. Now eqn(1) becomes,

$$\begin{aligned} i\hbar \frac{dL_x}{dt} &= c [y, p_y] p_z \alpha_y - c [z, p_z] p_y \alpha_z \\ &= i\hbar [\alpha_y p_z - \alpha_z p_y] \rightarrow (2) \end{aligned}$$

which shows that  $L_x$  is not a constant of motion. Similar equations hold good for  $L_y$  and  $L_z$ . Hence the orbital angular momentum  $L$  is not a

constant of motion. However, on physical grounds, the total angular momentum must be a constant of motion. Therefore, there must be another contribution to angular momentum, such that the commutator of its x-component with H is the negative to the RHS of eqn(2). This contribution comes from the operator  $\hbar\sigma'$  where

$$\sigma' = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix} \rightarrow (3)$$

Now the equation of motion of its x- component is

$$\begin{aligned} i\hbar \frac{d\sigma'_x}{dt} &= [\sigma'_x, \alpha p + \beta mc^2] \\ &= [\sigma'_x, \alpha_x p_x] + [\sigma'_x, \alpha_y p_y] + [\sigma'_x, \alpha_z p_z] \rightarrow (4) \end{aligned}$$

Since  $\sigma'_x$  commutes with  $\beta$ ,

$$\begin{aligned} [\sigma'_x, \alpha_x] &= 0, [\sigma'_x, \alpha_y] = 2i\alpha_z \\ [\sigma'_x, \alpha_z] &= -2i\alpha_y \rightarrow (5) \end{aligned}$$

Substitute eqn(5) in eqn(4); we get

$$\begin{aligned} i\hbar \frac{d\sigma'_x}{dt} &= -2i\alpha_y p_z - 2i\alpha_z p_y \\ \text{(or)} i\hbar \frac{d}{dt} \left( \frac{1}{2} \hbar \sigma'_x \right) &= -i\hbar (\alpha_y p_z - \alpha_z p_y) \rightarrow (6) \end{aligned}$$

Eqn(6) is the negative of RHS of eqn(2). Similar expressions hold true for  $\sigma'_y$  &  $\sigma'_z$ .

Combining eqn(2) and (6), we have

$$\begin{aligned} \frac{d}{dt} \left( L_x + \frac{1}{2} \hbar \sigma'_x \right) &= 0 \text{ (or)} \\ L_x + \frac{1}{2} \hbar \sigma'_x &= \text{constant} \end{aligned}$$

It is now obvious that  $L_x + \frac{1}{2} \hbar \sigma'_x$  commutes with the Hamiltonian and can therefore be taken as total angular momentum.

From eqn(3)

$$\sigma'^2_x = \sigma'^2_y = \sigma'^2_z = 1.$$

This gives the eigen values of  $\frac{1}{2} \hbar \sigma'$  as  $+\frac{1}{2} \hbar$  or  $-\frac{1}{2} \hbar$ . Hence the additional part

$$S = \frac{1}{2} \hbar \sigma' = \frac{1}{2} \hbar \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$$

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can be interpreted as the spin angular momentum of the electron. Thus the concept of spin angular momentum has evolved automatically from Dirac's Hamiltonian.

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### 9.3 CHECK YOUR PROGRESS

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1. What are holes?
2. Show that  $(\alpha.A)(\alpha.B) = (A.B) + i\sigma' . (AXB)$  where A and B commute with  $\alpha$  and  $\sigma' = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$

#### Let us sum up

The significance of negative energy states in pair production and pair annihilation, postulated by Dirac is explained. The contribution of spin to the conservation of angular momentum is described through Dirac's theory.

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### 9.4 UNIT-END EXERCISES

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1. Significance of negative energy states.
2. Explain how the existence of spin angular momentum can be proved by Dirac theory.

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### 9.5 ANSWERS TO CHECK YOUR PROGRESS

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1. They are the empty space created by the non-observable electrons when they get transferred to positive energy states.

$$2. \text{ We have } (\alpha.A)(\alpha.B) = (\alpha_x A_x + \alpha_y A_y + \alpha_z A_z)(\alpha_x B_x + \alpha_y B_y + \alpha_z B_z) \\ = \alpha_x^2 A_x B_x + \alpha_y^2 A_y B_y + \alpha_z^2 A_z B_z + \alpha_x \alpha_y A_x B_y + \alpha_x \alpha_z A_x B_z + \alpha_y \alpha_x A_y B_x + \alpha_y \alpha_z A_y B_z + \alpha_z \alpha_x A_z B_x + \alpha_z \alpha_y A_z B_y$$

Since  $\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = 1$ ,  $\alpha_x \alpha_y = -\alpha_y \alpha_x$  and the cyclic relations

$$(\alpha.A)(\alpha.B) = (A.B) + \alpha_x \alpha_y (A_x B_y - A_y B_x) + \alpha_y \alpha_z (A_y B_z - A_z B_y) + \alpha_z \alpha_x (A_z B_x - A_x B_z)$$

Where

$$\alpha_x \alpha_y = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} = \begin{pmatrix} \sigma_x \sigma_y & 0 \\ 0 & \sigma_x \sigma_y \end{pmatrix} = i \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} = i\sigma'_z$$

Using this results and the cyclic reactions, we get

$$(\alpha.A)(\alpha.B) = (A.B) + i\sigma' . (AXB)$$

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## 9.6 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldas- PHI learning Private limited, New Delhi 2008.
3. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.

*Dirac Particle*

**NOTES**

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# ***BLOCK IV: ELEMENTS OF FIELD QUANTIZATION AND SCATTERING THEORY***

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## **NOTES**

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## **UNIT-X RELATIVISTIC AND NON-RELATIVISTIC**

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### **Structure**

- 10.1 Elements of field quantization
- 10.2 Classical field equation - Lagrangian form
  - 10.2.1 Classical field equation-Hamiltonian form
- 10.3 Quantization of the field
- 10.4 Quantization of Non- relativistic schrödinger equation
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### **10.1 ELEMENTS OF FIELD QUANTIZATION**

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In general the fields are continuous mechanical systems with a non-denumerable infinite number of degrees of freedom. The degree of the field is called the field functions and these assume the role of the generalized coordinate  $q_i$  of a mechanical system.

A system of particle is specified by the position coordinate  $q_i$  and their dependence on time  $t$ , whereas a field is specified by its



amplitude  $\Psi(r,t)$  at all points of space and the dependence of these amplitudes on the time.

$\Psi(r,t)$  can be expanded in terms of some complete orthonormal set of functions  $u_k(r)$  as

$$\Psi(r, t) = \sum_k c_k(t) u_k(r)$$

Where  $c_k(t)$  can be considered as field coordinates,

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## 10.2 CLASSICAL FIELD EQUATION - LAGRANGIAN FORM

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Since the field Lagrangian is considered to be a function of the field amplitude  $\Psi(r,t)$ , Lagrangian density  $\mathcal{L}$  which is function of  $\Psi, \nabla\Psi, \dot{\Psi}$  and  $t$  is introduced in the field equation ,

$$(ie) \mathcal{L} = \mathcal{L}(\Psi, \nabla\Psi, \dot{\Psi}, t) \rightarrow (1)$$

The Lagrangian  $\mathcal{L}$  of the field would be an integral of  $\mathcal{L}$  over space

$$L = \int_v \mathcal{L}(\Psi, \nabla\Psi, \dot{\Psi}, t) d^3r \rightarrow (2)$$

According to the variational principle

$$\delta \int_{t_1}^{t_2} L dt = \delta \int_{t_1}^{t_2} \int_v \mathcal{L}(\Psi, \nabla\Psi, \dot{\Psi}, t) d^3r dt = 0$$

(or)

$$\int_{t_1}^{t_2} \int_v (\delta\mathcal{L}) d^3r dt = 0 \rightarrow (3)$$

Where the variation  $\delta\Psi$  of  $\Psi$  is subjected to the condition

$$\delta\Psi(r, t_1) = \delta\Psi(r, t_2) = 0 \rightarrow (4)$$

The variation in  $\mathcal{L}$  can easily be written from equation (1) as,

$$\begin{aligned} \delta\mathcal{L} &= \frac{\partial\mathcal{L}}{\partial\Psi} \delta\Psi + \frac{\partial\mathcal{L}}{\partial(\nabla\Psi)} \delta(\nabla\Psi) + \frac{\partial\mathcal{L}}{\partial\dot{\Psi}} \delta\dot{\Psi} \\ \delta\mathcal{L} &= \frac{\partial\mathcal{L}}{\partial\Psi} \delta\Psi + \sum_{x,y,z} \frac{\partial\mathcal{L}}{\partial(\frac{\partial\Psi}{\partial x})} \frac{\partial}{\partial x} (\delta\Psi) + \frac{\partial\mathcal{L}}{\partial\dot{\Psi}} (\delta\dot{\Psi}) \rightarrow (5) \end{aligned}$$

$$\text{Since } \delta\left(\frac{\partial\Psi}{\partial x}\right) = \frac{\partial}{\partial x} (\delta\Psi) \text{ and } \delta\dot{\Psi} = \delta\left(\frac{\partial\Psi}{\partial t}\right) = \frac{\partial}{\partial t} (\delta\Psi)$$

NOTES

Equation (5) reduces to

$$\delta\mathcal{L} = \frac{\partial\mathcal{L}}{\partial\psi} \delta\psi + \sum_{x,y,z} \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial x}\right)} \frac{\partial}{\partial x} (\delta\psi) + \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \frac{\partial}{\partial t} (\delta\psi) \rightarrow (6)$$

Substitute (6) in (3), we have

$$\int_{t_1}^{t_2} \int_v \left[ \frac{\partial\mathcal{L}}{\partial\psi} \delta\psi + \sum_{x,y,z} \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial x}\right)} \frac{\partial}{\partial x} (\delta\psi) + \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \frac{\partial}{\partial t} (\delta\psi) \right] d^3r dt = 0 \rightarrow (7)$$

Consider,

$$\int_{t_1}^{t_2} \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \frac{\partial}{\partial t} (\delta\psi) dt, \text{ integrating by parts we get}$$

$$\begin{aligned} \int_{t_1}^{t_2} \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \frac{\partial}{\partial t} (\delta\psi) dt &= \left[ \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \delta\psi \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} \frac{\partial}{\partial t} \left( \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \right) \delta\psi dt \\ &= - \int_{t_1}^{t_2} \frac{\partial}{\partial t} \left( \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \right) \delta\psi dt \rightarrow (8) \end{aligned}$$

Since the first term vanishes in accordance with equation (4)

Now integrating by parts the second term, we get

$$\begin{aligned} &\int_v \sum_{x,y,z} \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial x}\right)} \frac{\partial}{\partial x} (\delta\psi) d^3r \\ &= \sum_{x,y,z} \int \int \left[ \int \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial x}\right)} \frac{\partial}{\partial x} (\delta\psi) dx \right] dy dz \\ &= \sum_{x,y,z} \left[ \int \int \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial x}\right)} (\delta\psi) dy dz - \int_v \frac{\partial}{\partial x} \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial x}\right)} (\delta\psi) d^3r \right] \\ &= - \sum_{x,y,z} \int_v \frac{\partial}{\partial x} \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial x}\right)} (\delta\psi) d^3r \rightarrow (9) \end{aligned}$$

From equations (7),(8) and (9)

$$\int_{t_2}^{t_1} dt \int d^3r \left[ \frac{\partial\mathcal{L}}{\partial\psi} - \sum_{x,y,z} \frac{\partial}{\partial x} \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial x}\right)} - \frac{\partial}{\partial t} \left( \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \right) \right] \delta\psi = 0 \rightarrow (10)$$

This equation is valid for any arbitrary variation  $\delta\Psi$  at each point in space, therefore the integrand in the square bracket of equation (10) must vanish,

$$\therefore \frac{\partial \mathcal{L}}{\partial \Psi} - \sum_{x,y,z} \frac{\partial}{\partial x} \left( \frac{\partial \mathcal{L}}{\partial \left( \frac{\partial \Psi}{\partial x} \right)} \right) - \frac{\partial}{\partial t} \left( \frac{\partial \mathcal{L}}{\partial \dot{\Psi}} \right) = 0 \rightarrow (11)$$

Which is the classical field equation in terms of Lagrangian density.

The Lagrangian equation can be written in terms of its functional derivatives also. The value of a function at a point  $r$  depends on the value of its arguments whereas the value of a functional depends on the value of its arguments over a whole region. This can be obtained by replacing the volume integrals by summations over these cells. The volume of the  $i^{th}$  cell is denoted by  $\delta\tau_i$ . In the limit all the  $\delta\tau_i$  approach zero,

$$\sum_i \mathcal{L} [\Psi_i(\nabla\Psi_i)\dot{\Psi}_i, t] \delta\tau_i \rightarrow L(\Psi, \dot{\Psi})$$

Now the  $t$  integrand in equation (10) can now be written as

$$\sum_i \left\{ \frac{\partial \mathcal{L}}{\partial \Psi} - \sum_{x,y,z} \frac{\partial}{\partial x} \left( \frac{\partial \mathcal{L}}{\partial \left( \frac{\partial \Psi}{\partial x} \right)} \right) \right\} \delta\Psi_i \delta\tau_i + \sum_i \left( \frac{\partial \mathcal{L}}{\partial \dot{\Psi}} \right) \delta\dot{\Psi}_i \delta\tau_i \rightarrow (12)$$

Their function derivative can be defined as;

$$\frac{\delta L}{\delta \Psi} = \lim_{\delta\tau_i} \frac{\delta L}{\delta \Psi_j \delta \Psi_j} = \frac{\partial \mathcal{L}}{\partial \Psi} - \sum_{x,y,z} \frac{\partial}{\partial x} \left( \frac{\partial \mathcal{L}}{\partial \left( \frac{\partial \Psi}{\partial x} \right)} \right) \rightarrow (13)$$

$$\frac{\delta L}{\delta \dot{\Psi}} = \lim_{\delta\tau_j} \frac{\delta L}{\delta \dot{\Psi}_j \delta \Psi_j} = \frac{\partial \mathcal{L}}{\partial \dot{\Psi}}$$

Finally the classical field equation in terms of functional derivative is;

$$\frac{\partial}{\partial t} \left( \frac{\delta L}{\delta \dot{\Psi}} \right) - \frac{\delta L}{\delta \Psi} = 0 \rightarrow (14) \quad [from (11) And (13)]$$

### 10.2.1 Classical field equation-Hamiltonian form

The momentum  $P_i$  Conjugate to  $\Psi_i$  is defined by

$$P_i = \frac{\partial \mathcal{L}}{\partial \dot{\Psi}_i} \quad (or) \quad P_i = \left( \frac{\delta L}{\delta \dot{\Psi}_i} \right) \delta\tau_i$$

### NOTES

$$\text{and } P_i = \left( \frac{\partial L}{\partial \dot{\psi}_i} \right) \delta \tau_i$$

The Hamiltonian  $H = \sum_i P_i \dot{\psi}_i - L$

(ie)

$$\begin{aligned} H &= \lim_{\delta \tau_i \rightarrow 0} \left[ \sum_i \pi_i \dot{\psi}_i \delta \tau_i - \sum_i L_i \right] \delta \tau_i \\ &= \int \left[ \pi(r, t) \dot{\psi}(r, t) - \mathcal{L} \right] d^3 r \end{aligned}$$

$= \int \mathcal{H} d^3 r$  where  $\mathcal{H} = \pi \dot{\psi} - \mathcal{L}$  is the Hamiltonian density and  $\pi$  is called the conjugate field. (ie)

$$\pi = \frac{\partial L}{\partial \dot{\psi}} = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \rightarrow (1)$$

The classical field equation is

$$\frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{\psi}} \right) - \frac{\partial L}{\partial \psi} = 0$$

$$\frac{\partial \pi}{\partial t} - \frac{\partial \mathcal{L}}{\partial \psi} = 0 \rightarrow \text{from (1)}$$

(or)

$$\dot{\pi} = \frac{\partial \mathcal{L}}{\partial \psi}$$

$$\text{Now, } \delta L = \int \left( \frac{\partial L}{\partial \psi} \delta \psi + \frac{\partial L}{\partial \dot{\psi}} \delta \dot{\psi} \right) d^3 r$$

$$\delta L = \int \left( \dot{\pi} \delta \psi + \pi \delta \dot{\psi} \right) d^3 r$$

$$= \int \left( \pi \delta \dot{\psi} + \dot{\pi} \delta \psi \right) - \psi (\dot{\delta \pi}) d^3 r$$

$$H = \int \mathcal{H} d^3 r = \int (\pi \dot{\psi} - \mathcal{L}) d^3 r$$

$$\delta H = \int \delta (\pi \dot{\psi}) d^3 r - \delta \int \mathcal{L} d^3 r$$

$$\text{But } L = \int \mathcal{L} d^3 r$$

$$\therefore \delta L = \delta \int \mathcal{L} d^3 r$$

## NOTES

$$\therefore \delta H = \int \delta(\pi\dot{\Psi}) d^3r - \delta L$$

$$\delta H = \int \delta(\pi\dot{\Psi}) d^3r - \int \left[ \dot{\pi}\delta\Psi + \delta\dot{\pi}\Psi - \dot{\Psi}\delta\pi \right] d^3r$$

$$\delta H = \int \left( \dot{\Psi}\delta\pi - \dot{\pi}\delta\Psi \right) d^3r$$

Also

$$\delta H = \int \left( \frac{\partial H}{\partial \Psi} \delta\Psi + \frac{\partial H}{\partial \pi} \delta\pi \right) d^3r$$

$$\dot{\Psi} = \frac{\partial H}{\partial \pi} \text{ and } \dot{\pi} = -\frac{\partial H}{\partial \Psi}$$

These equations are referred to as classical field equation in Hamiltonian form.

## NOTES

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### 10.3 QUANTIZATION OF THE FIELD

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The field variables  $\psi$  and  $\pi$  are regarded as operator functions while quantizing a field. Hence the requirement of quantum conditions for canonical field variables will be,

$$\left. \begin{aligned} [\psi_i, \psi_j] &= [P_i, P_j] = 0 \\ \text{and} \\ [\psi_i, P_j] &= i\hbar\delta_{ij} \end{aligned} \right\} \rightarrow (1)$$

Assuming the cell volumes are small, (1) can be written as,

$$[\psi(r, t), \psi(r', t)] = [\pi(r, t), \pi(r', t)] = 0$$

&

$$[\psi(r, t), \pi(r', t)] = i\hbar\delta(r, r')$$

$\delta(r, r') = \frac{1}{\delta\tau_i}$  (if  $r$  and  $r'$  are in the same cell, otherwise it is zero)

$\delta(r, r')$  can be replaced by the 3D Dirac  $\delta$  function  $\delta(r - r')$ .

$\therefore$  we have,

$$\left. \begin{aligned} [\psi(r, t), \psi(r', t)] &= [\pi(r, t), \pi(r', t)] = 0 \\ \text{and} \\ [\psi(r, t), \pi(r', t)] &= i\hbar\delta(r - r') \end{aligned} \right\} \rightarrow (2)$$

The equation of motion for any dynamical variable  $F$  is given by,

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{1}{i\hbar} [F, H] \rightarrow (3)$$

Eqn. (2) & (3) completely describe the behavior of the quantized field specified by the Hamiltonian.

## NOTES

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### 10.4 QUANTIZATION OF NON-RELATIVISTIC SCHRÖDINGER EQUATION

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The name Schrödinger field is used for a field  $\psi(r, t)$  satisfying the equation,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \rightarrow (1)$$

This eqn. is already the quantized eqn. of motion of particle of mass  $m$  moving in a potential  $V$ . When this equation has been quantized for the second time by the procedure explained above, it is called as second quantization.

The classical field eqn. in terms of  $\mathcal{L}$  is ,

$$\frac{\partial \mathcal{L}}{\partial \psi} - \sum_{x,y,z} \frac{\partial}{\partial x} \left( \frac{\partial \mathcal{L}}{\partial \left( \frac{\partial \psi}{\partial x} \right)} \right) - \frac{\partial}{\partial t} \left( \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \right) = 0 \rightarrow (2)$$

The Lagrangian density  $\mathcal{L}$  takes the form,

$$\mathcal{L} = i\hbar \psi^* \dot{\psi} - \frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi - V(r,t) \psi^* \psi \rightarrow (3)$$

The variation with respect to  $\psi^*$  in eqn. (2) directly gives eqn. (1), while the variation with respect to  $\psi$  gives the complex conjugate of eqn. (1),

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* + V\psi^* \rightarrow (4)$$

The momentum canonically conjugate to  $\psi$  is,

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\hbar \psi^* \rightarrow (5) \text{ [from(3)]}$$

The Hamiltonian density  $\mathcal{H}$  can be written as,

$$\mathcal{H} = \pi \dot{\psi} - \mathcal{L} = \frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi + V\psi^* \psi \text{ [from(5)and (3)]}$$

Multiplying by  $-i^2 (=1)$

$$\mathcal{H} = -\frac{i\hbar}{2m} \nabla(i\hbar\psi^*)\nabla\psi - \frac{i}{\hbar} V(i\hbar\psi^*)\psi$$

$$\mathcal{H} = -\frac{i\hbar}{2m} \nabla\pi\nabla\psi - \frac{i}{\hbar} V\pi\psi \rightarrow (6)$$

The Hamiltonian  $H$  can also give by,

$$H = \int_v \mathcal{H} d^3r = \int_v \left( \frac{\hbar^2}{2m} \nabla\psi^*\nabla\psi + V\psi^*\psi \right) d^3r \rightarrow (7)$$

In terms of functional derivatives,

$$\left. \begin{aligned} \dot{\psi} &= \frac{\delta H}{\delta \pi} = \frac{\partial \mathcal{H}}{\partial \pi} - \nabla \cdot \frac{\partial \mathcal{H}}{\partial (\nabla \pi)} \\ \text{and} \\ \dot{\pi} &= -\frac{\delta H}{\delta \psi} = -\left( \frac{\partial \mathcal{H}}{\partial \psi} - \nabla \cdot \frac{\partial \mathcal{H}}{\partial (\nabla \psi)} \right) \end{aligned} \right\} \rightarrow (8)$$

From (8) and (6),

$$\dot{\psi} = -\frac{i}{\hbar} V\psi + \frac{i\hbar}{2m} \nabla^2 \psi$$

Multiplying by  $i\hbar$ ,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \rightarrow (9)$$

And also  $\dot{\pi} = \frac{i}{\hbar} V\pi - \frac{i\hbar}{2m} \nabla^2 \pi$

Using eqn. (5) the above eqn. becomes,

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* + V\psi^* \rightarrow (10)$$

Eqn. (9) and (10) are the classical equation. and it's complex conjugate for the Schrödinger (non- relativistic) field.

[∴  $\psi$  now operator,  $\psi^*$  is the Hermitian adjoint of  $\psi$  rather than its complex conjugate and it is denoted by  $\psi^\dagger$ .  $H$  is Hermitian and the quantized Hamiltonian is the operator]

The corresponding quantum condition is,

$$[\psi(r, t), \psi^\dagger(r', t)] = \delta(r - r') \rightarrow (11)$$

NOTES

It is easy to expand  $\psi$  in terms of some complete orthonormal set of functions  $\{u_k\}$  as,

$$\psi(r, t) = \sum_k a_k(t) u_k(r) \rightarrow \quad (12)$$

Where  $a_k(t) \rightarrow$  expansion co-efficient which depend on the time  $t$ .

Eqn. (5) now takes the form,

$$\psi^+(r, t) = \frac{1}{i\hbar} \pi(r, t) = \sum_k a_k^+(t) u_k^*(r) \rightarrow \quad (13)$$

The co-efficient  $a_k(t)$  and  $a_k^+(t)$  are operators.

#### 10.4.1 System of Boson

Multiplying (12) by  $u_l^*(r)$  and integrating over the whole range of the variable,

$$\int u_l^*(r) \psi(r, t) d^3r = \sum_k a_k(t) \int u_l^*(r) u_k(r) d^3r$$

Using the orthonormality of  $u_k^*$ ,

$$a_k(t) = \int u_k^*(r) \psi(r, t) d^3r \rightarrow \quad (14)$$

Similarly,

$$a_k^+(t) = \int u_k(r) \psi^+(r, t) d^3r \rightarrow \quad (15)$$

$$a_l^+(t) = \int u_l^*(r') \psi^+(r', t) d^3r'$$

Now,

$$[a_k, a_l^+] = \iint u_k^*(r) u_l(r') [\psi(r, t) \psi^+(r', t)] d^3r d^3r' \rightarrow \quad (16)$$

By eqn. (11), eqn. (16) reduces to,

$$\begin{aligned} [a_k, a_l^+] &= \iint u_k^*(r) u_l(r') \delta(r - r') d^3r d^3r' \\ &= \int u_k^*(r) u_l(r) d^3r = \delta_{kl} \rightarrow \quad (17) \end{aligned}$$

Similarly

$$[a_k, a_l] = [a_k^+, a_l^+] = 0 \rightarrow \quad (18)$$



The number operator, representing the total number of particles is defined by,

$$N = \int \psi^\dagger \psi d^3r \rightarrow (19)$$

Using eqns. (12) and (13),

$$\begin{aligned} N &= \sum_k \sum_l a_k^\dagger a_l \int u_k^* u_l d^3r \\ &= \sum_k \sum_l a_k^\dagger a_l \delta_{kl} = \sum_k a_k^\dagger a_k = \sum_k N_k \rightarrow (20) \end{aligned}$$

where,

$$N_k = a_k^\dagger a_k \rightarrow (21)$$

Let us consider,

$$\begin{aligned} [N_k, N_l] &= [a_k^\dagger a_k, a_l^\dagger a_l] \\ &= [a_k^\dagger a_k, a_l^\dagger] a_l + a_l^\dagger [a_k^\dagger a_k, a_l] \\ &= a_k^\dagger [a_k, a_l^\dagger] a_l + [a_k^\dagger, a_l^\dagger] a_k a_l + a_k^\dagger a_l^\dagger [a_k, a_l] + a_l^\dagger [a_k^\dagger, a_l] a_k \\ &= a_k^\dagger \delta_{kl} a_l + 0 + 0 + a_l^\dagger (-\delta_{kl}) a_k = 0 \end{aligned}$$

Hence  $N_k$  commutes with all others.

$\therefore N_k$  commutes with all others, they can have simultaneous eigenkets and can be diagonalized simultaneously. If  $n_1, n_2, \dots, n_k, \dots, \infty$  are the eigenvalues then the corresponding eigenkets are:

$$|n_1, n_2, \dots, n_k, \dots \rangle$$

The eigenvalue eqn. of  $N_k$  can be written as,

$$N_k \psi(n_k) = n_k \psi(n_k) \rightarrow (22)$$

Multiplying (22) by  $\psi^\dagger(n_k)$  and integrating over the entire space,

$$\begin{aligned} n_k &= \int \psi^\dagger(n_k) N_k \psi(n_k) d^3r \\ &= \int \psi^\dagger(n_k) a_k^\dagger a_k \psi(n_k) d^3r \quad [from (2)] \\ &= \int |a_k \psi(n_k)|^2 d^3r \geq 0 \end{aligned}$$

(i.e.,)  $n_k$  are all positive integers including zero

## NOTES

$$(ie)n_k=0,1,2,\dots,\infty$$

Therefore  $n_k$  has the value '0', there must exist an eigenket  $|0\rangle$  such that  $N_k|0\rangle=0$  for all  $k$ . The lowest normalized eigenket with no particle in the state  $|0\rangle$  is called the vacuum state.

Substituting the value of  $\psi(r, t)$  from equation (12) in the equation (7),

## NOTES

$$H = \sum_k \sum_l a_k^\dagger a_l \int \left( \frac{\hbar^2}{2m} \nabla u_k^* \nabla u_l + V u_k^* u_l \right) d^3 r \rightarrow (23)$$

Integrating the I term by parts, we have

$$\int \nabla u_k^* \nabla u_l d^3 r = \int u_k^* \nabla u_l ds - \int u_k^* \nabla^2 u_l d^3 r$$

Since  $u_k \rightarrow 0$  at the infinite bounding surface, the I term on RHS vanishes. (23) becomes

$$H = \sum_k \sum_l a_k^\dagger a_l \int u_k^* \left( -\frac{\hbar^2}{2m} \nabla^2 u_l + V u_l \right) d^3 r$$

Using the Schrödinger equation,

$$\begin{aligned} -\frac{\hbar^2}{2m} \nabla^2 u_l + V u_l &= E_l u_l \\ H &= \sum_k \sum_l a_k^\dagger a_l \int u_k^* E_l u_l d^3 r \\ &= \sum_k \sum_l a_k^\dagger a_l E_l \int u_k^* u_l d^3 r \\ H &= \sum_k a_k^\dagger a_k E_k = \sum_k N_k E_k \end{aligned}$$

The eigen value of the Hamiltonian H is,

$$E = \langle H \rangle = \sum_k n_k E_k \rightarrow (24)$$

It is evident from equation (24) that  $n_k$  is the number of particles in the state  $u_k$  with energy  $E_k$  and hence  $N_k$  can be regarded as the particle number operator in the  $k^{th}$  state. Since a given state  $u_k$  can be occupied by any number of particles of the same energy, the field represents an assembly of bosons.

### 10.4.2 Creation and annihilation operators

The commutator of  $a_k$  with  $N_k$  is,

$$[a_k, N_k] = [a_k, a_k^\dagger a_k] = [a_k, a_k^\dagger] a_k + a_k^\dagger [a_k, a_k] = a_k \rightarrow (25)$$

Similarly,

$$[a_k^\dagger, N_k] = -a_k^\dagger \rightarrow (26)$$

From equation (25) we have,

$$N_k a_k = a_k N_k - a_k$$

Allowing the operator equation to operate on  $\psi(n_k)$ ,

$$\begin{aligned} N_k a_k \psi(n_k) &= (a_k N_k - a_k) \psi(n_k) \\ &= a_k n_k \psi(n_k) - a_k \psi(n_k) \\ &= (n_k - 1) a_k \psi(n_k) \end{aligned}$$

This means that if  $\psi(n_k)$  is an eigenket of  $N_k$  with eigen value  $n_k$ ,  $a_k \psi(n_k)$  is also an eigenket of  $N_k$  with eigen value lowered by 1 (i.e.,) the number of particles in the  $k$  state is decreased by 1. Hence,  $a_k$  is considered as an annihilation or destruction operator for the  $k^{th}$  state of the field.

Similarly,

$$N_k a_k^\dagger \psi(n_k) = (n_k + 1) a_k^\dagger \psi(n_k)$$

(i.e.,)  $a_k^\dagger \psi(n_k)$  is also an eigenket of  $N_k$  with eigen value increased by 1 and the number of particles in the  $k^{th}$  state is increased by 1. Hence  $a_k^\dagger$  is considered as a creation operator for the  $k^{th}$  state of the field.

### 10.4.3 System of fermions

For a system of fermions, the number of particles  $n_k$  in any state should be restricted to 0 and 1, to be in accordance with Pauli's exclusion principle. In order to follow this the following anticommutation relation are used.

$$[a_k, a_l^\dagger]_+ = \delta_{kl} [a_k, a_l]_+ = [a_k^\dagger, a_l^\dagger]_+ = 0 \rightarrow (27)$$

From equation (27) we have,

$$\begin{aligned} a_k a_k^\dagger + a_k^\dagger a_k &= 1 \text{ and} \\ a_k a_k &= a_k^\dagger a_k^\dagger = 0 \end{aligned}$$

The particle number operator can be defined as,

$$N_k = a_k^\dagger a_k$$

### NOTES

**NOTES**

$\therefore N_k$  commutes with all others and therefore, they can be diagonalized simultaneously. The eigen value of  $N_k$  can be obtained by evaluating the square of  $N_k$ .

$$\begin{aligned} N_k^2 &= a_k^\dagger a_k a_k^\dagger a_k = a_k^\dagger (a_k a_k^\dagger) a_k = a_k^\dagger (1 - a_k^\dagger a_k) a_k \\ &= a_k^\dagger a_k = N_k \quad \therefore, \text{II term} = 0 \text{ (from equation (27))} \end{aligned}$$

$N_k$  is a diagonal with eigenvalue  $n_k$  and therefore  $N_k^2$  would also be a diagonal with eigen value  $n_k^2$ .

$$\text{(i.e.,)} \quad n_k^2 = n_k \text{ or } n_k^2 - n_k = 0$$

$$n_k(n_k - 1) = 0 \quad \Rightarrow n_k = 0, 1.$$

Thus the eigen values of  $N_k$  are 0 and 1. Thus number operator  $N$  representing total number of particles is given by,

$$N = \sum_k N_k$$

The expression for field Hamiltonian is same as in the case of bosons.

$$\text{(i.e.,)} \quad H = \sum_k \int d^3r a_k^\dagger a_l \int d^3r u_k^* \left( -\frac{\hbar^2}{2m} \nabla^2 u_l + V u_l \right) d^3r$$

$N_k$  can be represented by the diagonal matrix whose eigen value are 0 and 1.

$$N_k = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Matrices for  $a$  and  $a^\dagger$  satisfying the condition  $a_k a_k = a_k^\dagger a_k^\dagger = 0$  are,

$$a = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad ; \quad a^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

The kets representing the eigen values 0 and 1 are,

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad ; \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

---

## 10.5 CHECK YOUR PROGRESS

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1. Why do we require quantum field theory?
2. Define second quantisation.
3. Elements of quantisation.

### Let us sum up

The need of quantization, derivation of classical field equation both in Lagrangian and Hamiltonian form and the elements of field of

quantization are described in this unit. The procedure to quantize a non relativistic Schrodinger equation and how this field explains both the system of bosons and fermions is also described.

*Relativistic and non-relativistic*

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## 10.6 UNIT-END EXERCISES

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1. Explain the Lagrangian field theory to obtain the classical field equation.
2. For a system of fermions, define the number operator  $N_k$  and show that its eigen values are 0 and 1.

**NOTES**

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## 10.7 ANSWERS TO CHECK YOUR PROGRESS

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1. In any dynamical system, we have finite numbers of degrees of freedom, (ie) it has a fixed number of particles. Such formalism do not explain the processes such as beta decay, positron-electron pair creation etc.. Therefore a new theory is required which deals with a infinite number of particles.
2. As the initial fields are wave fields with amplitudes obeying classical wave equations, the process of their quantization is called first quantization. The wave-particle fields  $\psi$  obeying Schrodinger or Dirac equations can also be further quantized and the process is called second quantization.
3. The field variables  $\psi$  and  $\pi$  are regarded as operator functions while quantizing a field. Hence the requirement of quantum conditions for canonical field variables will be,

$$\left. \begin{aligned} [\psi(r, t), \psi(r', t)] &= [\pi(r, t), \pi(r', t)] = 0 \\ &\text{and} \\ [\psi(r, t), \pi(r', t)] &= i\hbar\delta(r - r') \end{aligned} \right\} \rightarrow (1)$$

The equation of motion for any dynamical variable F is given by,

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{1}{i\hbar} [F, H] \rightarrow (2)$$

Eqn. (1) & (2) completely describe the elements of the quantized field specified by the Hamiltonian.

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## 10.8 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.

*Relativistic and non-relativistic*

2. Quantum Mechanics-G. Aruldas- PHI learning Private limited, New Delhi 2008.

3. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.

## **NOTES**

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# UNIT-XI KLEIN-GORDON FIELD

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*Klein-Gordon field*

## Structure

- 11.1 Relativistic fields
- 11.2 The Klein-Gordon fields
- 11.3 The Dirac field
- 11.4 Quantization of electromagnetic fields
- 11.5 Check your progress
- 11.6 Unit – End Exercises
- 11.7 Answer to Check your progress
- 11.8 Suggested Readings

**NOTES**

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## 11.1 RELATIVISTIC FIELDS

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The relativistic field can consistently be quantized by using only one of the statistics because of the close relationship between the wave equation and spin of the particles and that between spin and statistics. Therefore, the field equation representing a system of bosons will be different from the one that represents a system of fermions.

In covariant form, it is practice to write,

$$\frac{\partial}{\partial t} \text{ as } \partial_t \text{ and } \frac{\partial}{\partial x_\mu} \text{ as } \partial_\mu$$

Natural, system of units is used in relativistic quantum field theory, in which there is only one fundamental unit, which is the unit of mass. Both  $c$  and  $\hbar$  are dimensionless and of magnitude  $\hbar=c=1$

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## 11.2 THE KLEIN-GORDON FIELDS

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The KG field is a relativistic field in which the spin of the particles is zero. The relativistic wave equation for KG field is,

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) \psi(\mathbf{r},t) = \frac{m^2 c^2}{\hbar^2} \psi(\mathbf{r},t) \rightarrow (1)$$

In terms of natural units, eqn.(1) can be written as

$$\left. \begin{aligned} (\partial_\mu \partial_\mu - m^2)\phi(X, t) = 0 \\ (or) (\partial_\mu \partial_\mu - m^2)\phi(x) = 0 \end{aligned} \right\} \rightarrow (2)$$

where  $X \rightarrow 3$  dimensional position vector

and  $x \rightarrow$  space-time coordinate force-vector ( $x, ict$ )

## NOTES

The interpretation of this equation as a single particle equation led to the occurrence of negative probability density. This difficulty can be removed if the KG field  $\phi(x)$  is quantized.

A suitable Lagrangian density that could reproduce the KG equation is

$$\mathcal{L}_{KG} = -(\partial_\mu \phi \partial_\mu \phi^* + m^2 \phi \phi^*) \rightarrow (3)$$

where  $\phi$  and  $\phi^*$  are independent fields.

In general, the field  $\phi(x)$  is complex. If  $\phi_1$  and  $\phi_2$  are real fields,  $\phi$  and  $\phi^*$  can be written as

$$\phi(x) = \frac{1}{\sqrt{2}} [\phi_1(x) - i\phi_2(x)] \rightarrow (4a)$$

$$\phi^*(x) = \frac{1}{\sqrt{2}} [\phi_1(x) + i\phi_2(x)] \rightarrow (4b)$$

$\phi_1$  and  $\phi_2$  satisfy equation 2. Now equation 3 becomes,

$$\begin{aligned} \mathcal{L}_{KG}(x) &= \frac{-1}{2} \partial_\mu (\phi_1 - \phi_2) \partial_\mu (\phi_1 + i\phi_2) - \frac{1}{2} m^2 (\phi_1 - i\phi_2) (\phi_1 + i\phi_2) \\ &= \frac{-1}{2} (\partial_\mu \phi_1 \partial_\mu \phi_1 + \partial_\mu \phi_2 \partial_\mu \phi_2) - \frac{1}{2} m^2 (\phi_1^2 + \phi_2^2) \\ &= \frac{-1}{2} \sum_{r=1}^2 (\partial_\mu \phi_r \partial_\mu \phi_r + m^2 \phi_r^2) \rightarrow (5) \end{aligned}$$

The conjugate momentum,

$$\pi_r(x) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}_r} = i \partial_4 \phi_r = \dot{\phi}_r \rightarrow (6)$$

The Hamiltonian density is defined by,

$$\mathcal{H} = \sum_{r=1}^2 (\pi_r(x) \dot{\phi}_r(x) - \mathcal{L})$$

$$\text{Now } H = \int_V H d^3x = - \sum_{r=1}^2 \int \partial_4 \phi_r \partial_4 \phi_r d^3x +$$

$$\frac{1}{2} \sum_{r=1}^2 \int \partial_\mu \phi_r \partial_\mu \phi_r + m^2 \phi_r^2 d^3x \rightarrow (7)$$



The canonical quantization rules for  $\phi_r$  and  $\pi_r$  are as follows

$$[\phi_r(x, t), \pi_s(x', t)] = i\delta_{rs}\delta(x - x')$$

$$[\phi_r(x, t), \phi_s(x', t)] = [\pi_r(x, t), \pi_s(x', t)] = 0 \rightarrow \text{(8)}$$

The expansion of  $\phi(x)$  in terms of a complete set of orthonormal solutions of the KG equations is necessary to quantize  $\phi_1$  and  $\phi_2$ .

Expanding  $\phi(x)$  in terms of the complete set of plane wave solutions, we have

$$\phi_r(x) = \sum_k \frac{1}{\sqrt{2v\omega_k}} [a_r e^{ikx} + a_r^+ e^{-ikx}]$$

Where the operators  $a_r$  and  $a_r^+$  are taken to be the Hermitian adjoints of each other. Using equation (8), we can obtain the commutation relations for  $a_r$  and  $a_r^+$  as

$$[a_r(k), a_s^+(k')] = \delta_{rs}\delta(k - k')$$

$$[a_r(k), a_s(k')] = [a_r^+(k), a_s^+(k')] = 0 \rightarrow \text{(9)}$$

These are the typical relations for bosons. Using equation 4(a) and (b) & equation (8) we have,

$$\varphi(x) = \frac{1}{\sqrt{2}} \sum_k \frac{1}{\sqrt{2v\omega_k}} [a_1 e^{ikx} + a_1^+ e^{-ikx}] - \frac{i}{\sqrt{2}} \sum_k \frac{1}{\sqrt{2v\omega_k}} [a_2 e^{ikx} + a_2^+ e^{-ikx}]$$

$$\varphi(x) = \sum_k \frac{1}{\sqrt{2v\omega_k}} \left[ \frac{1}{\sqrt{2}} (a_1 - ia_2) \right] e^{ikx} + \sum_k \frac{1}{\sqrt{2v\omega_k}} \left[ \frac{1}{\sqrt{2}} (a_1^+ - ia_2^+) \right] e^{-ikx}$$

$$= \sum_k \frac{1}{\sqrt{2v\omega_k}} [a e^{ikx} + b^+ e^{-ikx}]$$

$$\text{where } a(k) = \frac{1}{\sqrt{2}} (a_1 - ia_2)$$

$$b^+(k) = \frac{1}{\sqrt{2}} (a_1^+ - ia_2^+)$$

$$b(k) = \frac{1}{\sqrt{2}} (a_1 + ia_2)$$

$$a^+(k) = \frac{1}{\sqrt{2}} (a_1^+ + ia_2^+)$$

$$\text{Also } \varphi(x) = \sum_k \frac{1}{\sqrt{2v\omega_k}} [a^+ e^{-ikx} + b e^{ikx}]$$

The operators  $a(k)$ ,  $b(k)$  and their Hermitian adjoints  $a^+(k)$ ,  $b^+(k)$  satisfy the commutation relations,

## NOTES

## NOTES

$$[a(k), a^+(k')] = [b(k), b^+(k')] = \delta(k - k')$$

with all other commutators vanishing.

The charge  $Q$  and Hamiltonian  $H$  in terms of these operators are given

$$Q = e \sum_k [a^+ a - b^+ b] \text{ and}$$

$$H = \sum_k [a^+ a + b^+ b]$$

The operators  $a^+$  and  $a$  can be interpreted as the creation and destruction operators respectively for a positively charged particles and  $b^+$  and  $b$  are similar operators for a negatively charged particles. We have two numbers operators  $N^+$  and  $N^-$  defined by

$$N^+(k) = a^+ a ; N^-(k) = b^+ b$$

The eigen values of both these operators are

$$n_{\pm}(k) = 0, 1, 2, \dots, \infty$$

The positively and negatively charged particles have identical properties except for the sign of their charge. In relativistic quantum field theory, every charged particle is accompanied by an antiparticle having opposite charge. Example of particle and antiparticle pair are the charged  $\pi^+$  and  $\pi^-$  particles,  $k^+$  and  $k^-$  particles and so on. The electrically neutral  $k^0$  mesons has an antiparticle  $k^0$  which is also electrically neutral. These two particles carry opposite hypercharge.

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### 11.3 THE DIRAC FIELD

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In terms of natural units, the Dirac equation takes the form

$$(\gamma_{\mu} \partial_{\mu} + m) \psi(x) = 0 \rightarrow (1)$$

The Lagrangian density that reproduces equation (1) is,

$$\mathcal{L} = \bar{\psi}(x) (\gamma_{\mu} \partial_{\mu} + m) \psi(x) \rightarrow (2)$$

$$\text{Where } \bar{\psi}(x) = \psi^+(x) \gamma_4 \rightarrow (3)$$

Which is the Dirac adjoint of  $\psi$ . The conjugate fields of  $\psi$  and  $\bar{\psi}$  are,

$$\pi(x) = \frac{\partial}{\partial \dot{\psi}} \mathcal{L} = - \frac{\partial}{\partial \dot{\psi}} [\bar{\psi} \sum_{k=1}^3 \gamma_k \partial_k \psi + \bar{\psi} \frac{\gamma_4}{i} \dot{\psi} + \bar{\psi} m \psi]$$

$$= - \frac{1}{i} \bar{\psi} \gamma_4 = i \psi^+ \gamma_4 \gamma_4 = i \psi^+ \rightarrow (4)$$

$$\bar{\pi}(x) = \frac{\partial}{\partial \dot{\bar{\psi}}} \mathcal{L} = 0 \rightarrow (5)$$

The previously applied canonical quantization will not work for the Dirac equation.

$$\therefore [\bar{\psi}(x), \bar{\pi}(x')] = [\bar{\psi}(x), 0] = 0 \neq \delta(x - x')$$

Moreover, particles with  $s=1/2$  are fermions and in the non-relativistic limit these were quantized by means of anticommutation relations.

Now, the Hamiltonian density H is

$$\begin{aligned} H &= \pi\dot{\psi} - L = i\psi^+ \dot{\psi} + \bar{\psi}(\gamma_\mu \partial_\mu + m)\psi \\ &= i\psi^+ \dot{\psi} + \bar{\psi} \sum_{k=1}^3 \gamma_k \partial_k \psi + \bar{\psi} \frac{\gamma_4}{i} \dot{\psi} + m\bar{\psi}\psi \\ &= i\psi^+ \dot{\psi} + \bar{\psi} \sum_{k=1}^3 \gamma_k \partial_k \psi - i\psi^+ \dot{\psi} + m\bar{\psi}\psi \\ H &= \bar{\psi}(x) \sum_{k=1}^3 \gamma_k \partial_k \psi(x) + m\bar{\psi}(x)\psi(x) \rightarrow (6) \end{aligned}$$

and hence

$$H = \sum_{k=1}^3 \int \bar{\psi} \gamma_k \partial_k \psi d^3x + m \int_V \bar{\psi}\psi d^3x \rightarrow (7)$$

The plane wave solution of the Dirac equation is of the form

$$\psi_j(r, t) = u_j e^{i(kr - \omega t)}$$

Calculations give two independent solutions for the positive energy and another two independent solutions for the negative energy. Therefore, for a free particle in a volume V,

$$\varphi_r(p) = \sqrt{\frac{m}{VE_p}} u_r(p) e^{ipx}, \quad r=1,2, \rightarrow (8)$$

$$\varphi_{r+2}(p) = \sqrt{\frac{m}{VE_p}} v_r(p) e^{-ipx}, \quad r=1,2. \rightarrow (9)$$

where

$$u_r(p) = \left(\frac{E_p + m}{2m}\right)^{1/2} \begin{pmatrix} \chi_r \\ (\sigma \cdot p) \chi_r \\ E_p + m \end{pmatrix} \quad r=1,2$$

$$v_r(p) = \left(\frac{E_p + m}{2m}\right)^{1/2} \begin{pmatrix} (\sigma \cdot p) \chi_r \\ E_p + m \\ \chi_r \end{pmatrix} \quad r=1,2.$$

$$\text{with } \chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \chi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$E_p = \sqrt{p^2 + m^2}$$

## NOTES

## NOTES

$$px = p.X-Et$$

The functions  $\varphi_1$  and  $\varphi_2$  are the solutions of free particle. Dirac equation corresponding to positive energy and momentum ( $E_p, p$ ) while  $\varphi_3$  and  $\varphi_4$  correspond to negative energy and momentum, ( $-E_p, -p$ ).

The Dirac field operator  $\psi(x)$  and  $\bar{\psi}(x)$  can be written as

$$\psi(x) = \sum_p \sum_{r=1}^2 \sqrt{\frac{m}{vE_p}} [c_r(p)u_r(p)e^{ipx} + d_r^+(p)v_r(p)e^{-ipx}] \rightarrow (10)$$

$$= \psi^+(x) + \psi^-(x) \rightarrow (11)$$

where  $c_r(p)$  and  $d_r(p)$  are complex numbers, and here are operators

$$\bar{\psi}(x) = \sum_p \sum_{r=1}^2 \sqrt{\frac{m}{vE_p}} [c_r^+(p)u_r(p)e^{-ipx} + d_r(p)v_r(p)e^{ipx}] \rightarrow (12)$$

Substitute (10) and (12) in (7),

$$H = \sum_p \sum_{r=1}^2 E_p [c_r^+(p)c_r(p) - d_r(p)d_r^+(p)] \rightarrow (13)$$

$$\text{And } P = \sum_p \sum_{r=1}^2 p [c_r^+(p)c_r(p) - d_r(p)d_r^+(p)] \rightarrow (14)$$

In this theory, in order to obtain positive probability density and the Hamiltonian to be positive definite, anticommutation relations are considered.

$$[c_r(p), c_s^+(p')]_+ = [d_r(p), d_s^+(p')]_+ = \delta_{rs}\delta(p-p') \rightarrow (15)$$

$$\text{and } [c_r, c_s]_+ = [c_r^+, c_s^+]_+ = [d_r, d_s]_+ = [d_r^+, d_s^+]_+ = 0 \rightarrow (16)$$

Using (15) in (13), the Hamiltonian in terms of anticommutation relations is

$$H = \sum_p \sum_{r=1}^2 E_p [c_r^+(p)c_r(p) + d_r^+(p)d_r(p)] + E_0$$

$$P = \sum_p \sum_{r=1}^2 p [c_r^+(p)c_r(p) + d_r^+(p)d_r(p)] + P_0$$

where  $E_0 = -\sum_p \sum_{r=1}^2 E_p$  is the zero point energy and

$$P_0 = -\sum_p \sum_{r=1}^2 p \text{ is the zero point momentum.}$$

Subtracting out the zero point energy and momentum, the energy becomes positive definite. In this form all annihilation operators are written to the right of creation operators.

From equation (13)  $c_r^+(p)c_r(p)$  and  $d_r(p)d_r^+(p)$  are the number operators for the positive and negative energy respectively.

Therefore, from H and P it follows that  $d_r(p)$  creates a negative electron with  $(-E, -P)$  and  $d_r^+(p)$  is the corresponding annihilation operator.

According to Dirac's hole theory, the vacuum state is the one with all positive energy states empty and all negative energy states filled. When negative energy electron is annihilated, a hole is created which behaves as if it is a particle of positive charge, called positron.

The operator  $c_r^+(p)$  creates an electron and  $c_r(p)$  annihilates an electron. Similarly  $d_r^+(p)$  and  $d_r(p)$  creates and annihilates a positron respectively.

The number operators,

$$N_r^+(p) = c_r^+(p) c_r(p) \text{ and}$$

$$N_r^-(p) = d_r^+(p) d_r(p)$$

are the number operators for positive energy electrons and positive energy positrons respectively. The corresponding Hamiltonian and momentum are states filled. When a negative energy electron

$$H = \sum_p \sum_{r=1}^2 E_p [N_r^+(p) + N_r^-(p)] \text{ and}$$

$$P = \sum_p \sum_{r=1}^2 p [N_r^+(p) + N_r^-(p)]$$

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## 11.4 QUANTIZATION OF ELECTROMAGNETIC FIELDS

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The Maxwell's equation for the electric and magnetic fields are:

$$\nabla \cdot E = \rho \rightarrow (1)$$

$$\nabla \times E = -\frac{\partial B}{\partial t} \rightarrow (2)$$

$$\nabla \cdot B = 0 \rightarrow (3)$$

$$\nabla \times B = \frac{\partial E}{\partial t} + j \rightarrow (4)$$

These equations can be written in terms of A and  $\phi$ . Equation (3) can be written as:

$$B = \nabla \times A \rightarrow (5)$$

with this value, (2) becomes

## NOTES

$$\nabla \times \left( E + \frac{\partial A}{\partial t} \right) = 0 \rightarrow (6)$$

Therefore the curl of the gradient of a scalar function is zero (5) takes the form

$$E + \frac{\partial A}{\partial t} = -\nabla\phi$$

**NOTES**

(or)

$$E = -\frac{\partial A}{\partial t} - \nabla\phi \rightarrow (7)$$

Sub (7) in (1)

$$\nabla^2\phi + \frac{\partial(\nabla \cdot A)}{\partial t} = -\rho \rightarrow (8)$$

Sub (5)& (7) in (4)

$$\nabla \times (\nabla \times A) = \partial/\partial t \left( -\frac{\partial A}{\partial t} - \nabla\phi \right) + j$$

$$\nabla \times (\nabla \times A) + \partial/\partial t \left( \frac{\partial A}{\partial t} + \nabla\phi \right) = j$$

$$\nabla(\nabla \cdot A) - \nabla^2 A + \partial^2 A/\partial t^2 + \nabla \cdot \frac{\partial\phi}{\partial t} = j$$

$$\nabla^2 A - \frac{\partial^2 A}{\partial t^2} - \nabla \left( \nabla \cdot A + \frac{\partial\phi}{\partial t} \right) = -j \rightarrow (9)$$

The solutions of Maxwell's equation is thus reduced to solve the coupled equations (8) and (9) for A and  $\phi$ .

The potentials as defined earlier are not unique. We can decouple these 2 equations using Gauge invariance ( $A \rightarrow A'$ ,  $\phi \rightarrow \phi'$ )

It is understood that the transformations leave Maxwell's equations invariant.

One can use this invariance to select the family of potentials (A,  $\phi$ ) such that the coupling term in equation (9)

$$\left( \nabla \cdot A + \frac{\partial\phi}{\partial t} \right) = 0 \rightarrow (10)$$

This condition is known as Lorentz gauge condition.

Equation (10) can be written as:

$$\frac{\partial A_1}{\partial x_1} + \frac{\partial A_2}{\partial x_2} + \frac{\partial A_3}{\partial x_3} + \frac{\partial(i\phi)}{\partial(it)} = 0$$

$$\frac{\partial A_1}{\partial x_1} + \frac{\partial A_2}{\partial x_2} + \frac{\partial A_3}{\partial x_3} + \frac{\partial A_4}{\partial x_4} = 0 \rightarrow (11)$$

$$\frac{\partial A_\mu}{\partial x_\mu} = 0 \text{ (or) } \partial_\mu A_\mu = 0$$

The components of A and  $\phi$  form the four- vector potential

$$A = (A, i\phi)$$

From equation (5) we have

$$B_1 = \frac{\partial A_3}{\partial x_2} - \frac{\partial A_2}{\partial x_3} \rightarrow (11)(a)$$

$$B_2 = \frac{\partial A_1}{\partial x_3} - \frac{\partial A_3}{\partial x_1} \rightarrow (11)(b)$$

$$B_3 = \frac{\partial A_2}{\partial x_1} - \frac{\partial A_1}{\partial x_2} \rightarrow (11)(c)$$

From equation (7)

$$E_1 = -\frac{\partial A_1}{\partial t} - \frac{\partial \phi}{\partial x_1}$$

(or)

$$iE_1 = \frac{\partial A_1}{\partial(it)} - \frac{\partial(i\phi)}{\partial x_1}$$

(or)

$$iE_1 = \frac{\partial A_1}{\partial x_4} - \frac{\partial A_4}{\partial x_1} = F_{41}$$

$$iE_2 = \frac{\partial A_2}{\partial x_4} - \frac{\partial A_4}{\partial x_2} = F_{42}$$

$$iE_3 = \frac{\partial A_3}{\partial x_4} - \frac{\partial A_4}{\partial x_3} = F_{43}$$

In general,

$$F_{\mu\vartheta} = \frac{\partial A_\vartheta}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\vartheta}$$

## NOTES

$$F_{\mu\vartheta} = -F_{\vartheta\mu}$$

$F_{\mu\vartheta}$  is an anti-symmetric tensor which is given by

NOTES

$$F_{\mu\vartheta} = \begin{pmatrix} 0 & B_z & -B_y & -\frac{iE_x}{c} \\ -B_z & 0 & B_x & -\frac{iE_y}{c} \\ B_y & -B_x & 0 & -\frac{iE_z}{c} \\ \frac{iE_x}{c} & \frac{iE_y}{c} & \frac{iE_z}{c} & 0 \end{pmatrix}$$

which is the electromagnetic field four-tensor.

The electromagnetic field is an example of vector and can be classically expressed in terms of  $A$  ( $A, i\phi$ ) where  $A$  is the vector potential and  $\phi$  is the scalar potential.

To incorporate the principles of quantum theory into this classical field theory the field quantization is developed.

The relativistic wave equation for Klein Gordon field is

$$(\partial_\mu \partial_\mu - m^2)\phi(x) = 0 \rightarrow (1)$$

Since the electromagnetic quanta has zero rest mass, its classical wave equation can be written by setting  $m=0$  in equation (1)

$$\partial_\mu \partial_\mu A_\vartheta(x) = 0 \quad \vartheta = 1,2,3,4 \rightarrow (2)$$

Quantizing equation (2) is difficult due to the following reasons:

(1)Equation (2) is equivalent to Maxwell's equation only if it is combined with the Lorentz gauge condition, which implies that all the four components of  $A$  are not independent. However, canonical quantization procedure is valid only if they are independent.

(2)Since we have real and imaginary components for  $A_\mu$ , it is not possible to treat all the four components on the same footing.

(3)Invariance of the field under gauge transformation makes different quantization procedures for different gauge unavoidable.

To overcome the above difficulties one can use different gauges. Lorentz gauge defined by  $\partial_\mu \partial_\mu = 0$  is used and at first the imaginary character of  $A_4$  is ignored. Hence all the four  $A_\mu$ 's will be treated as independent and Hermitian



The Lagrangian density is given by

$$\mathcal{L}(x) = -\frac{1}{2} \partial_\mu A_\vartheta \partial_\mu A_\vartheta \rightarrow (3)$$

Expanding the field operator  $A_\mu(x)$  in terms of the complete set of plane wave solutions of equation (2), we have

$$A_\mu(x) = \frac{1}{\sqrt{v}} \sum_k \frac{1}{\sqrt{2\omega_k}} \sum_{r=1}^4 \left[ a_r(k) \epsilon_\mu^{(r)}(k) e^{ikx} + a_r^\dagger(k) \epsilon_\mu^{(r)*}(k) e^{-ikx} \right] \rightarrow (4)$$

For each  $k$   $\epsilon^{(r)}(k)$ ,  $r=1,2,3,4$  form a set of four linearly independent orthogonal vectors in the  $k$ -space.

Also,

$$\begin{aligned} \epsilon_\mu^{(r)*}(k) \epsilon_\mu^{(s)}(k') &= \delta_{rs} \delta_{kk'} \\ \sum_{r=1}^4 \epsilon_\mu^{(r)}(k) \epsilon_{\mu 1}^{(r)*}(k) &= \delta_{\mu 1} \end{aligned}$$

To understand about equation (4) definite choice of the polarization vectors  $\epsilon^{(r)}(k)$  has to be made.

Since  $\epsilon^{(r)}$  is arbitrary  $\epsilon^3(k)$  can be taken as the component along  $k$  and  $\epsilon^{(1)}(k)$  and  $\epsilon^{(2)}(k)$  perpendicular to it.  $\epsilon^{(1)}(k)$  and  $\epsilon^{(2)}(k)$  are called as transverse polarizations and  $\epsilon^{(3)}(k)$  as longitudinal polarization. Then it follows:

$$\epsilon_\mu^{(r)}(k) = \delta_{\mu r} \epsilon^{(r)}(k) \rightarrow (5)$$

Therefore equation (4) reduces to

$$A_\mu(x) = \frac{1}{\sqrt{v}} \frac{1}{\sqrt{2\omega_k}} \left[ a_\mu(k) \epsilon^{(\mu)}(k) e^{ikx} + a_\mu^\dagger(k) \epsilon^{(\mu)*}(k) e^{-ikx} \right] \rightarrow (6)$$

The required quantum conditions are

$$[a_\mu(k), a_\vartheta^\dagger(k')] = \delta_{\mu\vartheta} \delta(k - k')$$

$$[a_\mu(k), a_\vartheta(k')] = [a_\mu^\dagger(k), a_\vartheta^\dagger(k')] = 0 \rightarrow (7)$$

The operators  $a_\mu^\dagger, a_\mu$  and  $a_\mu^\dagger a_\mu = N(k)$  could be interpreted as creation, annihilation and number operators respectively.

The three polarization states in space indicate that photons have spin 1 with z-component of spin 1,0,-1. A photon with polarization along  $\epsilon^{(4)}$  is called a time like photon.

## NOTES

## NOTES

The momenta conjugate to the field  $A_\mu(x)$  is

$$\pi_\mu = \frac{\partial}{\partial \dot{A}_\mu} \mathcal{L}$$

From equation (3)

$$\begin{aligned} \mathcal{L} &= -\frac{1}{2} \partial_\mu A_\nu \partial_\mu A_\nu = -\frac{1}{2} \left[ \frac{\partial A_\nu}{\partial x_k} \cdot \frac{\partial A_\nu}{\partial x_k} + \frac{\partial A_\nu}{\partial x_4} \cdot \frac{\partial A_\nu}{\partial x_4} \right] \\ &= -\frac{1}{2} \left[ \frac{\partial A_\nu}{\partial x_k} \cdot \frac{\partial A_\nu}{\partial x_k} + \frac{\partial A_\nu}{\partial t} \cdot \frac{\partial A_\nu}{\partial t} \right] \\ &= -\frac{1}{2} \left[ \frac{\partial A_\nu}{\partial x_k} \cdot \frac{\partial A_\nu}{\partial x_k} - \dot{A}_\nu^2 \right] \rightarrow (8) \end{aligned}$$

Consequently

$$\pi_\mu = \dot{A}_\mu$$

The Hamiltonian density  $\mathcal{H}$  is given by

$$\mathcal{H} = \pi_\mu \dot{A}_\mu - \mathcal{L} = \pi_\mu + \frac{1}{2} \left[ \frac{\partial A_\mu}{\partial x_k} \cdot \frac{\partial A_\mu}{\partial x_k} - \dot{A}_\mu^2 \right]$$

$$\mathcal{H} = \pi_\mu \pi_\mu + \frac{1}{2} (\nabla \cdot A_\mu)(\nabla \cdot A_\mu) - \frac{1}{2} \pi_\mu \pi_\mu$$

$$\mathcal{H} = \frac{1}{2} \pi_\mu \pi_\mu + \frac{1}{2} (\nabla \cdot A_\mu)(\nabla \cdot A_\mu)$$

Therefore

$$H = \int \mathcal{H}(x) d^3X$$

becomes

$$\begin{aligned} H &= \sum_K \frac{1}{2} [a_\mu(k) a_\mu^+(k) + a_\mu^+(k) a_\mu(k)] \omega_k \\ &= \sum_k \frac{1}{2} [a_\mu(k) a_\mu^+(k)]_+ \omega_k \\ &= \sum_k \sum_\mu \left[ N_\mu(k) + \frac{1}{2} \right] \omega_k \end{aligned}$$

The total energy of the field is

$$E = \sum_k \sum_{\mu=1}^4 \left[ n_\mu(k) + \frac{1}{2} \right] \omega_k$$

where  $n_\mu(k) = 0, 1, 2, \dots, \infty$

*Klein-Gordon field*

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## 11.5 CHECK YOUR PROGRESS

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1. Differentiate relativistic and non Relativistic field.
2. Write down Lorentz gauge condition.
3. What is called as Hamiltonian density of a field?

### Let us sum up

This unit explains the quantization of relativistic fields like Klein Gordon Field, Dirac Field and electromagnetic field.

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## 11.6 UNIT-END EXERCISES

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1. Explain how to quantize a Klein-Gordon field.
2. Discuss the quantization of Dirac field energy and momentum.
3. Quantization of electromagnetic field.

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## 11.7 ANSWERS TO CHECK YOUR PROGRESS

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1. Relativistic mechanism deals with particles travelling at a speed close to that of light. Non relativistic mechanism deals with particles that do not travelling at a speed close to that of light.
2.  $(\nabla \cdot A + \frac{\partial \phi}{\partial t}) = 0$ .
3.  $H = \sum_{r=1}^2 \int \pi_x(x) \dot{\phi}_r(x) - L$

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## 11.8 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldas- PHI learning Private limited, New Delhi 2008.
3. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.

**NOTES**

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# UNIT-XII SCATTERING CROSS SECTION

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**NOTES**

## Structure

12.1 Scattering cross-section

12.2 Scattering Amplitude

12.3 Partial wave

12.3.1 Partial wave analysis

12.3.2 The Scattering Amplitude

12.3.3 The Scattering Cross-section

12.4 Check your progress

12.5 Unit – End Exercises

12.6 Answer to Check your progress

12.7 Suggested Readings

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## 12.1 SCATTERING CROSS-SECTION

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Both classical and quantum mechanical scattering phenomena are characterized by the scattering cross section,  $\sigma$ .

- Consider a collision experiment in which a detector measures the number of particles per unit time,  $N$   $d\Omega$  in direction  $(\theta, \phi)$ .
- This number is proportional to the incident flux of particles,  $j_i$  defined as the number of particles per unit time crossing a unit area normal to direction of incidence.
- Collisions are characterized by the differential cross section defined as the ratio of the number of particles scattered into direction  $(\theta, \phi)$  per unit time per unit solid angle, divided by incident flux,

$$\frac{d\sigma}{d\Omega} = \frac{N}{j_i}$$

- Total cross section by integrating over all solid angles,

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin\theta \frac{d\sigma}{d\Omega}$$

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## 12.2 SCATTERING AMPLITUDE

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The scattering amplitude is the probability amplitude of the outgoing spherical wave relative to the incoming plane wave in a stationary-state scattering process.

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

Where,  $r \equiv (x, y, z)$  is the position vector,  $e^{ikz}$  is the incoming plane wave with wave number  $k$  along  $z$  axis,  $\frac{e^{ikr}}{r}$  is the outgoing spherical wave,  $\theta$  is the scattering angle and  $f(\theta)$  is the scattering amplitude.

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## 12.3 PARTIAL WAVES

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A plane wave  $e^{ikz}$  can be expanded as a linear combination of spherical waves as

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta) \rightarrow (1)$$

$j_l(kr)$  is the spherical Bessel function of order  $l$  and  $P_l$  are the Legendre polynomials. Each term on the right-hand side represents a spherical wave. The plane wave is thus equivalent to the superposition of an infinite number of spherical waves and the individual waves are called partial waves. The waves with  $l=0, 1, 2, \dots$  are respectively called the s-wave, the p-wave, d-wave and so on. The notation is borrowed from atomic spectroscopy. Asymptotically,

$$j_l(kr) \rightarrow \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2}\right) \rightarrow (2)$$

Writing  $\sin\left(kr - \frac{l\pi}{2}\right)$  in terms of exponentials and substituting it in eqn.(1), we get

$$e^{ikz} = \sum_{l=0}^{\infty} \frac{i^l (2l+1)}{2ik} P_l(\cos\theta) \frac{1}{r} \left[ \exp\left(ikr - i\frac{l\pi}{2}\right) - \exp\left(-ikr + i\frac{l\pi}{2}\right) \right] \rightarrow (3)$$

This form shows that each partial wave can be represented as the sum of an incoming and an outgoing spherical wave.

In scattering problems, the first few spherical waves are the most important ones. The s-partial wave will be independent of the angle  $\theta$  and hence spherically symmetric about the origin. Results of

## NOTES

## NOTES

extremely low energy scattering can be explained satisfactorily with s-wave alone. If the energy is slightly higher, one needs p-wave also to explain the observed value.

### Scattered by a central potential

#### 12.3.1 Partial wave analysis

The method of partial wave is an elegant procedure for the analysis of elastic scattering. It is done in two steps. First, a wave function  $\psi$  which represents the sum of the incident and scattered waves is obtained in terms of the partial waves. Secondly, the asymptotic value of this  $\psi$  is equated to the  $\psi$  given in eqn.

$$\psi \xrightarrow{r \rightarrow \infty} A \left[ e^{ikz} + \frac{f(\theta)e^{ikr}}{r} \right] \rightarrow (4)$$

#### The Asymptotic Solution

The Schrodinger equation that describes the scattering is given by eqn. The wave function  $\psi$  has to be independent of  $\phi$ , as the incident particles are along the z-axis. Separating the variables, we get the solution of eqn. (1) as

$$\psi(r, \theta) = R_l(r) P_l(\cos\theta), \quad l=0,1,2,\dots \rightarrow (5)$$

Where  $R_l(r)$  satisfies the radial equation:

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR_l}{dr} \right) + \left[ \frac{2\mu E}{\hbar^2} - \frac{2\mu V}{\hbar^2} - \frac{l(l+1)}{r^2} \right] R_l = 0 \rightarrow (6)$$

Outside the range of the potential ( $r > r_0$ ), this equation reduces to the free-particle equation:

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r} \frac{dR_l}{dr} + \left[ k^2 - \frac{l(l+1)}{r^2} \right] R_l = 0 \rightarrow (7)$$

$$\text{where } k^2 = \frac{2\mu E}{\hbar^2} \rightarrow (8)$$

Differential equation (6) has two independent solutions  $j_l(kr)$  and  $n_l(kr)$ , where  $j_l(kr)$  is the spherical Bessel function and  $n_l(kr)$  is the spherical Neumann function. The general solution of eqn(6) is then

$$R_l(kr) = A' j_l(kr) - B' n_l(kr)$$

where  $A'$  and  $B'$  are constants. Though the function  $n_l(kr)$  is not finite at  $r = 0$ , it is retained as we are interested only in the asymptotic solution. Asymptotically, using this eqn, we have

$$R_l(kr) \underset{r \rightarrow \infty}{=} \frac{A'}{kr} \sin\left(kr - \frac{l\pi}{2}\right) + \frac{B'}{kr} \cos\left(kr - \frac{l\pi}{2}\right) \rightarrow (9)$$

We shall now investigate what happens when there is a potential. When  $V(r) \neq 0$ , the value of the constant  $B'_l/A'_l$  has to be determined by solving eqn. (6) inside the scattering region and then matching it with the asymptotic solution Eqn. (9). Writing the new constants  $A_l$  and  $\delta_l$  in terms of  $A'$  and  $B'$  by the relations

$A' = A_l \cos \delta_l$  and  $B' = A_l \sin \delta_l$ , we have the asymptotic solution of eqn(6) as

$$R_l(kr) = \frac{A_l}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right), \quad l=0,1,2,\dots \rightarrow (10)$$

where  $\delta_l$ 's are called phase shifts. The phase shifts  $\delta_l$  measures the amount by which the phase of the radial function for angular momentum quantum number  $l$  differs from the corresponding one for the  $V=0$  case. The most general asymptotic solution is then

$$\psi(r,\theta) = \sum_{l=0}^{\infty} \frac{A_l}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) P_l(\cos\theta) \rightarrow (11)$$

where  $A_l$  is the asymptotic amplitude.

### 12.3.2 The Scattering Amplitude

Equating this asymptotic form of the wave function with the  $\psi$  given by eqn (4)

$$e^{ikz} + f(\theta) \frac{e^{ikr}}{r} = \sum_{l=0}^{\infty} \frac{A_l}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) P_l(\cos\theta) \rightarrow (12)$$

Replacing  $e^{ikz}$  using equations (1) and (2), we have

$$\sum_{l=0}^{\infty} \frac{(2l+1)i^l}{kr} \sin\left(kr - \frac{l\pi}{2}\right) P_l(\cos\theta) + f(\theta) \frac{e^{ikr}}{r} = \sum_{l=0}^{\infty} \frac{A_l}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) P_l(\cos\theta) \rightarrow (13)$$

Writing the sine function in exponential form and equating the coefficients of  $e^{-ikz}$  on both sides, we get

$$\sum_{l=0}^{\infty} (2l+1) i^l e^{\frac{il\pi}{2}} P_l(\cos\theta) = \sum_{l=0}^{\infty} A_l e^{\frac{il\pi}{2}} \exp(-i\delta_l) P_l(\cos\theta) \rightarrow (14)$$

Since eqn(14) is valid for all values of  $\theta$ , using the orthogonal property of Legendre polynomials

$$A_l = i^l (2l+1) \exp(-i\delta_l) \rightarrow (15)$$

Comparison of the coefficient of  $e^{ikz}$  on both sides of eqn(13) gives,

## NOTES

$$\sum_{l=0}^{\infty} \frac{(2l+1)i^l e^{\frac{i l \pi}{2}}}{2ikr} P_l(\cos\theta) + \frac{f(\theta)}{r} = \sum_{l=0}^{\infty} \frac{(2l+1)i^l e^{2i\delta_l}}{2ikr} e^{-i l \pi/2} P_l(\cos\theta)$$

$$\text{(or) } f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) i^l e^{-\frac{i l \pi}{2}} [\exp(2i \delta_l) - 1] P_l(\cos\theta) \rightarrow \text{(16)}$$

$$\text{we have } i^l = e^{\frac{i l \pi}{2}}$$

**NOTES**

$$\exp(2i \delta_l) - 1 = \exp(i \delta_l) [\exp(i \delta_l) - \exp(-i \delta_l)] = 2i \exp(i \delta_l) \sin \delta_l \rightarrow \text{(17)}$$

Hence this equation (16) can be written as:

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp(i \delta_l) P_l(\cos \theta) \sin \delta_l \rightarrow \text{(18)}$$

Equation (18) represents the basic result of partial wave analysis which gives  $f(\theta)$  as a sum of contributions from all partial waves. Equation written in the exponential form allows a simple physical interpretation. Substituting the value of  $A_l$  in eqn.(11), we get

$$\Psi(r,\theta) = \sum_{l=0}^{\infty} \frac{(2l+1)i^l}{2ikr} \left\{ \exp \left[ i \left( kr - \frac{1}{2} l \pi + 2 \delta_l \right) \right] - \exp \left[ -i \left( kr - \frac{1}{2} l \pi \right) \right] \right\} P_l(\cos \theta) \rightarrow \text{(19)}$$

From equations (3) & (11), it follows that the effect of the scattering potential is to shift the phase of the outgoing waves relative to that of the incoming waves. This is reasonable, since at large distances the incoming waves are not aware of the potential that exists near the origin.

**12.3.4 The Scattering Cross-section**

The differential scattering cross-section

$$\sigma(\theta) = |f(\theta)|^2 = \frac{1}{k^2} \left| \sum_{l=0}^{\infty} (2l+1) \exp(i \delta_l) P_l(\cos \theta) \sin \delta_l \right|^2 \rightarrow \text{(20)}$$

Equation (20) was first derived by Faxen and Holtzmark. Lord Rayleigh derived a similar expression for wave diffraction. The total cross-section

$$\sigma = \int_0^\pi \sigma(\theta) d\Omega = \int_0^\pi \sigma(\theta) (2\pi \sin\theta) d\theta = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l \rightarrow \text{(21)}$$

In deriving equation (21), the orthogonal property of Legendre polynomial is used. The differential and total cross-sections are thus given in terms of the phase shifts  $\delta_l$  of the partial waves. For understanding the scattering problem, one should therefore know the phase shifts  $\delta_l, l=0,1,2,..$



For s-wave scattering, the differential scattering cross-section  $\sigma_0(\theta)$  and the total cross section  $\sigma_0$  are given by:

$$\sigma_0(\theta) = \frac{\sin^2 \delta_0}{k^2} \quad \text{and} \quad \sigma_0 = \frac{4\pi}{k^2} \sin^2 \delta_0 \rightarrow (22)$$

It may be noted that the both cross-sections do not depend on the angle  $\theta$ . Often s-wave contribution is the most dominant part in most of the experiments. It may also be noted from eqn (20) that  $\sigma(\theta)$  contains terms representing interference between differential partial waves whereas the total cross section  $\sigma$  in equation (21) does not contain such terms. If all phase shifts except  $\delta_0$  and  $\delta_l$  are negligible.

$$\sigma_0(\theta) = \frac{1}{k^2} [\sin^2 \delta_0 + 9 \sin^2 \delta_l \cos^2 \theta + 6 \sin^2 \delta_0 \sin^2 \delta_l \cos(\delta_0 - \delta_l \cos \theta) \rightarrow (23)$$

$$\text{and } \sigma = \frac{4\pi}{k^2} [\sin^2 \delta_0 + 3 \sin^2 \delta_l] \rightarrow (24)$$

As already mentioned, the first term on the right of eqn(23) is spherically symmetric. The second term has the factor  $\cos^2 \theta$  which has the same value  $\theta$  and  $\pi - \theta$  and therefore symmetric between forward and backward directions. The presence of  $\cos \theta$  in the third term produces a forward-backward asymmetry and may become large even if  $\sin \delta_0 \gg \sin \delta_l$ . Though, the p-wave contribution to the total cross-section is negligible, it is felt in the differential cross-section through cross-terms with the lower partial waves.

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## 12.4 CHECK YOUR PROGRESS

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1. Define scattering cross section and scattering amplitude.
2. What are partial waves? When do we call a scattering event as p wave scattering.

### Let us sum up

This unit describes one of the techniques to study the scattering namely partial wave analysis which is commonly employed to evaluate the scattering amplitude and scattering cross section. The asymptotic solution of this method is also obtained.

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## 12.5 UNIT-END EXERCISES

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1. General theory of partial wave analysis.

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## 12.6 ANSWERS TO CHECK YOUR PROGRESS

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1.  $\sigma = \frac{\text{No. of particles scattered per second}}{\text{No. of particles incident per second per unit area}}$

## NOTES

2. A plane wave is equivalent to the superposition of an infinite number of spherical waves and the individual waves are called partial waves. The waves with  $l=1$  is called p-wave scattering.

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## 12.7 SUGGESTED READINGS

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### NOTES

1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldhas- PHI learning Private limited, New Delhi 2008.
3. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.
4. Quantum Mechanics – Theory and Application – Ajoy Ghatak and S. Lokanathan – 5<sup>th</sup> edition – Trinity Press, 2012.

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# UNIT-XIII BORN APPROXIMATION

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*Born Approximation*

## Structure

- 13.1 Optical Theorem
- 13.2 Expression for phase shifts
- 13.3 Integral equation
- 13.4 Check your progress
- 13.5 Unit – End Exercises
- 13.6 Answer to Check your progress
- 13.7 Suggested Readings

## NOTES

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### 13.1 OPTICAL THEOREM

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For the case  $\theta = 0$ , we get from eqn.(18)

$$f(0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \exp(i \delta_l) \sin \delta_l \rightarrow (25)$$

The imaginary part of this scattering amplitude is given by

$$\text{Im}f(0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l \rightarrow (26)$$

Comparing equations (26) and (21), we get

$$\sigma = \frac{4\pi}{k} \text{Im} f(0) \rightarrow (27)$$

This relation is known as the optical theorem in analogy with the relation in optics between the absorption coefficient and the imaginary part of the complex index of refraction.

#### Ramsaur-Townsend Effect

If the bombarding energy is very small,  $kr_0 \ll 1$  and all phase shifts for  $l > 0$  are almost zero. If in addition, the potential is such that  $\delta_0 = \pi$ ,  $\sin \delta_0 = 0$  and the scattering cross-section vanishes. This phenomenon of no scattering is called the Ramsaur-Townsend effect. They observed extremely small scattering cross-section for electrons of rare gas atoms at a bombarding energy of 0.7 eV.

## 13.2 EXPRESSION FOR PHASE SHIFTS

To derive an expression for phase shift, let us consider the radial part of the Schrodinger equation that describes the scattering,

$$\frac{d^2 u_l(r)}{dr^2} + \left[ \frac{2\mu E}{\hbar^2} - \frac{2\mu V}{\hbar^2} - \frac{l(l+1)}{r^2} \right] u_l(r) = 0 \rightarrow (1)$$

### NOTES

Where  $u_l = r R_l(r)$ . In the incident wave region  $V = 0$  and therefore

$$\frac{d^2 u_l(r)}{dr^2} + \left[ k^2 - \frac{l(l+1)}{r^2} \right] u_l(r) = 0, \text{ where } k^2 = \frac{2mE}{\hbar^2} \rightarrow (2)$$

whose solution is

$$u_l(kr) = kr j_l(kr) \rightarrow (3)$$

Asymptotically,

$$u_l(kr) \xrightarrow{r \rightarrow \infty} \sin \left[ kr - \frac{l\pi}{2} \right] \rightarrow (4)$$

Similarly the asymptotic solution of

$$\frac{d^2 v_l}{dr^2} + \left[ k^2 - \frac{2\mu V(r)}{\hbar^2} - \frac{l(l+1)}{r^2} \right] v_l(r) = 0 \rightarrow (5)$$

is

$$v_l(kr) \xrightarrow{r \rightarrow \infty} \sin \left[ kr - \frac{l\pi}{2} + \delta_l \right] \rightarrow (6)$$

Multiplying eqn(2) by  $v_l$ , eqn(5) by  $u_l$  and subtracting, we get

$$v_l \frac{d^2 u_l}{dr^2} - u_l \frac{d^2 v_l}{dr^2} = -\frac{2\mu V}{\hbar^2} u_l v_l \rightarrow (7)$$

Integrating from  $r = 0$  to  $r$  and remembering that  $u_l(0) = v_l(0) = 0$

$$v_l \frac{du_l}{dr} - u_l \frac{dv_l}{dr} = -\frac{2\mu}{\hbar^2} \int_0^r V(r') u_l(r') v_l(r') dr'$$

Allowing  $\xrightarrow{r \rightarrow \infty}$  and substituting the values of  $u_l(r)$  and  $v_l(r)$  from eqn(4) and (6), we have

$$\begin{aligned} k \sin \left[ kr - \frac{l\pi}{2} + \delta_l \right] \cos \left[ kr - \frac{l\pi}{2} \right] - k \sin \left[ kr - \frac{l\pi}{2} \right] \cos \left[ kr - \frac{l\pi}{2} + \delta_l \right] \\ = -\frac{2\mu}{\hbar^2} \int_0^\infty V(r) u_l(kr) v_l(kr) dr \end{aligned}$$

$$\text{or } k \sin \delta_l = -\frac{2\mu}{\hbar^2} \int_0^\infty V(r) u_l(kr) v_l(kr) dr \rightarrow (8)$$

This expression for  $\sin \delta_l$  is exact. At high energies for weak potential, the phase shifts are small and

$$u_l(kr) \cong v_l(kr) \cong kr j_l(kr) \rightarrow (9)$$

As spherical Bessel function is related to the ordinary Bessel function by the relation

$$j_l(kr) = \left[ \frac{\pi}{2kr} \right]^{1/2} j_{l+(1/2)}(kr) \rightarrow (10)$$

$$\text{Then } \sin \delta_l = \delta_l = -\frac{2\mu k}{\hbar^2} \int_0^\infty V(r) j_l^2(kr) r^2 dr \rightarrow (11)$$

$$\sin \delta_l = \delta_l = -\frac{\pi\mu}{\hbar^2} \int_0^\infty [V(r) [j_{l+(1/2)}(kr)]^2 r dr \rightarrow (12)$$

This expression is known as the Born approximation for phase shifts which is valid only for weak potentials. It follows from eqn(12) that an attractive potential ( $V \leq 0$ ) leads to positive phase shifts whereas a repulsive potential ( $V \geq 0$ ) to negative phase shifts.

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### 13.3 INTEGRAL EQUATION

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The partial wave analysis of scattering which is based on the expansion of a plane wave in terms of spherical waves is more suitable for spherically symmetric potentials. Moreover, it is useful at relatively low energies. A more general analysis requires the expressing of the wave function in the form of an integral equation.

The Schrodinger equation for the scattering of a two-particle system can be written in the convenient form as

$$(\nabla^2 + k^2) \psi(r) = U(r) \psi(r) \rightarrow (13)$$

$$\text{Where } k^2 = \frac{2\mu E}{\hbar^2}, \quad U(r) = \frac{2\mu V(r)}{\hbar^2} \rightarrow (14)$$

We have to obtain a solution of eqn(13) whose asymptotic value has the form of eqn (15) as

$$\psi(r) = e^{ik.r} + \psi_s \rightarrow (15)$$

and substituting it in eqn (13), we get

$$(\nabla^2 + k^2)(e^{ik.r} + \psi_s) = U(r) \psi(r) \rightarrow (16)$$

Since  $(\nabla^2 + k^2) e^{ik.r} = 0$ , eqn (16) reduces to

$$(\nabla^2 + k^2) \psi_s = U(r) \psi(r) \rightarrow (17)$$

Equation (17) is an inhomogeneous equation wherein the inhomogeneous term itself depends on  $\psi(r)$ . Its solution is obtained by Green's function method. Let  $G(r,r')$  called the Green's formula, be the

### NOTES

solution of the inhomogeneous equation with a delta function source. That is,

$$(\nabla^2 + k^2) G(r, r') = \delta(r - r') \rightarrow (18)$$

The solution of the scattering equation for the density function  $\rho(r)$  can then be written as

$$\psi_s = \int G(r, r') \rho(r') d\tau \rightarrow (19)$$

## NOTES

Using Green's- function techniques and contour integration

$$G(r, r') = \frac{-\exp(ik|r-r'|)}{4\pi|r-r'|} \rightarrow (20)$$

It follows immediately that

$$\psi_s(r) = -\frac{1}{4\pi} \int \frac{-\exp(ik|r-r'|)}{|r-r'|} U(r') \psi(r') d\tau \rightarrow (21)$$

where  $r$  is the position of the scattered particle after being scattered in the region  $r' \cong 0$ . The scattered wave  $\psi_s$  at the point  $r$  has the form of the superposition of spherical waves originating from all points  $r'$  with amplitudes  $U(r') \psi(r')$ , figure illustrates the vectors  $r$  and  $r'$ . Let  $\hat{n}$  be the unit vector in the direction of the vector  $r$ . since  $r$  is very large, it follows from this figure

$$|r - r'| = r - \hat{n} \cdot r' \rightarrow (22)$$

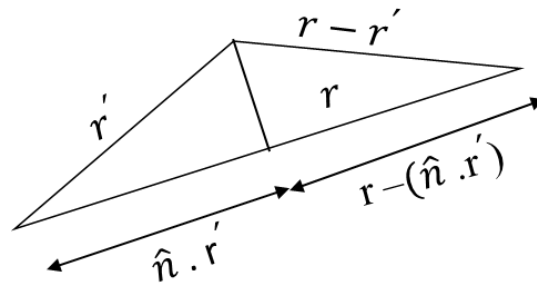


Figure. The vectors  $r$  and  $r'$  in a scattering problem

In the centre of mass system, the momentum  $K'$  of the elastically scattered particle is equal in magnitude to the momentum of the incident particle ( $k$ ). That is  $k' = k\hat{n}$ . hence

$$k|r - r'| = k(r - \hat{n} \cdot r') = kr - k' \cdot r' \rightarrow (23)$$

Replacing  $|r - r'|$  in the denominator of eqn (21) by  $r$ , the wave function for the scattering problem can be written as

$$\psi(r) \xrightarrow{r \rightarrow \infty} \exp(ik \cdot r) - \frac{1}{4\pi} \int \frac{\exp[i(\mathbf{k} - \mathbf{k}' \cdot \mathbf{r}')] U(\mathbf{r}') \psi(\mathbf{r}') d\tau' \rightarrow (24)$$

Eqn (24) is the integral equation for the wave function since  $\psi$  appears under the integral sign on the right-hand side. On comparing equations, we get, with the asymptotic solution  $\psi(r) \xrightarrow{r \rightarrow \infty} A \left[ e^{ikz} + \frac{f(\theta)e^{ikr}}{r} \right]$

$$f(\theta) = -\frac{1}{4\pi} \int \exp(-i\mathbf{k}' \cdot \mathbf{r}') U(\mathbf{r}') \psi(\mathbf{r}') d\tau' \rightarrow (25)$$

from which the differential scattering cross-section  $\sigma(\theta)$  can be calculated.

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### 13.4 THE BORN APPROXIMATION

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The wave function  $\psi(\mathbf{r}')$  is required to evaluate equation (25). Born used an iterative procedure for its evaluation. In this first Born approximation,  $\psi(\mathbf{r}')$  in the integral, eqn. (25) is replaced by the incoming plane wave,  $\exp(i\mathbf{k} \cdot \mathbf{r}')$ . This leads to an improved value for the wave function  $\psi(\mathbf{r})$  which is used in the integral in the second Born approximation. This iterative procedure is continued till both the input and output  $\psi$ 's are almost equal. As higher-order approximations are complicated, the discussion is restricted only to first Born approximation.

Replacing  $\psi(\mathbf{r}')$  in the integral in eqn. (25) by  $\exp(i\mathbf{k} \cdot \mathbf{r}')$ , we get

$$f(\theta) = -\frac{1}{4\pi} \int \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}'] U(\mathbf{r}') d\tau' \rightarrow (26)$$

where  $\mathbf{k}$  and  $\mathbf{k}'$  are the wave vectors in the incident and scattered directions, respectively. The quantity  $(\mathbf{k} - \mathbf{k}')\hbar = \mathbf{q}\hbar$  is then the momentum transfer from the incident particle to the scattering potential. In other words, the change in momentum  $\mathbf{q}\hbar$  due to collision is given by,

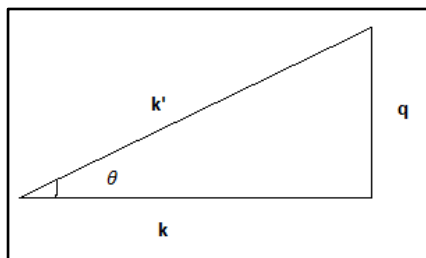
$$\mathbf{q}\hbar = (\mathbf{k} - \mathbf{k}')\hbar \text{ (or) } |q| = 2|k| \sin \frac{\theta}{2} \rightarrow (27)$$

Replacing  $(\mathbf{k} - \mathbf{k}')$  by  $\mathbf{q}$  in eqn.(A) we get

$$f(\theta) = -\frac{1}{4\pi} \int \exp(i\mathbf{q} \cdot \mathbf{r}') U(\mathbf{r}') d\tau' \rightarrow (28)$$

The angular integration in eqn.(C) can easily be carried out by taking the direction of  $\mathbf{q}$  as the polar axis, Denoting the angle between  $\mathbf{q}$  and  $\mathbf{r}'$  by  $\theta'$ .

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Representation of the wave vectors  $\mathbf{k}$ ,  $\mathbf{k}'$  and  $\mathbf{q}$ . The vector  $\mathbf{k}$  points in the incident direction,  $\mathbf{k}'$  in the scattered direction.

$$f(\theta) = -\frac{1}{4\pi} \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} \exp(iq r' \cos \theta) U(r') r'^2 \sin \theta' d\phi' d\theta' dr' \rightarrow (29)$$

Integration over  $\phi$  gives  $2\pi$ . The  $\theta$ -integral can easily be evaluated by writing

$$\cos \theta' = x \text{ or } -\sin \theta' d\theta' = dx$$

We get

$$\begin{aligned} \int_0^{\pi} \exp(iq r' \cos \theta) \sin \theta' d\theta' &= \int_{-1}^1 \exp(iqr' x) dx \\ &= \frac{\exp(iqr') - \exp(-iqr')}{iqr'} \\ &= \frac{2\sin(qr')}{qr'} \rightarrow (30) \end{aligned}$$

Substituting the value of the angular part in eqn (29)

$$f(\theta) = -\frac{2\mu}{\hbar^2} \int_0^{\infty} \frac{\sin(qr')}{qr'} V(r') r'^2 dr' \rightarrow (31)$$

from which  $\sigma(\theta)$  can be calculated. It may be noted from eqn(31) that the only variable parameter in  $f(\theta)$  is the magnitude of the momentum transfer  $q\hbar$ , where  $q$  is given by eqn (27). Thus, the scattering cross-section depends on the momentum of the incident particle  $k\hbar$  and the scattering angle  $\theta$  through the combination  $q=2k \sin (\theta/2)$ .

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**13.4 CHECK YOUR PROGRESS**

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1. Express the optical theorem.
2. State Ramsaur- Townsend effect.



3. Express Green's function.

*Born Approximation*

### Let us sum up

The optical theorem and Ramsaur-Townsend effect at the outset of partial wave analysis are stated and explained. An approach to evaluate scattering amplitude namely Born approximation is explained.

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## 13.5 UNIT-END EXERCISES

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1. Discuss the theory of scattering using the Born approximation.

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## 13.6 ANSWERS TO CHECK YOUR PROGRESS

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1.  $\sigma = \frac{4\pi}{k} \text{Im } f(0)$

2. If the bombarding energy is very small,  $kr_0 \ll 1$  and all phase shifts for  $l > 0$  are almost zero. If in addition, the potential is such that  $\delta_0 = \pi$ ,  $\sin \delta_0 = 0$  and the scattering cross-section vanishes. This phenomenon of no scattering is called the Ramsaur-Townsend effect. They observed extremely small scattering cross-section for electrons of rare gas atoms at a bombarding energy of 0.7 eV.

3.  $G_{k'}(\mathbf{r}, \mathbf{r}') = \int \frac{\Psi_{k'}^*(\mathbf{r}') \Psi_{k'}(\mathbf{r}) dk'}{(k'^2 - k^2)}$

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## 13.7 SUGGESTED READINGS

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.

2. Quantum Mechanics-G. Aruldas- PHI learning Private limited, New Delhi 2008.

3. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.

4. Quantum Mechanics – Theory and Application – Ajoy Ghatak and S. Lokanathan – 5<sup>th</sup> edition – Trinity Press, 2012.

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## UNIT-XIV DIFFUSION SCATTERING

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### Structure

14.1 Scattering by screened coulomb potential

14.2 Validity of Born approximation

14.3 Check your progress

14.4 Unit – End Exercises

14.5 Answer to Check your progress

14.6 Suggested Readings

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### 14.1 SCATTERING BY SCREENED COULOMB POTENTIAL

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As an example of Born approximation, the scattering of a particle having charge  $Z'e$  by an atomic nucleus of charge  $Ze$  is considered the interaction between the two is usually screened by the atomic electrons surrounding the nucleus. The potential representing the interaction can be written as

$$V(r) = -\frac{ZZ'e^2}{r}e^{-\alpha r}$$

Where  $\alpha$  is the parameter which determines the screening by atomic electrons. With this value of  $V(r)$ , the scattering amplitude  $f(\theta)$  becomes

$$\begin{aligned} f(\theta) &= \frac{2\mu ZZ'e^2}{\hbar^2 q} \int_0^{\infty} \sin(qr) \exp(-\alpha r) dr \\ &= \frac{2\mu ZZ'e^2}{\hbar^2 q} \frac{q}{q^2 + \alpha^2} \\ &= \frac{2\mu ZZ'e^2}{\hbar^2 (q^2 + \alpha^2)} \end{aligned}$$

Therefore,

$$\sigma(\theta) = |f(\theta)|^2 = \left( \frac{2\mu Z Z' e^2}{\hbar^2} \right)^2 \frac{1}{(q^2 + \alpha^2)^2}$$

If the momentum transfer  $q \gg \alpha$ ,

$$q^2 + \alpha^2 \cong q^2 = 4k^2 \sin^2 \frac{\theta}{2}$$

$$\text{and } \sigma(\theta) = \frac{\mu^2 Z^2 Z'^2 e^4}{4\hbar^4 k^4 \sin^4(\theta/2)}$$

which is Rutherford's scattering formula for scattering by a pure Coulomb potential  $-ZZ'e^2/r$ .

## 14.2 VALIDITY OF BORN APPROXIMATION

In the Born approximation,  $\psi(r')$  in eqn.(25) was replaced by  $\exp(i\mathbf{k}\cdot\mathbf{r}')$ , which is valid only if the scattered wave  $\psi_s$  in eqn(21) is small compared to the plane wave. The scattered wave  $\psi_s$  is likely to be maximum in the interaction region, where  $r \cong 0$ . With  $r \cong 0$  in eqn.(21) the condition reduces to

$$\left| \frac{1}{4\pi} \int \frac{\exp(-ikr')}{r'} U(r') \exp(i\mathbf{k}\cdot\mathbf{r}') d\tau \right| \ll 1 \rightarrow (32)$$

Where  $\mathbf{k}\cdot\mathbf{r}' = kr' \cos\theta'$  and  $d\tau' = r'^2 \sin\theta' d\theta' d\phi' dr'$ . Integration over  $\phi'$  gives  $2\pi$ . Integration over  $\theta'$  can be done using the substitution  $\cos\theta' = x'$ . Carrying out the angular integration, eqn(32) reduces to

$$\left| \int_0^\infty \frac{\exp(ikr')}{r'} U(r') \frac{\sin(kr')}{kr'} r'^2 dr' \right| \ll 1$$

$$\text{or } \frac{2\mu}{\hbar^2} \left| \int_0^\infty \exp(r') \sin(kr') V(r') dr' \right| \ll 1 \rightarrow (33)$$

If the energy is sufficiently high,  $\sin(kr')$  will be a rapidly varying function and the value of the integral in eqn (33) will be very small. A weak potential also makes the integral small. When energy is high the factor  $2\mu/(k\hbar^2)$  will also be very small. Hence Born approximation is valid for weak potentials at high energies.

## 14.3 CHECK YOUR PROGRESS

1. Write down the validity of Born approximation.

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**Let us sum up**

Rutherford's scattering formula is derived using the theory of scattering by screened coulomb potential. The validity of Born approximation is also explained.

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**14.4 UNIT-END EXERCISES**

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1. Derive the Rutherford's formula for scattering by a coulomb potential.

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**14.5 ANSWERS TO CHECK YOUR PROGRESS**

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1.  $\frac{2\mu}{k\hbar^2} \left| \int_0^\infty \exp r') \sin (kr')V(r')dr' \right| \ll 1$ , If the energy is sufficiently high,  $\sin(kr')$  will be a rapidly varying function and the value of the integral in eqn(33) will be very small. A weak potential also makes the integral small. When energy is high the factor  $2\mu/(k\hbar^2)$  will also be very small. Hence Born approximation is valid for weak potentials at high energies.

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**14.6 SUGGESTED READINGS**

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1. A textbook of quantum mechanics- P.M. Mathews and K.Venkatesan, McGraw hill, New Delhi 2010.
2. Quantum Mechanics-G. Aruldhas- PHI learning Private limited, New Delhi 2008.
3. Quantum mechanics – VK Thankappan – 4<sup>th</sup> edition – New Age International Publishers, New Delhi.
4. Quantum Mechanics – Theory and Application – Ajoy Ghatak and S. Lokanathan – 5<sup>th</sup> edition – Trinity Press, 2012.