LESSION – 1: INTRODUCTION TO QUANTUM MECHANICS

CONTENTS

1.0. Aims and Objectives:

In this unit, we are going to discuss

- The inadequacy of classical mechanics
- Birth of quantum mechanics
- Basic formalism of quantum mechanics
- Introduction to quantum mechanical operators

1.1. Quantum Mechanics: An Introduction

The concepts and formulation of quantum mechanics are not elementary in the sense that they are easily understood. They are based on the outcome of considerable theoretical research supported by experimental evidence. The quantum mechanical approach to physical problems cannot be explained in simple non-mathematical terms. Simple and elegant mathematical techniques have been used to elucidate the physical concepts.

1.2. Difficulties with Classical Physics

Classical Physics deals primarily with macroscopic phenomena. Most of the effects with which classical theory is concerned are either directly observable or can be made observable with relatively instruments. There is a close link between the world of classical physics and the world of sensory perception.

During the decades of 20^{th} century, Physicists turned their attention to the study of atomic systems, which are inherently inaccessible to direct observation. It soon became clear that the concepts and methods of classical macroscopic physics could not be applied directly to atomic phenomena.

1.3. The Birth of Quantum Mechanics

The early development of atomic theory consisted of efforts to overcome these difficulties by modifying the laws of Classical Physics. These efforts reached their successful conclusion in the period from 1925 to 1930, when an entirely new theoretical discipline, Quantum Mechanics was developed by Schrödinger, Heisenberg, Dirac and others.

Quantum Mechanics can be regarded as the fundamental theory of atomic phenomena. The experimental data on which it is based are derived from physical events that lie almost entirely beyond the range of human perception. It is not surprising, that the theory embodies physical concepts that are foreign to common daily experience.

1.4. State Vectors

The values of Schrödinger wave functions $\psi(x)$ at various points x are akin to the components of a vector. While the components are numbers which depend on the choice of coordinate system or basis in the vector space, the vector itself is an abstract geometrical object with an existence and significance independent of coordinate systems. In the quantum mechanics, the abstract mathematical object which is

associated with the physical entity, the quantum state, is known as the **State Vector**. The different kinds of wave functions for a given state (in the configuration space, momentum space) are simply the sets of components of the state vector as referred to different 'coordinate systems' or bases in the state vector space. This notation was introduced by Dirac. It is used to relate different representations. The notation is very general and suitable for handling of systems which have no classical counterpart, e.g. spin angular momentum.

1.5. Hilbert Space

It is an abstract space. The vector spaces of quantum mechanics are called **Hibert Space**. The mathematical concept of a Hilbert Space, named after the German mathematician David Hilbert, generalizes the notion of Euclidean space in a way that extends methods of vector algebra from the two-dimensional plane and three-dimensional space to infinite-dimensional spaces. In more formal terms, a Hilbert space is an inner product space an abstract vector space in which distances and angles can be measured which is "complete", meaning that if a sequence of vectors approaches a limit, then that limit is guaranteed to be in the space as well.

1.6. Dirac Notation

Bra-ket notation is the standard notation for describing quantum states in the theory of quantum mechanics. It can also be used to denote abstract vectors and linear functionals in pure mathematics. It is so called because the inner product (or dot product) of two states is denoted by a bracket, consisting of a left part, called **the Bra**, and a right part, called **the Ket**. The notation was invented by Paul Dirac, and is also known as Dirac notation.

Dirac introudced the symbol $|\psi\rangle$ to denote an abstract state vector distinct from its representation, the wave functions. The state vectors constitute a complex vectors space, i.e. if $|\psi\rangle$, $|\chi\rangle$ are state vectors, so that $c|\psi\rangle + c'|\chi\rangle$ for any complex numbers c and c'. all vectors $c|\psi\rangle$, c 0, which have the same direction $|\psi\rangle$, correspond to the same physical state. The set of all such vectors constitute a space

called a ray in the space. Therefore, we can say that any physical state is represented by a ray (rather than a single vector) in the vector space.

Corresponding to every vector $|\psi\rangle$ there is a conjugate vector $|\overline{\psi}\rangle$ for which Dirac used to notation $\langle\psi|$.

i.e. $\langle\psi| \equiv |\overline{\psi}\rangle, \langle\overline{\psi}|$ $|\psi\rangle$ (1)

The relation between any vector and its conjugate may be visualized readily if we consider examples of their representations. In the Schrödinger picture $|\psi\rangle \to \psi(x$ $\rangle\langle$ $|, \overline{\psi}$ $(^*$ $)$. It is to be mentioned that the relation between $|\psi\rangle$ and $\langle\psi|$ is not a linear.

1.7. Norm and Scalar Product

The length or norm of the vector $|\psi\rangle$ is denoted by $\langle\psi|\ \psi\rangle$. By definition $\langle\psi|\ \psi\rangle$ is a real non-negative number.

i.e. $\langle\psi|$ $\psi\rangle \geq 0\langle$ $|,\overline{\psi}\rangle$ 0 if and only if $|\psi\rangle = 0$. (2a)

In general if the vector $|\psi\rangle$ and its conjugate $\langle\phi|$ of some vector $|\phi\rangle$ are juxtaposed in such a was as to form a closed bracket $\langle\phi|\ \psi\rangle$, this symbol represents a single (real or complex) number which is defined to be the scalar product of $|\phi\rangle$ and $|\psi\rangle$, taken in that order. Vectors of type $\langle\psi|$ which forms the first half of the closed brackets are called **Bra Vectors** and those of the type $|\psi\rangle$ which forms the second half are called **Ket Vectors**. The conjugate of a bra vector is a ket vector, and vice versa.

In the Schrödinger picture, $\langle\phi|$ $\rangle\psi \to \int \phi^*(x)\psi x($ d. It is to be noted that

$\langle\phi|$ $\psi\rangle \neq \langle\psi|$ $\phi\rangle$ but $\langle\phi|$ $\psi\rangle = \langle\psi|$ $\phi\rangle^*$ (2b)

The scalar product of two vectors is linear in the second vector.

$$\langle \phi | (c|\psi\rangle + d|\chi\rangle) = c\langle \phi|\psi\rangle + d\langle \phi|\chi\rangle \qquad (2c)$$

Any vector space (in general infinite dimensional) such that between any two vectors of the space a scalar product which satisfies equation (2) is called a Hibert space. The space of ket vectors (or bra vectors) representing quantum mechanical states is thus a Hilbert space.

1.8. Dynamical variables as Operators

Each dynamical variable A (x,p) is represented in quantum mechanics by a linear operator $\hat{A} = A(\hat{x}, \hat{p}) = A(x, -i\hbar\nabla)$ The operator acts on the wave function of the system. The effect of an operator $\hat{A}$ on a wave function ψ is to convert it into another wave function denoted by A ψ. Linearity of the operator means that a linear combinations of A ψ_1 and A ψ_2. is

$$A(c_1\psi_1 + c_2\psi_2) = c_1(A\psi_1) + c_2(A\psi_2)$$

dynamic variables in quantum mechanics do not commute with each other that is

AB BA.

1.9. Change of Basis

If the vectors e^i are on orthonormal basis for a N – dimensional space,

$$(e^i, e^j) = \delta_{ij}, \quad i, j = 1, 2, \ldots N \qquad (1)$$

Then a new basis can be constructed by forming N linear combinations of these vectors,

$$e^i = \sum_{j=1}^{N} u_i^j e_j \qquad (2)$$

in which u_i are suitably chosen complex numbers. This new basis are also orthonormal, provided that

$$(e^{i'}, e^{j'}) = \delta_{ij} \qquad (3)$$

If Equation (2) is substituted the above condition becomes

$$\sum_{k,\ l} u_i \quad \overset{*}{u}_k \left(\overset{k}{e}_j , \overset{l}{e}_l \right) = \delta_j \tag{4}$$

Using equation (1) we get

$$\sum_k u_i \quad {}_k \overset{*}{u}_j = \delta_i \tag{5}$$

In other words, the matrix $U = u_{i\ j}$ must satisfy

$$U \quad \overset{\dagger}{U} = 1$$

It follows that, U must be non singular and

$$U^{-1} = U^{\dagger} \tag{6}$$

It is also apparent that this conditions is sufficient to insure that the vectors $e^{i'}$ formed according to equation (2) are orthonormal. Hence the necessary and sufficient conditions for the vectors $e^{i'}$ to form an orthonormal basis is that the matrix U is unitary. Since $U^{-1}U = U^{1}\ U = \quad 1 \quad$, the equation (6) becomes

$$U \quad \overset{\dagger}{U} = \overset{\dagger}{U} \quad U \quad 1 \tag{7}$$

Such a unitary transformation has the effect of substituting the basis $\left\{ e' \right\}$ for the basis $\left\{ e \right\}$.If a vector x is represented with respect to the basis $\left\{ e \right\}$ by

$$x = \sum_i \quad {}_i \dot{e} \tag{8}$$

and with respect to basis $\left\{ e' \right\}$ by

$$x = \sum_i \quad {}_i' \dot{e}' \tag{9}$$

Then, since these expression representatives of one and the same vector,

$$\sum_j x_i \quad {}_i \overset{j}{e} = \sum_{j,} x_i \quad {}^{j'} u_j^{\ *} \ e \tag{10}$$

hence by orthogonality of e^j,

$$x_j = \sum_i U_{ij}^* x_i' \tag{11}$$

This equation provides the connection between the components x_i and x_i' of the vector with respect to the bases $\{e\}$ $\{e'\}$. Since U is the unitary matrix, equation (11) can be solved for x_i' in terms of x_i.

1.10. LET US SUM UP

In this unit, we have studied

- The inadequacy of classical mechanics
- Birth of quantum mechanics
- Basic formalism of quantum mechanics
- Introduction to quantum mechanical operators
- Hilbert's space and Dirac notation

1.11. LESSON END ACTIVITIES

1. List the inadequacy of classical mechanics
2. Briefly discuss about Hilbert's space
3. Give an account on Dirac notation
4. What are conditions under which an operator can be represented by a diagonal matrix.?
5. What are bra and ket vectors?
6. Define a linear operator in Hilbert space.

1.12. References

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LESSON - 2

EQUATION OF MOTION

2.0. Aims and Objectives:

In this lesson we are going to study

- Schrodinger picture
- Heinsenberg's picture
- Interaction picture

2.1. Schrödinger Picture

In the Schrödinger picture, the state vectors are assumed to be time dependent and the dynamical variables are assumed to be time independent. The wave equation in the Schrödinger picture is

$$i\hbar \frac{d}{dt}|\alpha_s(t)\rangle = H|\alpha_s(t)\rangle \qquad (1)$$

The subscript's' refers to the ket as viewed is Schrödinger picture. The total time derivative in used here, since the dependence of ket on co-ordinate or other variable does not appear explicitly.

The Hermitian adjoint wave equation will be

$$-i\hbar\frac{d}{dt}\langle\alpha_s(t)| = \langle\alpha_s(t)|H^{\dagger}$$

$$= \langle\alpha_s(t)|H \tag{2}$$

Since $H^{\dagger} = H$ because H is hermitian. Assuming H to be independent of time the solution for the above equations will be of the form

$$|\alpha_s(t)\rangle = e^{-i\frac{H}{\hbar}t}|\alpha_s(0)\rangle \text{ and} \tag{3}$$

$$\langle\alpha_s(t)| = \langle\alpha_s(0)|e^{-i\frac{H}{\hbar}t} \tag{4}$$

This can be easily verified by differentiating equation (3) and getting the equation (1)

$$\frac{d}{dt}|\alpha_s(t)\rangle = \frac{-i}{\hbar}H e^{-i\frac{H}{\hbar}t}|\alpha_s(0)\rangle$$

$$i\hbar\frac{d}{dt}|\alpha_s(t)\rangle = H|\alpha_s(t)\rangle$$

The operator $e^{-i\frac{H}{\hbar}t}$ is an infinite sum of powers of H , each of which is a dynamical variable, that can be expressed as an operator or square matrix. It is essential to remember that the operator $e^{-i\frac{H}{\hbar}t}$ is not an unitary transformation in the ordinary sense of rotation of axes in Hilbert's space as U, V, W. But it represents the change of in to some other ket $|\alpha_s(0)\rangle$. Thus the series as a whole is also a dynamical variable. The time rate of change of matrix element of a dynamical variable Ω_s in the Schrödinger picture can be found out as

$$\frac{d}{dt}\langle\alpha_s(t)|\Omega_s|\beta_s(t)\rangle = \frac{d}{dt}\{\langle\alpha_s(t)|\Omega_s|\beta_s(t)\rangle\} + \{\langle\alpha_s(t)|\frac{\partial\Omega_s}{\partial t}|\beta_s(t)\rangle\} + \{\langle\alpha_s(t)|\Omega_s\frac{d}{dt}|\beta_s(t)\rangle\}$$

$$= \frac{-1}{i\hbar}\langle\alpha_s(t)|\Omega_s H|\beta_s(t)\rangle + \{\langle\alpha_s(t)|\frac{\partial\Omega_s}{\partial t}|\beta_s(t)\rangle\} + \frac{1}{i\hbar}\{\langle\alpha_s(t)|\Omega_s H|\beta_s(t)\rangle\}$$

$$= \langle\alpha_s(t)|\frac{\partial\Omega_s}{\partial t}|\beta_s(t)\rangle + \frac{1}{i\hbar}\langle\alpha_s(t)|[\Omega_s, H]|\beta_s(t)\rangle$$

The first term on the right hand side arises due to any explicit time dependence Ω_s may have. The second term on the right hand side arises due to the change in the state vectors with time.

A special case of interest will b when Ω_s is time independent, and when Ω_s commutes with H. In such a case right hand side will be zero and all the matrix elements of Ω_s are constant in time. Such a dynamical variable is said to be a constant of the motion.

2.2. Heisenberg Picture

In Heisenberg Picture, the state vectors are assumed to be independent of time and the dynamical variables are time dependent. We know that the time rate of change of matrix element in Schrödinger picture is given by the equation.

$$\frac{d}{dt}\langle \alpha_s | \Omega_s | \beta_s \rangle = \langle \frac{\partial \alpha_s}{\partial t} | \Omega_s | \beta_s \rangle + \langle \alpha_s | \frac{\partial \Omega_s}{\partial t} | \beta_s \rangle + \frac{1}{i\hbar}\langle \alpha_s | \Omega_s H - H \Omega_s | \beta_s \rangle$$

with $|\alpha_s(t)\rangle = e^{\frac{-iHt}{\hbar}} |\alpha_s(0)\rangle$ and $\langle \alpha_s(t)| = \langle \alpha_s(0)| e^{\frac{iHt}{\hbar}}$

substituting for ket and bra vectors

$$\frac{d}{dt}\langle \alpha_s | \Omega_s | \beta_s \rangle = \langle \alpha_s(0) | e^{\frac{iHt}{\hbar}} \frac{\partial \Omega_s}{\partial t} e^{\frac{-iHt}{\hbar}} | \beta_s(0) \rangle + \frac{1}{i\hbar}\langle \alpha_s(0) | e^{\frac{iHt}{\hbar}} \Omega_s H e^{\frac{-iHt}{\hbar}} | \beta_s(0) \rangle - \frac{1}{i\hbar}\langle \alpha_s(0) | e^{\frac{iHt}{\hbar}} H \Omega_s e^{\frac{-iHt}{\hbar}} | \beta_s(0) \rangle$$

Assuming H to commute with $e^{\frac{-iHt}{\hbar}}$ and also choosing the state vectors in Heisenberg picture to be time independent as

$$|\alpha_H\rangle = |\alpha_s(0)\rangle = e^{\frac{iHt}{\hbar}} |\alpha_s(t)\rangle$$

since $|\alpha_H(t)\rangle$ does not depend on time, the explicit mention of t may be omitted. The dynamical variable Ω_H and its derivative to be

$$\Omega_H = e^{\frac{iHT}{\hbar}} \Omega_s e^{\frac{-iHT}{\hbar}} \quad \text{and}$$

$$\frac{\partial \Omega_H}{\partial t} = e^{\frac{iHt}{\hbar}} \frac{\partial \Omega_s}{\partial t} e^{\frac{-iHt}{\hbar}}$$

$$\frac{d}{dt}\langle \alpha_H | \Omega_H | \beta_H \rangle = \langle \alpha_H | \frac{\partial \Omega_H}{\partial t} | \beta_H \rangle + \frac{1}{i\hbar}\langle \alpha_H | e^{\frac{iHt}{\hbar}} \Omega_s H e^{\frac{-iHt}{\hbar}} - e^{\frac{iHt}{\hbar}} H \Omega_s e^{\frac{-iHt}{\hbar}} | \beta_H \rangle$$

$$\frac{d}{d}\langle\alpha_H|\Omega_H|\beta_H\rangle = \langle\alpha_H|\frac{\partial\Omega_H}{\partial t}|\beta_H\rangle + \frac{1}{i\hbar}\langle\alpha_H|[\Omega_H, H_H]|\beta_H\rangle$$

since the state vectors in Heisenberg's picture are independent of time $\frac{d}{d}$ can be brought inside the ket $\langle\alpha_H|$ in the above equations and we will have

$$\langle\alpha_H|\frac{d\Omega_H}{d}|\beta_H\rangle = \langle\alpha_H|\frac{\partial\Omega_H}{\partial t}|\beta_H\rangle + \frac{1}{i\hbar}\langle\alpha_H|[\Omega_H, H_H]|\beta_H\rangle$$

This equation is true for arbitrary bra and ket vectors and hence we can write

$$\frac{d\Omega_H}{d} = \frac{\partial\Omega_H}{\partial t} + \frac{1}{i\hbar}[\Omega_H, H]$$

This equation is called equation of motion in Heisenberg's picture. This is similar to the classical equation of motion for the dynamical variable F given by

$$\frac{d}{d} = \frac{F}{t}\frac{\partial F}{\partial t} + \{F, H\}$$

where $\{F, H\}$ is poisson bracket.

So the transition from classical to quantum mechanical picture can be made by replacing the poisson bracket with commutator bracket divided by $i\hbar$

2.3. Interaction Picture (or Dirac Picture)

We know that the state vectors alone or the dynamical variable alone are not central to describe the development of a physical system with time. Both the state vectors and the dynamical variables can be altered by means of the unitary transformation operator $e^{\frac{i}{\hbar}H_s}$.

The quantities that are not altered are the matrix element of the dynamical variable and this provides the physical content of the system since eigenvalues, expectation values, and transition probabilities can be obtained from the matrix element.

In the interaction picture, the Hamiltonian is split up into two parts as H = H_0 + H' where H_0 is usually chosen to be independent of time. H_0 may be simple

structure as the coloumb interaction and H' may be the external electromagnetic field varying with time. In the interaction picture we define the state vectors and the dynamical variables as

$$|\alpha_I(t)\rangle = e^{\frac{-iH_s t}{\hbar}}|\alpha_s(t)\rangle \qquad (1)$$

$$\Omega_I(t) = e^{\frac{iH_s t}{\hbar}}\Omega_s e^{\frac{-iH_s t}{\hbar}}$$

Differentiating equation (1)

$$i\hbar\frac{d}{dt}|\alpha_I(t)\rangle = i\hbar\frac{d}{dt}\left[e^{\frac{iH_s t}{\hbar}}|\alpha_s(t)\rangle\right] = i\hbar\left[\frac{iH_s}{\hbar}e^{\frac{iH_s t}{\hbar}}|\alpha_s(t)\rangle + e^{\frac{iH_s t}{\hbar}}\frac{d}{dt}|\alpha_s(t)\rangle\right]$$

$$= -H_s e^{\frac{iH_s t}{\hbar}}|\alpha_s(t)\rangle + e^{\frac{iH_s t}{\hbar}}H_s|\alpha_s(t)\rangle$$

$$= -H_s e^{\frac{iH_s t}{\hbar}}|\alpha_s(t)\rangle + e^{\frac{iH_s t}{\hbar}}H_s|\alpha_s(t)\rangle$$

$$= -H_s|\alpha_I(t)\rangle + H_s|\alpha_I(t)\rangle$$

$$= H'|\alpha_I(t)\rangle$$

$$\frac{d\Omega_I}{dt} = \frac{i}{\hbar}H_s e^{\frac{iH_s t}{\hbar}}\Omega_s e^{-\frac{iH_s t}{\hbar}} - e^{\frac{iH_s t}{\hbar}}\frac{\partial}{\partial t}\left(i\Omega_s e^{\frac{iH_s t}{\hbar}}\right)e^{-\frac{iH_s t}{\hbar}}\left(H_s - \frac{i}{\hbar}H_s\right)e^{\frac{iH_s t}{\hbar}}$$

$$= \frac{\partial\Omega_I}{\partial t} + \frac{1}{i\hbar}(\Omega_I H_s - H_s\Omega_I)$$

$$= \frac{\partial\Omega_I}{\partial t} + \frac{1}{i\hbar}[\Omega_I, H_s]$$

$$= \frac{\partial\Omega_I}{\partial t} + \frac{1}{i\hbar}[\Omega_I, H_I]$$

In interaction picture, part of the time dependence is assigned to the state vectors and another part to the dynamical variables instead of having one constant and the other time dependent.

2.4. LET US SUM UP

In this lesson we have discussed

- Schrodinger picture
- Heinsenberg's picture
- Interaction picture

in detail.

2.5. LESSON END ACTIVITIES

1. Obtain the equation of motion in Schrodinger's picture
2. Obtain the equation of motion in Heinsenberg's picture
3. Compare the equation of motion in Schrodinger's picture with that of Heinsenberg's picture
4. Obtain the equation of motion in Dirac's picture

2.7. Problems:

Show that If the Hamiltonain H of a system does not contain time explicitly

$$|\alpha(t)\rangle = e^{\left(\frac{i}{\hbar}H\right)t}$$

Solution

$$|\alpha(t)\rangle = |\alpha(0)\rangle + \int_0^t \frac{d}{dt'}|\alpha(t')\rangle dt'$$

$$= |\alpha(0)\rangle + \frac{1}{i\hbar}\int_0^t H|\alpha(t')\rangle dt'$$

$$= |\alpha(0)\rangle + \frac{1}{i\hbar}\int_0^t H\left[|\alpha(0)\rangle + \int_0^{t'}\frac{d}{dt''}|\alpha(t'')\rangle dt''\right] dt'$$

$$= |\alpha(0)\rangle + \frac{1}{i\hbar}H|\alpha(0)\rangle t + \frac{1}{(i\hbar)^2}\int_0^t\int_0^{t'} H^2|\alpha(t'')\rangle dt'' dt'$$

$$= \left(1 + \frac{1}{i\hbar}Ht + \frac{1}{2!}\left(\frac{1}{i\hbar}\right)^2 H^2 t^2 + \cdots\right)|\alpha(0)\rangle$$

$$= e^{\left(\frac{-i}{\hbar}H\right)t}|\alpha(0)\rangle$$

since H is hermitian U is unitary, where U is $e^{\left(\frac{-i}{\hbar}H\right)t}$

2.8. Do it yourself

Obtain the equation of motion for <A> in the Schrodinger's picture and also in the Heisenberg's picture.

2.9. References

1. A text book of Quantum Mechanics **P.M. Mathews and K. Venkatesan**. Tata McGraw –Hill Publishers.
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LESSON 3

MATRIX MECHANICS

3.1. Aims and objectives:

In this lesson, we are going to solve the linear harmonic oscillator by the method of matrix mechanics. Also we are going to study the Kronig Penny model.

3.2. One Dimensional Linear Harmonic Oscillator in Matrix Mechanics

The Linear Harmonic oscillator can be treated by manipulating the matrix equations directly the Hamiltonian for a linear harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2} k x^2 \qquad (1)$$

where $\omega = \sqrt{\frac{k}{m}}$

The commutator of x with H is

$$[x, H] = \left[x, \frac{p^2}{2m}\right] + \left[x, \frac{1}{2} k x^2\right]$$

$$= \frac{1}{2m}\{p[x, p] + [x, p]p\} + 0 \qquad \text{since } [x,x] = 0$$

$$= \frac{1}{2m}\{i\hbar p\} + \{i\hbar p\}$$

$$= \frac{2i\hbar p}{2m}$$

$$= \frac{i\hbar p}{m} \qquad (2)$$

The commutator of p with H

$$[p, H] = \left[p, \frac{p^2}{2m} + \frac{1}{2}kx^2\right]$$

$$= 0 + \frac{1}{2}k\{x[p,p] + [p,x]x\} \qquad \text{since } [p,p] = 0$$

$$= \frac{1}{2}k\{-i\hbar x - i\hbar x\}$$

$$= \frac{-2i\hbar k}{2}$$

$$= -i\hbar kx \qquad (3)$$

3.3. Energy Representations

If there are transition from the initial state $|l\rangle$ to the final state $|k\rangle$

$$\langle k|[x, H]|l\rangle = \langle k|\left[x, \frac{p^2}{2m} + \frac{1}{2}kx^2\right]|l\rangle$$

$$= \frac{i\hbar}{m}\langle k|p|l\rangle \qquad (4)$$

But $\langle k|[x, H]|l\rangle = \langle k|xH - Hx|l\rangle = \langle k|xH|l\rangle - \langle k|Hx|l\rangle$

Introducing a dummy operators, $|l\rangle\langle l|$ and $|k\rangle\langle k|$

$$= \langle k|x|l\rangle\langle l|H|l\rangle\langle l| - \langle k|H|k\rangle\langle k|x|l\rangle$$

$$= (E_l - E_k)\langle k|x|l\rangle \qquad (5)$$

From equations (4) and (5)

$$E_l - E_k\langle k|x|l\rangle = \frac{i\hbar}{m}\langle k|p|l\rangle$$

$$\langle k|x|l\rangle = \frac{i\hbar}{m}\frac{\langle k|p|l\rangle}{E_l - E_k} \qquad (6)$$

Similarly

$$\langle k|[p, H]|l\rangle = \langle k|i\hbar kx|l\rangle = i\hbar k\langle k|x|l\rangle \qquad (7)$$

But

$$\langle k|[p, H]|l\rangle = \langle k|pH - Hp|l\rangle = \langle k|pH|l\rangle - \langle k|Hp|l\rangle$$

$$= (E_l - E_k)\langle k|p|l\rangle \qquad (8)$$

From equations (7) and (8)

$$\langle k|\ |p\rangle = \frac{-i\hbar\ k}{(E_l - E_k)}\langle x|\ |l\rangle \qquad (9)$$

$$\langle k|\ p|\ \rangle l = \frac{-i\hbar\ k}{(E_l - E_k)}\frac{\hbar i}{m}\frac{\langle k|\ p|\ \rangle l}{(E_k - E_l)}$$

$$= \frac{\hbar^2 k}{m}\frac{1}{(E_l - E_k)^2}\langle k|\ p|\ \rangle$$

$$\langle k|\ |p\rangle = \frac{\hbar^2\omega^2\ k}{(E_l - E_k)^2}\langle p|\ |l\rangle$$

$$(E_l - E_k) = \pm\hbar\omega$$

Thus we see that the energy difference between successive levels will be $\pm\hbar\omega$. Therefore the energy change can takes place in units of $\hbar\omega$

3.4. Raising and Lowering operator

Multiplying equation (6) by $-i\hbar\omega$ then we get

$$\langle k|-i\ \ m\omega\ x|\ \rangle l\ \frac{\hbar\omega\langle k|\ p|\ \rangle}{(E_l - E_k)}$$

(10)

Rewriting equation (9) as

$$\langle k|\ |p\rangle = \frac{-i\hbar\omega^2 m}{(E_l - E_k)}\langle x|\ |l\rangle$$

$$= \frac{\hbar\omega}{(E_l - E_k)}\langle k|\ i\ \ m\omega\ x|\ \rangle \qquad (11)$$

(10) + (11) $\Rightarrow$

$$\langle k|\ p - i\omega\ m|\ \rangle x = \frac{\hbar\omega}{(E_l - E_k)}\langle\ |i\ \ m\ \ x|\ \rangle l$$

$$(E_l - E_k\ \ \hbar\omega)p\langle\ |i\ -\omega m\ \ 0x|=\rangle l$$

We see that $\langle k|\ p - i\ \ m\omega\ |x\rangle$ is not equal to zero only when $E_k = E_l - \hbar\omega$

Therefore the operator $(p - im\omega x)$ on $|l\rangle$ decreases the eigenvalue by $\hbar\omega$.

Thus each operation on $|l\rangle$ will successively reduce the eigenvalue by units of $\hbar\omega$.

But this cannot be done indefinitely.

Thus $(p-i)\ \ 0\rangle\ \ 0$

Now operating $(p+im\omega x)$ from the left we get

$$(p+i\ \ )(-p\ \omega i\ \ m\ )\ 0\rangle\ \ 0$$

$$\{p^2+i\ \ m\omega^2(x-p^{\ 2}p)\omega\ x^{\ 2}m\ \ x\}\ 0\rangle\ \ 0$$

Dividing throughout by 2m $\Rightarrow$

$$\left(\frac{p^2}{2m}+\frac{i\ ^2\omega m}{2m}i\hbar+\frac{m\ ^2x}{2m}\right)\ 0\rangle\ \ 0$$

$$\left(\frac{p^2}{2m}-\frac{1}{2}\hbar\omega\ \ \frac{1}{2}\right)+m\omega\ \ ^2x^2\ 0\rangle\ \ 0$$

$$\left(\frac{p^2}{2m}+\frac{1}{2}m\ \omega^2x^2\right)\frac{1}{2}\ \ \omega\hbar\ \ 0\rangle\ \ 0$$

$$\left(H-\frac{1}{2}\hbar\omega\ \ 0\rangle\right)\ \ 0$$

$$H\ 0\rangle=\frac{1}{2}\hbar\omega\ \ \rangle$$

Thus $\frac{1}{2}\hbar\omega$ is the eigenvalue of the operator H, corresponding to the eigenket $|0\rangle$.

We can also similarly prove that $(p+i\ \ m\ )$ increases the eigenvalue by $\hbar\omega$. Since this is the lowest eigenvalue and each operation of $(p+im\omega x)$ increases the eigen value by $\hbar\omega$, we can write

$$E_n=\left(n\ +\frac{1}{2}\right)\ \hbar\omega \qquad\qquad \text{n=0,1,2,.....}$$

$(p+im\omega x)$ is called the raising operator or creating operator and $(p-im\omega x)$ is called the lowering operator or annihilation operator for the above mentioned reasons.

It is a customary practice to represent the raising and lowering operators as dimensionless quantity. Therefore we multiply the raising operator $(p+im\omega x)$ by the factor $\frac{-i}{\sqrt{2m\hbar\omega}}$ and the lowering operator $(p-im\omega x)$ by the factor $\frac{i}{\sqrt{2m\hbar\omega}}$

The creation and annihilation operator is defined as

$$a^{\dagger} = \frac{1}{\sqrt{2m\hbar\omega}}\{-i\omega p + m\omega x\}$$

$$a = \frac{1}{\sqrt{2m\hbar\omega}}\{+i\omega p + m\omega x\}$$

$$a^{\dagger}a = \frac{1}{2m\hbar\omega}\{+i\omega p + m\omega x\}\{-i\omega p + m\omega x\}$$

$$= \frac{1}{2m\hbar\omega}\{m^2\omega^2 x^2 + i^2\omega^2 p^2 + im\omega(x\,p - p\,x)\}$$

$$= \frac{1}{\hbar\omega}\left\{\frac{1}{2}m\omega^2 x^2 + \frac{i\omega}{2m}(-i\hbar) + \frac{p^2}{2m}\right\}$$

$$= \frac{1}{\hbar\omega}\left\{H + \frac{1}{2}\hbar\omega\right\}$$

$$= \frac{H}{\hbar\omega} + \frac{1}{2}$$

$$\hbar\omega a^{\dagger}a + \frac{1}{2}\hbar\omega = H \qquad (12)$$

$$aa^{\dagger} = \frac{1}{2m\hbar\omega}\{+i\omega p + m\omega x\}\{-i\omega p + m\omega x\}$$

$$= \frac{1}{2m\hbar\omega}\{m^2\omega^2 x^2 + i^2\omega^2 p^2 + im\omega(x\,p - p\,x)\}$$

$$= \frac{1}{\hbar\omega}\left\{\frac{1}{2}m\omega^2 x^2 + \frac{i\omega}{2m}(-i\hbar) + \frac{p^2}{2m}\right\}$$

$$= \frac{1}{\hbar\omega}\left(H + \frac{1}{2}\hbar\omega\right)$$

$$= \frac{H}{\hbar\omega} - \frac{1}{2}$$

$$H = \hbar\omega a^{\dagger}a + \frac{1}{2}\hbar\omega \qquad (13)$$

Post multiply by a in (12) $\Rightarrow$

$$Ha = \hbar\omega a^{\dagger}aa + \frac{1}{2}\hbar\omega a \qquad (14)$$

Premultiply by a in(13)

$$aH = \hbar\omega aa^{\dagger}a + \frac{1}{2}\hbar\omega a \qquad (15)$$

Since $aH - Ha = [a, H]$ we have

$$[a, H] = \hbar\omega a$$

Similarly

$$a^{\dagger} H = \hbar\omega a^{\dagger} a^{\dagger} a^{\dagger} + \frac{1}{2} a^{\dagger}$$

$$H a^{\dagger} = \hbar\omega a^{\dagger} a^{\dagger} + \frac{1}{2} a^{\dagger}$$

Since $a^{\dagger} H - H a^{\dagger} = a^{\dagger}\left[a^{\dagger}, H\right]$ we have

$$\left[a^{\dagger}, H\right] = \hbar\omega a^{\dagger}$$

$$\left[a, a^{\dagger}\right] = a a^{\dagger} - a^{\dagger} a$$

$$a^{\dagger} a = \frac{H}{\hbar\omega} + \frac{1}{2}$$

$$a a^{\dagger} = \frac{H}{\hbar\omega} - \frac{1}{2}$$

$$\left[a, a^{\dagger}\right] = 1$$

This is called the number operator

Eigen values of raising and lowering operator $\left[a, a^{\dagger}\right]$

Let $a|\psi_n\rangle = \alpha_n |\psi_n\rangle$

$$a^{\dagger}|\psi_n\rangle = \beta_n |\psi_{n+1}\rangle$$

where α_n and β_n are the eigenvalues,

Let us find

$$\langle\psi_n | a^{\dagger} a | \psi_n\rangle = \langle\psi_n | \frac{H}{\hbar\omega} - \frac{1}{2} | \psi_n\rangle$$

$$= \langle\psi_n | \frac{(n + 1/2)\hbar\omega}{\hbar\omega} - \frac{1}{2} | \psi_n\rangle$$

$$= n\langle\psi_n | \psi_n\rangle$$

$$= n \qquad (16)$$

$$\langle\psi_n | a^{\dagger} a | \psi_n\rangle = \langle a\psi_n | a\psi_n\rangle$$

$$= \alpha_n^{*} \alpha_n \langle\psi_{n-1} | \psi_{n-1}\rangle$$

$$= |\alpha_n|^2 \qquad (17)$$

Comparing equations (16) and (17)

$$\alpha_n = \sqrt{n}$$

$$a|\psi_n\rangle = \sqrt{n}|\psi_{n-1}\rangle$$

In a similar manner let us find

$$\langle\psi_n | a a^{\dagger} | \psi_n\rangle = \langle\psi_n | \frac{H}{\hbar\omega} + \frac{1}{2} | \psi_n\rangle$$

$$= \langle\psi_n | \frac{H}{\hbar\omega} + \frac{1}{2} | \psi_n\rangle$$

$$= \langle\psi_n | \frac{(n+1/2)\hbar\omega}{\hbar\omega} + \frac{1}{2} | \psi_n\rangle$$

$$= (n+1)\langle \psi_n | \psi_n \rangle$$

$$= n+1 \qquad (18)$$

$$\langle \psi_n | a^{\dagger} | \psi_n a \rangle = \langle a^{\dagger} | a \psi_n \rangle$$

$$= \beta_n^{\dagger} \beta_n \langle \psi_{n+1} | a \psi_{n+1} \rangle$$

$$= |\beta_n|^2 \qquad (19)$$

Comparing equations (18) and (19)

$$\beta_n = \sqrt{n+1}$$

$$a^{\dagger} | \psi_n \rangle = \sqrt{n+1} | \psi_{n+1} \rangle$$

3.5. Matrix representation for $a^{\dagger}, x, a$ and p

$$\langle \psi'_n | a | \psi_n \rangle = \langle \psi'_n | \sqrt{n} | \psi_{n-1} \rangle$$

$$= \sqrt{n}\delta_{n', n-1}$$

$$a = \begin{pmatrix} 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 \\ 0 & 0 & 0 & 0 & \sqrt{5} \end{pmatrix}$$

$$\langle \psi'_n | a^{\dagger} | \psi_n \rangle = \sqrt{n+1} \langle \psi'_{n+1} | \psi_{n+1} \rangle$$

$$= \sqrt{n+1}\delta_{n', n+1}$$

$$= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{4} & 0 & 0 \end{pmatrix}$$

$$a^{\dagger} = \frac{1}{\sqrt{2m\hbar\omega}} (-i\omega x + p)$$

$$a = \frac{1}{\sqrt{2m\hbar\omega}} (+i\omega x + p)$$

$$a^{\dagger} + a = \frac{1}{\sqrt{2m\hbar\omega}} (2\omega x)$$

$$= \sqrt{\frac{2m\omega}{\hbar}} x$$

$$\Rightarrow x = \sqrt{\frac{\hbar}{2m\omega}}\left\{ a^{\dagger} \quad a \right\}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left\{\begin{pmatrix} 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 \\ 0 & 0 & 0 & 0 & \sqrt{5} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{4} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{5} & 0 \end{pmatrix}\right\}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & \sqrt{2} & 0 & 0 \\ \sqrt{2} & 0 & \sqrt{3} & 0 \\ 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & \sqrt{4} & 0 \end{pmatrix}$$

Similarly $\left(a^{\dagger} - \right)a = \frac{1}{\sqrt{2\hbar\omega m}}\left(p \right)$

Or $p = i\sqrt{\frac{m\hbar\omega}{2}}\left(\pm a \right)$

$$= i\sqrt{\frac{m\hbar\omega}{2}}\begin{pmatrix} 0 & -\sqrt{2} & 0 & 0 \\ \sqrt{2} & 0 & -\sqrt{3} & 0 \\ 0 & \sqrt{3} & 0 & -\sqrt{4} \\ 0 & 0 & \sqrt{4} & 0 \end{pmatrix}$$

3.6. An infinite array of square wells The Kronig – Penney Model

When the array of potential wells extends to infinity on both sides, we have to make sure that the wave functions does not diverge as $x \to \pm$. We know that this is possible only if $|\mu| = 1$ For, if $|\mu| < 1 \mu^{N} \to \infty$ as $N \to -$ and $\mu^{-N} \to$ as $N \to +$. When $\mu > 1$ the situation is reversed. In either case, the wave function in the N^{th} well will diverge in one or both of the limits $N \to +$ and $N \to -$. Hence we must have

$$\mu = e^{i\theta} \quad (\theta \text{ real}) \tag{1}$$

Also we have

$$c\ \theta = \frac{1}{2}\left(\mu s^{-1} \right) \alpha\ '\ \omega\ c = \beta\ s\ \omega\ s\ i\ n\ \omega h\ '\beta = f\ s\ \omega\ i\ n\beta - c\ \omega\ s\varphi(\tag{2}$$

where

$$f = (\cosh^2 \alpha\omega' \cdot \sinh^2 \alpha\omega')^{\frac{1}{2}} \qquad \tan\varphi = s \tanh \alpha\omega' \tag{3}$$

The above equation (3) determines the allowed energy levels since α and β (and hence f and φ also) depend on the parameter E. From the structure of this equation it is immediately evident that the allowed energies form continuous bands with gaps in between. For, since the value of the left hand side of equation (2) is restricted to $-1 \le \cos\theta \le 1$ the equation can be satisfied only when the right hand side also is within this range. As the parameter E is varied , the right hand side, $f \cos(\beta\omega - \varphi)$ as oscillates between the bounds + f (E) and - f (E) which lie outside the limits +1 and -1 admissible for cosθ, since $|f| \ge \cosh \alpha\omega'$. The intervals of E for which $|f \cos(\beta\omega - \varphi)| \le 1$ constitute the 'allowed' energy bands, and those for which $|f \cos(\beta\omega - \varphi)| > 1$ are the 'forbidden' regions. These form energy gaps, between allowed bands. The variation of $f \cos(\beta\omega - \varphi)$ with E, and the identification of energy bands and gaps are illustrated in Figure 3.1

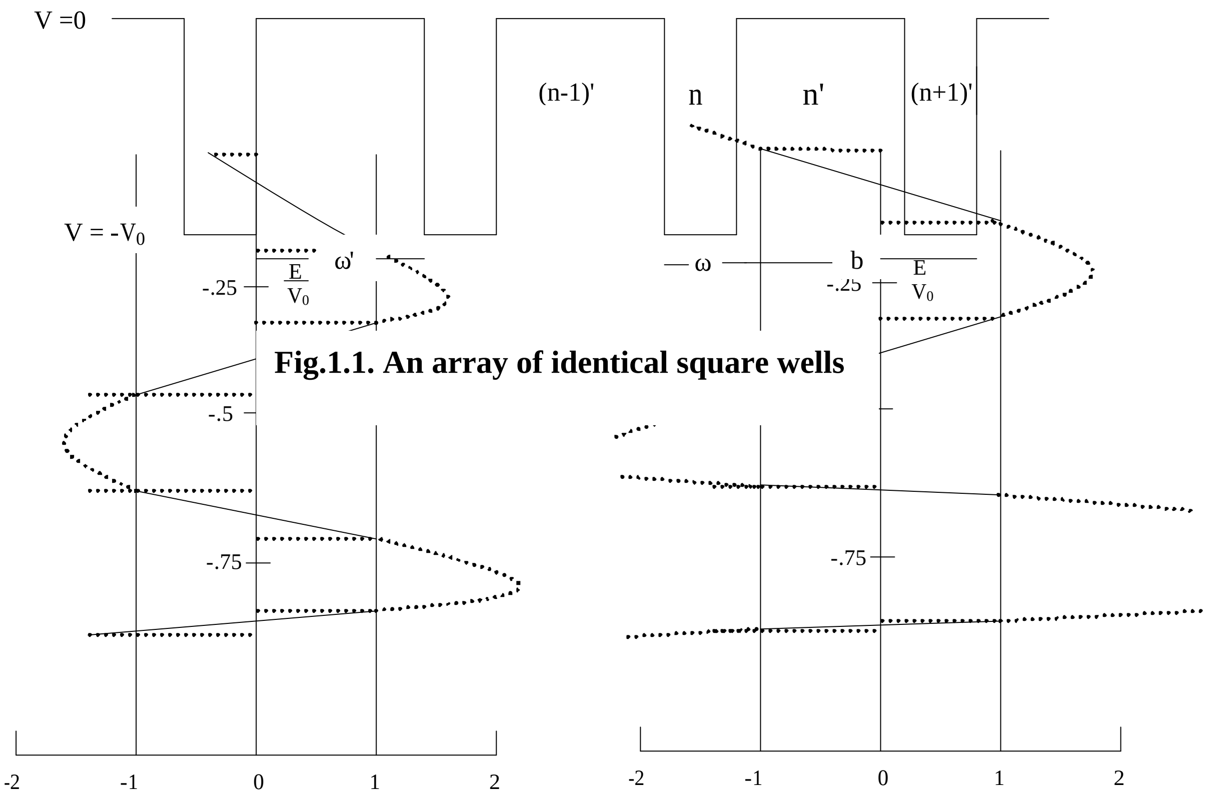

Fig.1.1. An array of identical square wells

Fig.1 fcos(βω-φ)

b) fcos(βω-φ)

Fig.3.1 Energy bands and gaps or $V_0\omega^2 = 2$ (a) $\omega' = 0.1$ and (b) $\omega' = 0.2$ Bands of allowed energies are shown as thickened sections on the energy axis. Note the narrowing of the bands as ω' increases. In the limit $\omega' \to \infty$ they reduce to points at the positions of the energy levels of a single potential well, shown by arrows in the figure

The nature of the energy eigenfunctions u(x) corresponding to any energy E within an allowed band can now be easily seen. We recall that we have already imposed the necessary continuity conditions on the wave function, which resulted in the 'transfer' equation

$$\begin{pmatrix} A_n^+ \\ A_n^- \end{pmatrix} = M \begin{pmatrix} A_0^+ \\ A_0^- \end{pmatrix} \tag{4}$$

and also the condition of finiteness at infinity which gave us the restriction equation (2) on the eigenvalues of the transfer matrix M. There are no further conditions on the wave function, and in particular, there is nothing to prevent us from choosing the two coefficients (A^+, A^- or B^+, B^-) in any one of the regions in Figure.1.2. Suppose then that we choose some energy E within an allowed band, and after finding α,β,c,s for this E using

$$\frac{2m}{\hbar^2} = \alpha^2 \quad \frac{2m}{\hbar^2}(V_0 - E) = \beta^2 \tag{5}$$

determine θ from equation (2) and the matrix M itself from equation (4). Now let us avail ourselves of the freedom of choosing the coefficients, and take A_0^+, A_0^- to be such that the column made up of these is the eigenvector belonging to the eigenvalue $e^{i\theta}$ of M, i.e.

$$M \begin{pmatrix} A_0^+ \\ A_0^- \end{pmatrix} = e^{i\theta} \begin{pmatrix} A_0^+ \\ A_0^- \end{pmatrix} \tag{6}$$

The θ-dependence of the coefficients so defined is explicitly indicated here**.** From

$$\begin{pmatrix} A_N^+ \\ A_N^- \end{pmatrix} = M^N \begin{pmatrix} A_0^+ \\ A_0^- \end{pmatrix} \tag{7}$$

we have

$$\begin{pmatrix} A_n^+ \\ A_n^- \end{pmatrix}_\theta = e^{in\theta} \begin{pmatrix} A^+ \\ A^- \end{pmatrix}_\theta \qquad (8)$$

i.e. the coefficients depend on n only through the simple factor $e^{in\theta}$. It is obvious that a similar result holds good for B_n^+ and B_n^- also. If we think of a well and the adjacent barrier together, as forming a 'unit cell' of the repeating pattern, the result just obtained may be stated in the following instructive form: The wave functions at corresponding points x and x + nb of wells (or barriers) separated by n unit cells differ only by the constant factor $e^{in\theta}$:

$$u_\theta(x+n) = e^{in\theta} u_\theta(x) \qquad (9)$$

This property is often expressed in the form

$$u_\theta(x) = e^{i\theta x/b} v_\theta(x) \text{ and } v_\theta(x+n) = v_\theta(x) \qquad (10)$$

Equation (10) may be thought of as the definition of $v_\theta(x)$, and when it is introduced in equation (9), the periodicity of $v_\theta(x)$ follows. Besides $u_\theta(x)$ there is another independent solution $u_{-\theta}(x)$ obtained by using the eigenvalue $e^{-i\theta}$ of M instead of $e^{i\theta}$ in equation (6). The most general eigenfunction for a given energy E is a linear combination $c_1 u_\theta(x) + c_2 u_{-\theta}(x)$, with arbitrary complex coefficients c_1 and c_2.

The above results are of considerable physical importance in the study of crystalline solids where in the array of atoms produces a potential forming a regular repeating pattern. In the usual situation, the number of atoms is so large that the idealization to infinite number may be made to simplify matters. The Kronig-Penny model makes the further idealization of treating the potential due to each atom as a square well. But the fundamental specifically, the occurrence of allowed energy bands and forbidden gaps follows just from the periodicity property, V(x) = V(x + nb), of the potential. The general form equation (10) of the eigenfunctions, are called Bloch wave functions. But the explicit structure of the function $v_\theta(x)$ in equation (10) depends on the actual shape of the potential function.

3.7. LET US SUM UP

From this lesson one can get an clear idea on linear harmonic oscillator in detail. We can calculate the energy eigenvalues. The Kronig – Penny model, is discussed in detail which find application field of nuclear physics and material science.

3.8. Test Yourself

1. What are raisnig and lowering operators? Explain why they are so called.
2. Give the matrix theory of harmonic oscillator and obtain the energy eigenvalue spectrum.
3. Explain Kronig Penny model.
4. Write down the matrices for the ladder operators a, a^+ of the harmonic oscillator in the representation which diagonalises the Hamiltonian.

3.9. References

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LESSON 4

STATIONARY PERTURBATION THEORY

4.1 Aim and Objectives

In this lesson, we are going to give an introduction to various approximation methods and going to study Stationary perturbation theory and its applications in detail

4.2. INTRODUCTION

In quantum mechanics, there are many physical systems for which, the equation of motion cannot be solved exactly. So, one has to resort to approximation methods. There are three most important approximation methods in quantum mechanics. They are

4.2.1. The Perturbation Method

This method is applicable, when the Hamiltonian can be written as sum of two parts. i.e.

$H = H_o + H'$

Where $H_O \rightarrow$ unperturbed Hamiltonian

& $H' \rightarrow$ perturbed Hamiltonian & is assumed to be very small.

Applications : - Stark effect, Zeeman effect

4.2.2. Variational Method

It gives good estimate of the ground state energy by choosing an appropriate trial function. The main disadvantage of this method is that, Pt cannot be extended higher excited states.

Applications :- Ground state of Hydrogen, Helium.

4.2.3. W.K.B. Approximation

This method gives an approximate but direct solution of Schrödinger equation. This method is applicable. When the potentials are such that, the Schrödinger equation is separable to a one dimensional equation and when the potential is a smoothly varying function.

Applications :- Barrier penetration problem, Alpha decay problem.

Approximation methods, therefore, plays an important role in all applications of theory. This enhances rather than, diminishes, the importance of those problems for which exact solutions can be found out. Also, the exact solutions are often useful as starting points for approximate calculations. They may also help to establish limits of validity for various approximation methods. These methods can be broadly classified in to two, according as they deal with bound states or with scattering states.

4.3. Time Independent Perturbation Theory or Stationary Perturbation Theory

The stationary perturbation theory is concerned with finding the changes in the discrete energy levels and eigenfunctions of a system when a small disturbance is applied. It is assumed that the Hamiltonian H is the Schrödinger equation can be written as sum of two parts.

$$\text{i.e. } H = H_o + H' \qquad (1)$$

where H_o is unperturbed Hamiltonian & is of sufficiently simple structure, that its Schrödinger equation can be solved.

& H' is perturbed Hamiltonian & is small enough so that it can be regarded as a perturbation on H_o.

Let $U_k \& E_k$ be the orthonormal eigenfunctions & eigenvalues of the unperturbed Hamiltonian H_o. Let $\psi \& W$ be the wave function and energy level of perturbed Hamiltonian Therefore we can write.

$$H_0 \; U_k = E_k \; U_k$$
$$H\psi \quad W\psi$$

4.3.1. Non degenerate case

The assumption that H' is small suggests that, we expand the perturbed eigenfunction & eigenvalues as power series in H'. This is easily accomplished in-terms of a parameter λ, such that, the zero, first, second…….. powers of λ correspond to zero, first, second …….. orders of perturbations. We replace H' by $\lambda H'$ and express Ψ and W as power series in λ. We assume that, these two series are continuous analytic function of λ for λ between zero and one. The different orders of perturbation approximation are then given by the coefficients of corresponding powers of λ. In the final result, λ is set equal to one.

The perturbed wave function & energy level are written as

$$\psi = \psi_0 + \lambda \psi_1 + \lambda^2 \psi_2 + \lambda^3 \psi_3 + \ldots\ldots \quad (3a)$$

$$W = W_0 + \lambda W_1 + \lambda^2 W_2 + \lambda^3 W_3 + \ldots\ldots \quad (3b)$$

using (2) and (3) in equation (1) we get

$$(H_o' + \lambda H') (\psi_0 + \lambda \psi_1 + \lambda^2 \psi_2 + \ldots) = (W_0 + \lambda W_1 + \lambda^2 W_2 + \ldots)(\psi_0 + \lambda \psi_1 + \lambda^2 \psi_2 + \ldots) \quad (4)$$

The above equation is valid for a continuous range of λ. We now, equate the coefficients of equal powers of λ on both sides to obtain a series of equations that represent successively higher orders of perturbation.

$$\lambda^0 \Rightarrow H_0 \psi_0 = W_0 \psi_0$$

$$\Rightarrow (H_0 - W_0)\psi_0 = 0 \quad (5a)$$

$$\lambda^1 \Rightarrow H_0 \psi_1 + H' \psi_0 = W_0 \psi_1 + W_1 \psi_0$$

$$\Rightarrow (H_0 - W_0)\psi_1 = (W_1 - H')\psi_0 \quad (5b)$$

similarly for λ^2 (5c)

$$\lambda^3 \Rightarrow (H_0 - W_0)\psi_3 = (W_1 - H')\psi_2 + W_2 \psi_1 \quad (5d)$$

……

……

The first of the above set of equations means that ψ_0 is any one of the unperturbed eigenfunctions. Therefore, we can write,

$$\psi_0 \quad u_m = \&_o \Psi W_m E \tag{6}$$

This state u_m is discrete, since we are dealing with the perturbation of a bound state. It is assumed to be non degenerate as well, although, others of the unperturbed eigenfunctions may be degenerate or continuous.

4.3.2. First order Perturbation

The first order perturbation equation is given by

$$(H_0 - W_0\psi)(\psi_1 = W_1 - H'\psi)$$

Expressing $\psi_1 = a_n \sum u_n \psi \& = u_m$

$$\Rightarrow (H_0 - W_0)\sum a_n = (u^1)(w - H'_m)u$$

$$\Rightarrow a_n \sum H^1_0 u - a_n W \sum u_0 \Psi W_n u_1 - H_m' u$$

$$\Rightarrow a_n \sum E^1_n u - a_n E \sum u_m \Psi W_n u_1 - H_m' u$$

$$\Rightarrow a_n \sum [E^1_n - E_m] u = W_1 u - H'_m u$$

Multiplying by - & rearranging we get

$$\Rightarrow a_n \sum [E_m - E_n] u_k = W_1 u - H'_m u$$

Multiplying the above equation u^*_k and integrating we get,

$$\Rightarrow a_n \sum [E_m - E_n] \int u_k u \, d\tau = \int u^*_k W_1 u \, d\tau - \int u^*_k H' u \, d\tau$$

$$W \cdot I \int \psi^*_\ell T \psi_m \, d\tau = \delta_{m\ell} = 0 \neq i \neq m$$

$$\Rightarrow a_n (E^1_m - E_k \delta_k E_n + 1) \delta W_m - H_k' m'$$

Carrying out the summation we get

$$a_k (E^1_m - E_k + 1) \delta W_k - H'_m \tag{7}$$

$$where H'_k = \int \psi^*_k H'_m u \, d\tau = \langle k | H' | m \rangle$$

When k = m equation (7) becomes

$$W_1 = H'_m = m \mid H' \mid m \tag{8}$$

which represents the first order perturbation of the energy.

For k ≠ m, equation (7) gives

$$a_k^{(1)} = \frac{H'_{km}}{(E_m - E_k)} \qquad (9)$$

Noticethatwehavenotbeenabletodetermine $a_m^{(1)}$ hence we assume that $a_m^{(1)} = 0$

4.3.3. Second order perturbation

The second order perturbation equation is given by

$$\Rightarrow (H_0 - E_0)\psi_2 + (H_1 - E_1)\psi_1 = E_2\psi_0$$

Expressing $\psi_2 = \sum_n a_n^{(2)} u_n$, $\psi_1 = \sum_n a_n^{(1)} u_n$, $\psi_0 = u_m$

we get

$$\Rightarrow \sum_n a_n^{(2)} (H_0 - E_0) u_n + \sum_n a_n^{(1)} (H_1 - E_1) u_n = E_2 u_m$$

$$\Rightarrow \sum_n a_n^{(2)} (E_n - E_0) u_n + \sum_n a_n^{(1)} (H_1 - E_1) u_n = E_2 u_m$$

$$\Rightarrow \sum_n a_n^{(2)} (E_n - E_m) u_n + \sum_n a_n^{(1)} (H_1 - E_1) u_n = E_2 u_m$$

Rearranging we get

$$\Rightarrow \sum_n a_n^{(2)} (E_n - E_m) u_n = E_2 u_m - \sum_n a_n^{(1)} (H_1 - E_1) u_n$$

Multiplying by u_k^* & integrating we obtain.

$$\sum_n a_n^{(2)} (E_n - E_m) \int u_k^* u_n d\tau = E_2 \int u_k^* u_m d\tau$$

$$- \sum_n a_n^{(1)} \int u_k^* (H_1 - E_1) u_n d\tau$$

$$\sum_n a_n^{(2)} (E_n - E_m) \delta_{kn} = E_2 \delta_{km} - \sum_n a_n^{(1)} H'_{kn} + \sum_n a_n^{(1)} H'_{km} \delta_{kn}$$

Carrying out summation we get

$$a_k^{(2)} (E_k - E_m) = E_2 \delta_{km} - \sum_n a_n^{(1)} H'_{kn} + a_m^{(1)} H'_{km} \qquad (10)$$

For m = k, we get,

$$E_2 = \sum_n a_n^{(1)} H'_{mn} - a_m^{(1)} H'_{mm}$$

$$= \sum_{\substack{n \\ n \neq m}}' a_n^{(1)} H'_{mn}$$

where prime over the summation indicates that, we have omitted the term n = m. Substituting the value of $a_n^{(1)}$ from first order perturbation equation we have,

$$E_2 = \sum_n' \frac{|H'_{mn}|^2}{(E_m - E_n)}$$

where we used the relation $H'_{mn} = (H'_{nm})^*$. The above equation gives the second order perturbation to the energy eigenvalue.

For k ≠ m, equation (10) gives

$$a_k^{(2)} = \sum_{m,n} \frac{H'_{kn} H'_{nm} H'_{mk}}{(E_m - E_k)(E_n - E_k)} - \frac{H'_{mm} H'_{mk}}{(E_m - E_k)^2}$$

$$a_k^{(2)} = \sum_{n} \frac{\langle k | H' | n \rangle \langle n | H' | m \rangle \langle m | H' | k \rangle}{(E_m - E_k)(E_n - E_k)} - \frac{\langle m | H' | m \rangle \langle m | H' | k \rangle}{(E_m - E_k)^2} \qquad (12)$$

Similarly we can obtain $W_3, W_4 \ldots\ldots$

With this, the energy and wavefunction to second order in H' is given by

$$W = E_m + \langle m | H' | m \rangle + \sum' \frac{|\langle m | H' | n \rangle|^2}{E_m - E_n} \qquad (13\ a)$$

$$\psi_m = u_m + \sum' \left[\frac{\langle k | H' | m \rangle}{E_m - E_k} + \left(\frac{\langle m | H' | m \rangle}{E_m - E_k} \right) \frac{\langle k | H' | n \rangle \langle n | H' | m \rangle}{(E_m - E_k)(E_m - E_n)} \right] u_k \qquad (13\ b)$$

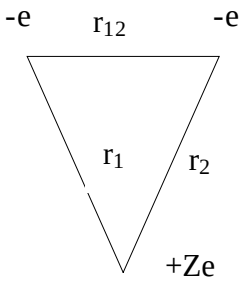
The primes in the above equation denote the omission of k = m or n = m. It is to be noted that, the wave function ψ is not normalised since

$$(\psi, \psi) = 1 + \sum_k' \frac{|\langle k | H' | m \rangle|^2}{(E_m - E_k)^2} \qquad (14)$$

to the second order in H'. This occured because each condition $(\psi_0, \psi_n) = 0$, s

Applications of Stationary Perturbation Theory

The Normal Helium Atom Or Ground State Of Helium Atom



NUCLEUS

Consider the normal state of helium atom which contains a nucleus of charge Ze and two electrons each having a charge –e. The potential energy of such a system is given by

$$V = -\frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{r_{12}} \qquad (1)$$

in which r_1 and r_2 are the distances of electrons 1 and 2, respectively from nucleus

and r_{12} is the separation of the two electrons as shown in Figure 1.

Considering the nucleus at rest, the wave equation for the two electrons becomes

$$\left(\frac{\partial^2\psi}{\partial x_1^2}+\frac{\partial^2\psi}{\partial y_1^2}+\frac{\partial^2\psi}{\partial z_1^2}+\frac{\partial^2\psi}{\partial x_2^2}+\frac{\partial^2\psi}{\partial y_2^2}+\frac{\partial^2\psi}{\partial z_2^2}\right) + \frac{2m}{\hbar^2}\left[E+\frac{Ze^2}{r_1}+\frac{Ze^2}{r_2}-\frac{e^2}{r_{12}}\right]\psi = 0 \tag{2}$$

The variables x_1, y_1, z_1 are Cartesian coordinates of one electron and x_2, y_2, z_2 those of the other. If the term $\frac{e^2}{r_{12}}$ is omitted, the wave equation can be solved exactly; hence this term may be regarded as perturbation term

$$H^{(1)} = \frac{e^2}{r_{12}} \tag{3}$$

The unperturbed wave equation can be separated into two equations by substituting

$$\psi^{(0)}(x_1y_1z_1, x_2y_2z_2) = u_1^{(0)}(x_1y_1z_1)u_2^{(0)}(x_2y_2z_2) \tag{4}$$

Considering the wave functions in polar coordinates r_1, θ_1, ϕ_1, and r_2, θ_2 ϕ_2 and in normal state,

$$\psi_{100,100}^{(0)} = \psi_{100}^{(0)}(r_1,\theta_1,\phi_1)\psi_{100}^{(0)}(r_2,\theta_2,\phi_2)$$

$$= \psi_{1s}^{(0)}(r_1,\theta_1,\phi_1)\psi_{1s}^{(0)}(r_2,\theta_2,\phi_2)$$

and corresponding eigenvalue is

$$E_{100,100}^{(0)} = E_1^{(0)} + E_2^{(0)} = -2Z^2E_H \tag{5}$$

The first order perturbed energy $E^{(1)}$ is the average value of the perturbation function $H^{(1)} = \frac{e^2}{r_{12}}$ over the unperturbed state of the system. Hence

$$E^{(1)} = \int \psi_n^{(0)*} H^{(1)} \psi_n^{(0)} d\tau = \int \psi_{100,100}^{(0)2} \frac{e^2}{r_{12}} d\tau \tag{6}$$

we know that

$$u_{1s}^{(0)} = \psi_{100} = \sqrt{\left(\frac{Z^3}{\pi a_0^3}\right)}\, e^{-\rho/2} \tag{7}$$

in which $\rho = 2Zr / a_0$ and $a_0 = h^2 / (4\pi^2 me^2)$

$$\psi^{(0)}_{100,100} = \frac{Z^3}{\pi a_0^3} e^{(-\rho_1/2)} e^{(-\rho_2/2)}. \quad (8)$$

The volume element is

$$d\tau = r_1^2 dr_1 \sin\theta_1 d\theta_1 d\phi_1 r_2^2 \sin\theta_2 d\theta_2 d\phi_2 \quad (9)$$

So that the integral for $E^{(1)}$ becomes

$$E^{(1)} = \frac{Z^2 e}{2^5 \pi^2 a_0} \int_0^\infty \int_0^\pi \int_0^{2\pi} \int_0^\pi \int_0^\pi \int_0^{2\pi} \frac{e^{(-\rho_1 - \rho_2)}}{\rho_{12}} \rho_1^2 \rho_2^2 \sin\theta_1 d\theta_1 d\phi_1 \sin\theta_2 d\theta_2 d\phi_2 d\rho_1 d\rho_2 \quad (10)$$

in which $\rho_{12} = 2Zr_{12} / a_0$.

The value of the integral can be calculated by considering the electrostatic interaction energy of two spherically symmetrical distributions of electricity, with density functions $e^{(-\rho 1)}$ and $e^{(-\rho 2)}$ respectively, Solving the integral, we have

$$E^{(1)} = \frac{5}{4} Z E_H \quad (11)$$

Thus the total energy of the system is

$$E^{(1)} = \left(-2Z + 5/4 Z \right) E_H \quad (12)$$

Thus we can calculate the energy of He, Li^+, Be^{++}, etc. with Z = 2,3,4 etc. respectively.

4.4.2. Stark effect in Hydrogen: Linear or First order Stark Effect

The ground state of hydrogen atom is non – degenerate, but the n = 2 energy levels of hydrogen atom is four – fold degenerate. On the application of an external electric field, the degeneracy is partly removed. The splitting of atomic energy levels due to the application of external electric field is known as Stark effect and it has been discovered as early as 1913. It is found that the splitting of energy levels of the hydrogen atom for weak electric field is proportional to the field strength, and hence it is known as Linear Stark Effect or First order Stark Effect.

The splitting of energy level for all other atom is proportional to second power of the field strength and that is known as Quadratic Stark Effect.

Let us denote the eigenfunctions of the hydrogen atom, by $\psi_{n\,l\,m}(r, \theta, \phi)$. The ground state $\psi_{1\,0}$ is non – degenerate, but, the first excited state $\psi_{2\,l\,m}$ with n = 2 is four fold degenerate. We shall write down explicitly the degenerate eigenfunctions,

$$\left.\begin{aligned} u_1 &= \psi_{2\,0\,0} = R_{2\,0}(r)\,Y_{0\,0}(\theta, \phi) \\ u_2 &= \psi_{2\,1\,0} = R_{2\,1}(r)\,Y_{1\,0}(\theta, \phi) \\ u_3 &= \psi_{2\,1\,1} = R_{2\,1}(r)\,Y_{1\,1}(\theta, \phi) \\ u_4 &= \psi_{2\,1\,-1} = R_{2\,1}(r)\,Y_{1\,-1}(\theta, \phi) \end{aligned}\right\} \qquad (1)$$

where, $Y_{l\,m}(\theta, \phi)$ are the spherical harmonics and $R_{21}(r)$ and $R_{20}(r)$ are the radial part of the wave functions. The radial functions are given by ,

$$R_{2\,0}(r) = \frac{1}{\sqrt{2a_0^{\,3}}}\left(1 - \frac{r}{2a_0}\right) e^{-r/2a_0} \qquad (2)$$

$$R_{2\,1}(r) = \frac{1}{2\sqrt{6a_0^{\,3}}}\frac{r}{a_0} e^{-r/2a_0} \qquad (3)$$

$$a_0 = \hbar^2 / \mu_e^{\,2} \qquad (4)$$

The Hamiltonian of the hydrogen atom is taken as the unperturbed Hamiltonian H_0 and the applied electric field as the perturbation H'. If the electric field E is along the z – axis, the perturbation is given by

$$H' = -eE_z$$

$$= -e\,Er\cos\theta$$

$$H'_{e} = \sqrt{\frac{4\pi}{3}}\,|\,|\,Er\,Y_{1\,0}(\theta\ \varphi) \qquad (5)$$

where, $-e-$ is a positive quantity.

Since, H' is of odd parity, the matrix elements between the states of same parity (same l value) vanish. The same result can be arrived at by considering the angular integration involving the spherical harmonics. The only surviving matrix elements are,

$$\left.\begin{aligned} &\langle \psi_{2\,0\,0} | H' | \psi_{2\,1\,0} \rangle \\ &\langle \psi_{2\,1\,0} | H' | \psi_{2\,0\,0} \rangle \end{aligned}\right\}$$

It can be easily seen that this two matrix elements are equal. Let us evaluate one of them

$$\langle \psi_2 | H_0 | \psi_2 \rangle = \int \psi_2^* H_0 \psi_2 \, d\tau_0$$

$$= \int R_2(r_0) R_2(r_0) r_0^2 dr_0 \int Y_{00}(\theta_0, \phi_0) H_0 Y_{00}(\theta_0, \phi_0) d\Omega_0$$

$$= \sqrt{\frac{4\pi}{3}} |e| E \int R_2(r_0) r_0^2 dr_0 \int Y_{00}(\theta_0, \phi_0) Y_{10}(\theta_0, \phi_0) d\Omega_0$$

where, $Y_{00}(\theta, \phi) = \sqrt{\frac{1}{4\pi}}$

$$\int Y_{10} Y_{10} d\Omega = 1$$

and hence the angular integration yields $\frac{1}{\sqrt{4\pi}}$. The radial integral can be performed by substituting the radial function from equations (2) and (3)

$$\int_0^\infty R_2(r_0) R_2(r_0) r_0^3 dr_0 = \frac{1}{4\sqrt{3}} \int_0^\infty \left(1 - \frac{r}{2a_0}\right)^2 r^4 e^{\frac{-r}{a_0}} dr$$

Letting $x = \frac{r}{a_0}$ the integral becomes,

$$= \frac{a_0}{4\sqrt{3}} \int_0^\infty \left(1 - \frac{x}{2}\right)^2 x^4 e^{-x} dx$$

$$= \frac{a_0}{4\sqrt{3}} \left[4 - \frac{5}{2}\right]!$$

$$= \frac{9a_0}{4\sqrt{3}} \qquad (7)$$

$$\langle \psi_2 | H_0 | \psi_2 \rangle = \sqrt{\frac{4\pi}{3}} E |e| \left(\frac{9a_0}{\sqrt{3}}\right) \frac{1}{\sqrt{4\pi}}$$

$$= |e| E \sqrt{\frac{4\pi}{3}}$$

$$\langle \psi_2 | H_0 | e \rangle = 3 |E| a_0 \qquad (8)$$

Denoting the matrix elements $\langle \psi_2 | H_0 | \psi_2 \rangle$ and $\langle \psi_2 | H_0 | \psi_2 \rangle$ as H_1' and H_2' because of the definition equation (1) and denoting the quantity $3|e|E a_0$ by P_1 we have,

$$H_1' = H_2' = P_2 \quad e \quad 3E \, a_0 \qquad (9)$$

Substituting the values of H_1' and H_2' in the secular equation,

$$\begin{vmatrix} -W_1 & -P & 0 & 0 \\ -P & -W_1 & 0 & 0 \\ 0 & 0 & -W_1 & 0 \\ 0 & 0 & 0 & -W_1 \end{vmatrix} = 0$$

The roots of the above secular equations are ,

$$W_1 = P, -P, 0 ,$$

Let us write down explicitly the set of linear equations

$$\left.\begin{aligned} -W_1 C_1 - P C_2 &= 0 \\ -P C_1 - W_1 C_2 &= 0 \\ -W_1 C_3 &= 0 \\ -W_1 C_4 &= 0 \end{aligned}\right\} \qquad (10)$$

If $W_1 = P$, then $C_1 = - C_2$ and $C_3 = C_4 = 0$

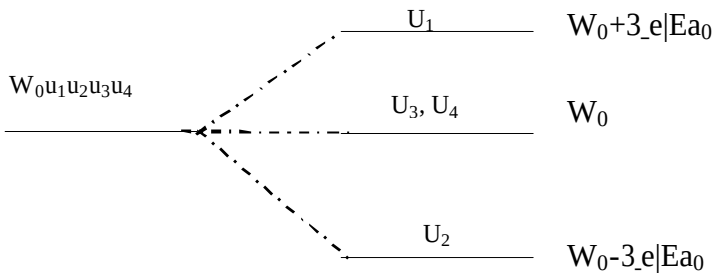
If $W_1 = -P$, then $C_1 = C_2$ and $C_3 = C_4 = 0$

If $W_1 = 0$, then $C_1 = C_2 = 0$ and C_3 and C_4 are indeterminate

Then it follows that,

$$\left.\begin{aligned} U_1 &= \frac{1}{\sqrt{2}}(u_1 - u_2) \\ U_2 &= \frac{1}{\sqrt{2}}(u_1 + u_2) \\ U_3 &= C_3 u_3 + C_4 u_4 \\ U_4 &= C_3' u_3 + C_4' u_4 \end{aligned}\right\} \qquad (11)$$

give respectively the first order correction to the energy and the corresponding zeroth order eigenfunctions. It is seem that out of the four degenerate states only the two states $\psi_{2\,0}$ and $\psi_{2\,-1}$ are split but the other two states $\psi_{2\,1}$ and $\psi_{2\,-1}$ continue to be degenerate. This is diagrammatically shown in the following figure.



in absence of electric field in presence of electric field

4.5. LET US SUM UP

It is very clear that this lesson gives an exposure on stationary perturbation theory and its application such as normal state of Helium and Stark effect.

4.6. LESSON END ACTIVITIES

Check your progress

1. 'There is no first order stark effect in the ground state of an atom' – Illustrate.
2. Explain briefly stationary perturbation theory.
3. Define the degeneracy of an energy eigenvalue and illustrate its removal by considering the stark effect in the n = 2 level of the hydrogen atom.
4. Obtain the expressions for the first order corrections to the energy and wave function making the use of the non-degenerate stationary perturbation theory.

4.7. References

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LESSON 5

VARIATIONAL METHOD AND WKB APPROXIMATION

5.1. Aims and Objectives

In this lesson also, we are going to concentrate on the other two approximation methods namely Variational method and WKB approximation.

5.2. Variational Method:

The variation method is specially applicable for determining the lowest energy of the system. According to this method, the integral

$$W = \int \phi^* H \phi \, d\tau \geq E_0 \qquad (1)$$

is an upper limit to the lowest energy state of the system. In the above equation, H is the complete Hamiltonian operator for the system and the function ϕ is any normalised function of the co-ordinates of the system. The choice of the function ϕ is quite arbitrary but the more wisely H is chosen, the more closely W will approach the energy E_o. If we use the true wave function ψ_o of the lowest state instead of ϕ, then W will be equal to E_o.

It ϕ is not equal to ψ_o, we may expand ϕ is terms of the complete set of normalised orthogonal functions $\psi_o, \psi_1, \ldots \psi_n \ldots$.

$$\phi = \sum_n a_n \psi_n \qquad \int \phi^* \phi \, d\tau = \sum_n a_n^* a_n = 1 \qquad (2)$$

Substituting in equation (1) we

$$W = \sum_n \sum_m a_n^* a_m \int \psi_n^* H \psi_m \, d\tau$$

$$= \sum_n \sum_m a_n^* a_m \int \psi_n^* E_m \psi_m \, d\tau$$

$$= \sum_n \sum_m a_n^* a_m E_m \delta_{nm}$$

$$= \sum_n a_n^* a_n E_n$$

$$W = \sum_n |a_n|^2 E_n \qquad (3)$$

Subtracting the ground state energy from the both

$$W - E_0 = \sum_n |a_n|^2 E_n - E_0 \quad \because \sum_n |a_n|^2 = 1$$

$$= \sum_n |a_n|^2 (E_n - E_0) \tag{4}$$

As $|a_n|^2$ is positive and $E_n \geq E_0$, the R.H.S is positive or Zero. Thus the have proved that W is an upper bound to the lowest value of energy E_0.

$$\because W \geq E_0 \tag{5}$$

Note :-

If the function ϕ is not normalised, then W is given by the expression

$$W = \frac{\int \phi^* H \phi \, d\tau}{\int \phi^* \phi \, d\tau}$$

The variation of ϕ is performed by first choosing a suitable functional form for ϕ. Depending on a number of parameters $\lambda_1, \lambda_2 \ldots \lambda_n \ldots$

$$W(\lambda_1, \lambda_2 \ldots \lambda_n \ldots) = \int \phi_i^* (\lambda_1, \lambda_2 \ldots \lambda_n \ldots) H \phi_i (\lambda_1, \lambda_2 \ldots \lambda_n \ldots) \tau$$

As the parameters are varied, the value of W also varies. Minimization of W is then accomplished by finding the values of $\lambda_1, \lambda_2 \ldots \lambda_n \ldots$ for which

$$\frac{\partial W}{\partial \lambda_1} = \frac{\partial W}{\partial \lambda_2} = \ldots \frac{\partial W}{\partial \lambda_n} = \ldots$$

5.3. Application of Varitional Method :

5.3.1. Ground state energy of the Hydrogen atom.

In this case wave function is of the general form

$$\psi = e^{-a} \tag{1}$$

For the ground state of hydrogen atom, the potential energy term will be $-e^2/r$ and hence the form of the Hamiltonian operator $\hat{H}$ will be

$$\hat{H} = -\frac{h^2}{8\pi^2 m}\nabla^2 - \frac{e^2}{r} \tag{2}$$

as the energy occurs in the radial equation, we need only to consider the radial part of the Laplacian operator ∇^2. Hence

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) \tag{3}$$

The value of $\nabla^2\psi$ will be

$$\nabla^2\psi = \left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right] e^{-ar}$$

$$= \frac{1}{r^2}\left[2r\frac{\partial}{\partial r} + r^2\frac{\partial^2}{\partial r^2}\right]e^{-ar}$$

$$= \frac{1}{r^2}\left[2r\frac{\partial}{\partial r}\left(e^{-ar}\right) + r^2\frac{\partial^2}{\partial r^2}\left(e^{-ar}\right)\right]$$

$$= \frac{1}{r^2}\left[2r(-a)e^{-ar} + r^2a^2e^{-ar}\right]$$

$$= e^{-ar}\left\{a^2 - \frac{2a}{r}\right\} \qquad (4)$$

According to variational method, the energy E is given by

$$E = \frac{\int \psi^* \hat{H}\psi \, d\tau}{\int \psi^* \psi \, d\tau}$$

$$= \frac{\int_0^\infty e^{-ar}\left[-\frac{h^2}{8\pi^2 m}\left\{a^2 - \frac{2a}{r}\right\} - \frac{e^2}{r}\right] r^2 \, d(4\pi r)}{\int_0^\infty e^{-2ar} 4\pi r^2 \, dr}$$

where $4\pi r^2 dr$ is the volume of a spherical shell at a distance r and r+dr from the nucleus. The limit of integration varies from 0 to ∞ as r goes form zero to infinity.

$$= \frac{\int_0^\infty -\frac{h^2}{8\pi^2 m} r^2 a^2 e^{-ar} dr + \int_0^\infty \frac{h^2}{8\pi^2 m} 2ar e^{-ar} dr - \int_0^\infty e^2 r e^{-ar} dr}{\int_0^\infty r^2 e^{-2ar} dr} \qquad (5)$$

Applying the relation $\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$

The values of the above integrals can be obtained as

$$= \frac{-\frac{h^2a^2}{8\pi^2 m}\left\{\frac{2}{8a^3}\right\} + \frac{h^2a}{4\pi^2 m}\left\{\frac{1}{4a^2}\right\} - e^2\left\{\frac{1}{4a^2}\right\}}{\left\{\frac{2}{8a^3}\right\}}$$

$$= \frac{h^2a^2}{8\pi^2 m} - e^2a \qquad (6)$$

Now we shall choose a in such manner as to give a minimum energy. Thus

$$\frac{\partial E}{\partial a} = \frac{2h^2}{8\pi^2 m}a - e^2 = 0$$

$$\text{Or} \quad a = \frac{4\pi^2 me^2}{h^2} \tag{7}$$

Substituting the value of a in equation (6), we have

$$E_{\min} = \frac{h^2}{8\pi^2 m}\left\{\frac{4\pi^2 me^2}{h^2}\right\}^2 - e^2\left\{\frac{4\pi^2 me^2}{h^2}\right\}$$

$$E_{min} = \frac{2\pi^2 m^4 e}{h^2} \tag{8}$$

This is same value as we have obtained by other methods.

5.4. The W.K.B. Approximation

5.4.1. Introduction

In the development of Quantum Mechanics, the Bohr- Sommerfield quantization rules of the old Quantum theory, occupy a position intermediate between classical & Quantum Mechanics. It is interesting that, there is an approximate treatment of the Schrödinger wave equation that shows its connection with the quantization rules. It is based on an expansion of wave function in powers of $\hbar$, which has asymptotic nature is nevertheless useful for the approximate solution of quantum mechanical problems in appropriate cases. This method is called the "Wentzel – kramer –Brillouin " or WKB approximation. It is applicable to potentials which are such that, the Schrödinger equation is separable to one dimensional equations. Further, the potential, should be slowly varying such that

$$\left|\frac{1}{k(x)}\frac{dk}{dx}\right| < k$$

where $K(x) = \frac{1}{\hbar} p_x = \left[\frac{m}{\hbar^2}(E - V(x))\right]^{1/2}$ represents the local wave number. It is of interest to mention that the motion of a particle in a varying potential is analogous to the behaviour of light in a medium of varying refractive index. If the refractive index changes rapidly, one has reflections. If the change is gradual, the trajectory is not straight, but there are practically no reflections. The behaviour of particle in a varying potential is quite similar.

This is the approximate method of solution of wave function based on the expansion, of which, the first term leads to classical results, the second term to the old

quantum theory results and the higher terms, to the characteristics of the new mechanics.

One dimensional Schrödinger equation is written as

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+(V-E)\psi=0 \qquad (1)$$

The WKB approximation takes advantage of the fact that the wavelength is changing slowly, by assuming that the wave function is not changed much from the form it would take of V were constant, namely

$$\psi = e^{\left(\frac{ip x}{\hbar}\right)} \text{ where } p=\sqrt{2m(E-V)}$$

This suggests that, when E > V, it will be convenient to write, the wave function in the form

$$\psi = e^{\left(\frac{iS}{\hbar}\right)} \qquad (2)$$

where S is a function of x (S may be complex).

It V is nearly constant, we may expect that s is roughly equal to p_2 x. Now, S can be expanded as

$$S=S_0(x)+\hbar S_1(x)+\hbar^2 S_2(x)+\ldots\ldots\ldots \qquad (3)$$

Using equation (2) and (3)

$$\psi = e^{\left(\frac{iS}{\hbar}\right)} \Rightarrow \frac{\partial\psi}{\partial x}=e^{\left(\frac{iS}{\hbar}\right)}\frac{i}{\hbar}\frac{\partial S}{\partial x}$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2}=\frac{i}{\hbar}\frac{\partial\psi}{\partial x}\frac{\partial S}{\partial x}+e^{\left(\frac{iS}{\hbar}\right)}\frac{i}{\hbar}\frac{\partial^2 S}{\partial x^2}$$

$$=\frac{-1}{\hbar^2}e^{\left(\frac{iS}{\hbar}\right)}\left(\frac{\partial S}{\partial x}\right)^2+e^{\left(\frac{iS}{\hbar}\right)}\frac{i}{\hbar}\frac{\partial^2 S}{\partial x^2}$$

equation(1)becom

$$\left[\frac{1}{2m}\left\{\left(\frac{\partial S}{\partial x}\right)^2-i\hbar\frac{\partial^2 S}{\partial x^2}\right\}+V-E\right]e^{\left(\frac{iS}{\hbar}\right)}=0$$

$$\frac{1}{2m}\left[\left(\frac{\partial S}{\partial x}\right)^2-i\hbar\frac{\partial^2 S}{\partial x^2}\right]+V-E=0$$

$$\Rightarrow \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2-\frac{i\hbar}{2m}\frac{\partial^2 S}{\partial x^2}+V-E=0 \qquad (4)$$

SubstitutingthevalueofSfromequation(3)in(osecondorderin$\hbar$)inequation(4)we

$$\frac{1}{2}\left[\left(\frac{\partial S_o}{\partial x}+\hbar\frac{\partial S_1}{\partial x}+\right)\right]+\frac{\hbar\partial^2 S}{2\partial x}^2$$

$$+(\quad -V\frac{i\hbar}{2}\left[\frac{\partial^2 S_o}{\partial x^2}E\ \hbar\frac{\partial^2 S_1}{\partial x^2\ 2}\right])+\frac{\partial^2 S}{\partial x^2}0$$

$$\Rightarrow\frac{1}{2}\left[\left(\frac{\partial S_o}{\partial m}+\quad\right)^2\frac{\hbar^2}{\partial x}\left(\frac{\partial S_1}{x}+\left[\frac{\partial^2 S_o}{2}\ h\frac{\hbar}{x}\frac{\partial S_2}{\partial}\right]\right)+\frac{\partial^2 S}{x}\left(\frac{\partial}{\partial x}\right)\right]$$

$$+(\ V\ E\ )\frac{i}{2}\left[\hbar\left(\frac{\partial^2 S_o}{\partial x^2}\right)+\hbar\quad^2\left(\frac{\partial^2 S_1}{\partial x^2}\right)\right]=0$$

$$\Rightarrow\frac{1}{2}\left[\left(\frac{\partial S_o}{m\partial}\right)^2\right]x\ (-V\frac{\partial S}{\partial m}E\ )\frac{i\ \hbar}{x}\left[\frac{\partial}{\partial}\frac{\partial S_1}{x}\ 2\right]\frac{2}{\partial x^2}$$

$$+\frac{\hbar^2}{2}\left[\frac{\partial S_o}{m\partial}+\frac{\partial S_2}{x\partial}\ x\left(\frac{\partial S_1}{\partial x}\right)\right]^2\ \partial_i\frac{S^2}{\partial x^2}=0 \qquad (5)$$

Since this equation must be satisfied, independently to the value of $\hbar$, it is necessary that, the coefficient of each power of $\hbar$ be separately equal to zero. This requirement leads to the following series of equations.

$$\Rightarrow\ \frac{1}{2}\left(\frac{\partial S_o}{m\partial x}\right)^2-(\ V\pm E\ )\ (\qquad (6)$$

$$\Rightarrow\ \frac{1}{m}\left[\frac{\partial S_o}{\partial x}\frac{\partial S_1}{\partial x}\frac{\partial S}{2}\right]\frac{2}{\partial x^2}\quad 0$$

$$(\qquad \frac{\partial S_o}{\partial x}\frac{\partial S_1}{\partial x}-\frac{\partial S}{2}\frac{2}{\partial x^2}=0 \qquad (7)$$

$$\Rightarrow\frac{1}{2}\left[\frac{\partial S_o}{m\partial}+\frac{\partial S_2}{x\partial}\ x\left(\frac{\partial S_1}{\partial x}\right)\right]^2\ \partial_i\frac{S^2}{\partial x^2}=0\quad (\ o\ r$$

$$\frac{\partial S_o}{\partial x}\frac{\partial S_2}{\partial x}-\frac{\partial_1 S}{\partial x}\ {}^2i\frac{\partial S_1}{\partial x^2}=0 \qquad (8)$$

Fromequation(6)weha

$$\frac{\partial S_o}{\partial x}=\ [2\pm m\ (-E\ V]^{1/2}$$

$$\Rightarrow\ S_0\ [=2\int_{x_0}^{x}m\pm(\ E-V\ )^{1/}]^2 d\ : \qquad (9)$$

From equation (7) we have

$$\frac{\partial S_1}{\partial x}=\frac{i}{2S}\frac{1}{(\ _o\partial x}\frac{\partial^2 S_o}{)\partial x^2}$$

$$=\frac{i}{2}\frac{\partial}{\partial x}\left(1\ o\left(\frac{\partial}{g}\frac{S_o}{\partial x}\right)\right)$$

$$S_1=\frac{i}{2}1\ o\left(g\frac{\partial S_o}{\partial x}\right) \qquad (10)$$

$$i_1 S = \frac{-1}{2} \log \left[\frac{\partial S_o}{\partial x} \log \left[\frac{\partial S_o}{\partial x} \right] \right]^{-1/2}$$

$$or \quad i_1 S = \frac{1}{\sqrt{\partial S_o / \partial x}} \quad \frac{1}{[2m(E-V)]^{1/4}}$$

similarly from equation (8) we can show that

$$S_2 = \frac{1}{2} \frac{m(\partial v/\partial x)}{[2m(E-V)]} \frac{1}{2} \int \frac{m^2(\partial v^2/\partial x)}{[2m(E-V)^{5/2}]} \qquad (11)$$

Neglecting S_2, the sol n of equation (1) is given by

$$\psi = e^{\frac{i}{\hbar}(S_0 + \hbar S_1)} = e^{\frac{i}{\hbar} S_0} e^{i S_1}$$

As S_0 has positive as well as negative valu

$$\psi = A e^{(i_0 S/\hbar)} + B e^{(-i S/\hbar)}$$

$$= \frac{A}{[(2m)(E-V)]^{1/4}} e^{+\frac{i}{\hbar}\left[\int_{x_0}^{x} 2m(E-V)^{1/2}\right]^2 dx} + \frac{B}{[(2m)(E-V)]^{1/4}} e^{-\frac{i}{\hbar}\left[\int_{x_0}^{x} 2m(E-V)^{1/2}\right]^2 dx}$$

$$= \frac{A}{\sqrt{p_2}} e^{\frac{i}{\hbar}\left(\int_{x_0}^{x} p_2 dx\right)} + \frac{B}{p_2 \sqrt{\quad}} e^{\frac{i}{\hbar}\int_{x_0}^{x} p dx} \qquad (12)$$

where A & B are two arbitrary constants and $P_2 = \sqrt{m(E-V)}$. The positive exponential represents a wave moving in the positive X direction while the negative exponential, a wave moving is the negative X direction. When V is a constant, the exponential reduces respectively to plane waves,

$$e^{\frac{i}{\hbar}(p_1 x)} \quad e^{\frac{i}{\hbar}(-p_2 x)}$$

When V > E, the W.K.B approx possesses real exponential solution. The solution is

$$\psi = \frac{A}{\sqrt{p_1}} e^{\frac{i}{\hbar}\int_{x_0}^{x} p_1 dx} + \frac{B}{p_2 \sqrt{\quad}} e^{\frac{i}{\hbar}\int_{x_0}^{x} p dx} \qquad (13)$$

where $p_1 = \sqrt{2m(V-E)}$

5.5. LET US SUM UP

By reading this lesson one can get an understanding on the two approximation methods namely variational method and WKB approximation and its applications. Variational method is applicable to study the ground state of system. WKB method find its application in alpha decay paradox.

5.6. LESSON END ACTIVITIES

Check your progress

1. Explain how ground state energy could be evaluated using the variation method.
2. Briefly discuss an application of WKB method.
3. Briefly outline the variation method.
4. Explain how the ground state energy could be evaluated using the variation method and hence find the ground state energy of helium atom.
5. Explain the main stages involved in the WKB approximation. Use the technique to obtain the asymptotic solution of the one dimensional Schrödinger equation. Also arrive at the solution near a turning point.

5.7. References

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LESSON 6

TIME DEPENDENT PERTURBATION THEORY AND ITS APPLICATIONS

6.1. Aims and Objectives

We are going to discuss

- Time dependent perturbation theory and its applications
- Fermi Golden rule
- Harmonic perturbation
- Constant perturbation
- Selections rules

6.2. Time Dependent Perturbation Theory

If the Hamiltonian of the system is time dependent, the energy is no longer a constant of motion. In such case we have to solve time dependent Schrödinger equation.

$$E\psi \quad \hat{H} \quad \psi$$

$$i\hbar \frac{\partial \quad \psi}{\partial t} \hat{H} \quad \psi \qquad (1)$$

In many physical problems, the time dependence of the Hamiltonian arises due to an external agency. For example, an atom irradiated by light, by applying electric field to atomic system etc. In such cases, Hamiltonian is written as,

$$H = H_0 + V(t) \qquad (2)$$

where, H_0 is the sum of Hamiltonian of the two systems in isolation and V(t) is their interaction.

At a particular instant of time t = 0, the system may be regarded as being approximately in an eigenstate of H_0 as ‘i’. We have to calculate the probability of finding the system at a later time t in an eigenstate ‘f’. If ψ_n denotes the complete set of eigen functions, then, we have

$$H_0 \psi_n = E_n \psi_n$$
$$= \hbar \omega_n \psi_n$$

The wave function corresponding to the actual state can be expanded in terms of ψ_n

$$\psi_n(t) = \sum_n C_n(t) \psi_n(r) e^{-i\omega_n t} \quad (3)$$

where, $\omega_s - \omega_n = \frac{E_s - E_n}{\hbar}$ is the Bohr angular frequency between the states s and n. If the perturbation V(t) is absent, all the co-efficients C_n will be constant in time. On the other hand, the perturbation V(t) makes them vary with time and for this reason, this method is called the method of variation of constants.

Suppose the perturbation begins to act at time t. Initially at t = 0, the system is in the unperturbed state say, 'i' before the perturbation is turned on. In such a case,

$$C_n(0) = 0 \text{ for } n \neq i$$
$$C_n(0) = 1 \text{ for } n = i$$
$$\frac{\partial}{\partial t} C_f = \frac{1}{i\hbar} V_{fi}(t) e^{+i\omega_{fi} t}$$

Integrating the above equation between the limits 0 and t, we get,

$$\int_0^t \frac{\partial C_f}{\partial t} dt = \frac{1}{i\hbar} \int_0^t V_{fi}(t) e^{i\omega_{fi} t} dt$$

$$C_f(t) - C_f(0) = \frac{1}{i\hbar} \int_0^t V_{fi}(t) e^{i\omega_{fi} t} dt$$

$$C_f(t) - C_f(0) = \frac{1}{i\hbar} \int_0^t V_{fi}(t) e^{i\omega_{fi} t} dt \qquad \because C_f(0) = 0$$

$$C_f(t) = \frac{1}{i\hbar} \int_0^t V_{fi}(t) e^{i\omega_{fi} t} dt, \text{ for } f \neq i$$

This gives the probability amplitude for states of later time other than the initial state.

6.3. Fermi – Golden Rule (or) Closely Spaced Levels (or) Transition to continuum

If transitions are taking place to a set of closely spaced levels 'f' then, $P_f(t)$ will be obtained by summing over, all final state levels 'f' Therefore,

$$P_f(t) = |C(t)|^2$$

$$= \sum_f \frac{|V_{if}|^2}{\hbar^2} \sin^2\left(\frac{(\omega_f - \omega_i)t}{2}\right) \Big/ \left(\frac{\omega_f - \omega_i}{2}\right)^2$$

If the level spacing is very close, then, the summation can be replaced by integration.

$$\sum_f = \int \rho(E_f)\, dE_f$$

where $\rho(E_f)$ is the density of the final states around E_f (i.e) the number of energy levels per unit energy interval.

Therefore, $P_f = \int \frac{|V_{if}|^2}{\hbar^2} \rho(E_f) \sin^2\left(\frac{(\omega_f - \omega_i)t}{2}\right) \Big/ \left(\frac{\omega_f - \omega_i}{2}\right)^2 dE$

$$= \frac{|V_{if}|^2}{\hbar^2} \int \rho(E_f) \sin^2\left(\frac{(\omega_f - \omega_i)t}{2}\right) \Big/ \left(\frac{\omega_f - \omega_i}{2}\right)^2 dE$$

Assuming $\rho(E_f)$ does not vary around E, we have

$$P_f = \frac{|V_{if}|^2}{\hbar^2} \rho(E_f) \int_{-\infty}^{\infty} \sin^2\left(\frac{(\omega_f - \omega_i)t}{2}\right) \Big/ \left(\frac{\omega_f - \omega_i}{2}\right)^2 dE$$

$$P_f = \frac{|V_{if}|^2}{\hbar^2} \rho(E_f) \int_{-\infty}^{\infty} \sin^2\left(\frac{(\omega_f - \omega_i)t}{2}\right) \Big/ \left(\frac{\omega_f - \omega_i}{2}\right)^2 \hbar\, d\omega \quad \because [\omega = E/\hbar]$$

$$P_f = \frac{|V_{if}|^2}{\hbar^2} (\rho E \hbar) \int_{-\infty}^{\infty} \sin^2\left(\frac{(\omega_f - \omega_i)t}{2}\right) \Big/ \left(\frac{\omega_f - \omega_i}{2}\right)^2 d\omega \qquad (1)$$

Since the integral is practically zero outside ω_f, the limits are chosen from $-\infty$ to $+\infty$, consider, the integral,

$$\int_{-\infty}^{+\infty} \sin^2\left(\frac{(\omega_f - \omega_i)t}{2}\right) \Big/ \left(\frac{\omega_f - \omega_i}{2}\right)^2 d\omega_f$$

$$\text{put } x = (\omega_f - \omega_i)t / 2$$

$$dx = \frac{d\omega_f\, t}{2}$$

$$\Rightarrow \int_{-\infty}^{\infty} \sin^2\left(\frac{(\omega_f - \omega_i)t}{2}\right) \Big/ \left(\frac{\omega_f - \omega_i}{2}\right)^2 = \int_{-\infty}^{\infty} \frac{\sin^2 x}{(x/t)^2} \frac{2}{t} dx$$

$$= \frac{2}{t} t^2 \int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx$$

$$= 2t \int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx$$

we can show that $\int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx = \pi$;

$$\int_{-\infty}^{+\infty} \sin^2\left(\frac{(\omega_f - \omega_i)t}{2}\right) \Big/ \left(\frac{\omega_f - \omega_i}{2}\right)^2 d\omega_f = 2\pi t$$

substituting the integral value on equation (1) we get

$$P_f(t) = \frac{|V_{fi}(0)|^2}{\hbar^2}\left(\frac{\sin^2(\omega_{fi}t/2)}{(\omega_{fi}/2)^2}\right)\pi^2 t$$

$$= \frac{2\pi}{\hbar}|V_{fi}(0)|^2 \left(\frac{\sin^2(\omega_{fi}t/2)}{(\omega_{fi}/2)^2}\right) t$$

Therefore the transition probability per unit time, will be,

$$\frac{P_f(t)}{t} = \frac{2\pi}{\hbar}|V_{fi}(0)|^2 \left(\frac{\sin^2(\omega_{fi}t/2)}{(\omega_{fi}/2)^2}\right)$$

This is called the Fermi Golden rule

6.4. Constant Perturbation

If the perturbation last from time t = 0 to t = t, and during this time, it is constant, then, we have,

$$C_f(t) = \frac{1}{i\hbar}V_{fi}(0)\int_0^t e^{i\omega_{fi}t}\,dt$$

$$= \frac{1}{i\hbar}V_{fi}(0)\left[\frac{e^{i\omega_{fi}t}}{i\omega_{fi}}\right]_0^t$$

$$C_f(t) = \frac{V_{fi}(0)}{\hbar\omega_{fi}}\left[e^{i\omega_{fi}t} - 1\right]$$

Thus, the probability of finding the system, in the state 'f' at time 't' is given by,

$$P_f(t) = |C_f(t)|^2$$

$$P_f(t) = \frac{V_{fi}^2(0)}{\hbar^2\omega_{fi}^2}\left(e^{i\omega_{fi}t} \times e^{i\omega_{fi}t} - 1\right)\left(e^{i\omega_{fi}t} - 1\right)$$

where $\left(e^{i\omega_{fi}t} - e^{-i\omega_{fi}t}\right)\left(e^{i\omega_{fi}t} - 1\right) = e^{i\omega_{fi}t} - 1 - 1 + e^{-i\omega_{fi}t}$

$$= 2 - \left[e^{i\omega_{fi}t} + e^{-i\omega_{fi}t}\right]$$

$$= 2 - 2\cos\omega_{fi}t$$

$$= 2\left[1 - \cos\omega_{fi}t\right]$$

$$= 2\left[2\sin^2\left(\frac{\omega_{fi}t}{2}\right)\right]$$

$$= 4\sin^2\left(\frac{\omega_{fi}t}{2}\right)$$

$$\therefore P_f(t) = \frac{|V_{fi}(0)|^2}{\hbar^2\omega_{fi}^2}\,4\sin^2\left(\frac{\omega_{fi}t}{2}\right)$$

$$= \frac{|V_{fi}(0)|^2}{\hbar^2}\sin^2\left(\frac{\omega_{fi}t/2}{\omega_{fi}t/2}\right)^2 2^2$$

In such a case the probability amplitude will be,

$$C_f(t) = \frac{-V_0}{\hbar}\left[\frac{e^{i(\omega_f-\omega_i)t}-1}{\omega_f-\omega_i} + e^{i(\omega_f+\omega)t}\frac{e^{i(\omega_f+\omega)t}-1}{\omega_f+\omega}\right]$$

Thereforethetransitionprobabil

$$P_f(t) = |c(t)|^2 = \frac{V_0^2}{\hbar^2}\left|\left[\frac{e^{i(\omega_f-\omega_i)t}-1}{(\omega_f-\omega_i)} + \frac{e^{i(\omega_f+\omega)t}-1}{(\omega_f+\omega)}\right]\right|^2$$

We find that the terms inside the box, while squaring will not contribute anything because when ω_f approximately equal to ω only one term (IInd term) will contribute while the other (Ist term) vanishes. Similarly, when ω_f approximately equals - ω, the contribution by the two terms will exchange. Thus, the above discussion treating the terms independently is valid.

6.5. Harmonic Perturbation

We know that the probability amplitude for transition from initial state 'i' to the final state 'f' will be,

$$C_f(t) = \frac{1}{i\hbar}\int_0^t V_i(t)\,e^{i\omega_{fi}t}\,dt$$

we introduce a harmonic perturbation given by

$$V_f(t=t_0) = \bar{V}e^{i(\omega t)}, \quad C$$

$$C_f(t) = \frac{1}{i\hbar}\int_0^t V^{-i(\omega t)}e^{i\omega_{fi}t}\,dt$$

$$= \frac{V_o}{i\hbar}\int_o^t e^{i(\omega_f-\omega_i)\omega t}\,t$$

$$= \frac{V_o}{i\hbar}\left[\frac{e^{i\omega(\omega_f-\omega_i)\omega t}}{i\,\omega_f(\omega_i-\omega)}\right]_o^t$$

$$= \frac{V_o}{i\hbar\,i\omega_f(\omega_i-\omega)}\left[e^{i(\omega_f-\omega)\omega t}-1\right]$$

$$= \frac{V_o}{\hbar}\left[\frac{e^{i(\omega_f-\omega)t}-1}{\omega_f-\omega}\right]$$

This expression differs in having $\omega_f - \omega$ for harmonic perturbation instead of just ω_f for constant perturbation. The entire discussion of constant perturbation can be carried for harmonic perturbation, with $(\omega_f-\omega)$ replacing ω_f. We conclude that for large t, only those transitions in which $\omega_f - \omega \approx 0$ can take place with appreciable

probability In other words, only when $E_f - E_i = \hbar\omega$, the transitions will be appreciable. Thus, the harmonic perturbation $V_0 e^{-i\omega t}$ can induce transitions to a level E_f whose energy is higher than E_i by $\hbar\omega$. Such a transition can be described as absorption of energy $\hbar\omega$ by the system from the external agency.

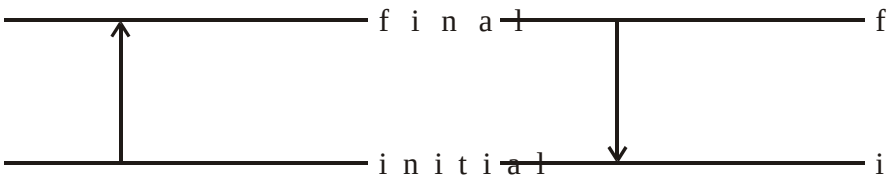
On the otherhand, if the Hermitian adjoint $V_0 e^{i\omega t}$ is used for harmonic perturbation, then we will have, $(\omega_f + \omega_i)$ instead of $(\omega_f - \omega_i)$. In such a case, the probability amplitude is given by,

$$C_f(t) = \frac{-V_o}{\hbar}\left[\frac{e^{i(\omega_f + \omega)t} - 1}{\omega_f + \omega}\right]$$

This induces a transition in which

$$\omega_f + \omega = 0$$
$$\Rightarrow \hbar\omega_f = -\hbar\omega$$
$$\Rightarrow E_f - E_i = -\hbar\omega \quad (\text{or})$$
$$E_i - E_f = \hbar\omega$$

In this case we find that E_f is lower than E_i by $\hbar\omega$ and this describes the emission of energy, Here, the energy is given by the system to the external agency.



In reality, the actual potential has to be Hermitian and must be,

$$V_0(e^{i\omega t} + e^{-i\omega t})$$

6.6. Selection Rules

In many cases of interest, $V_f(t)$ can be expressed in the form,

$$V_f(t) = V_i(\omega)e^{i\omega t}$$

where $V_i(0)$ is independent of t

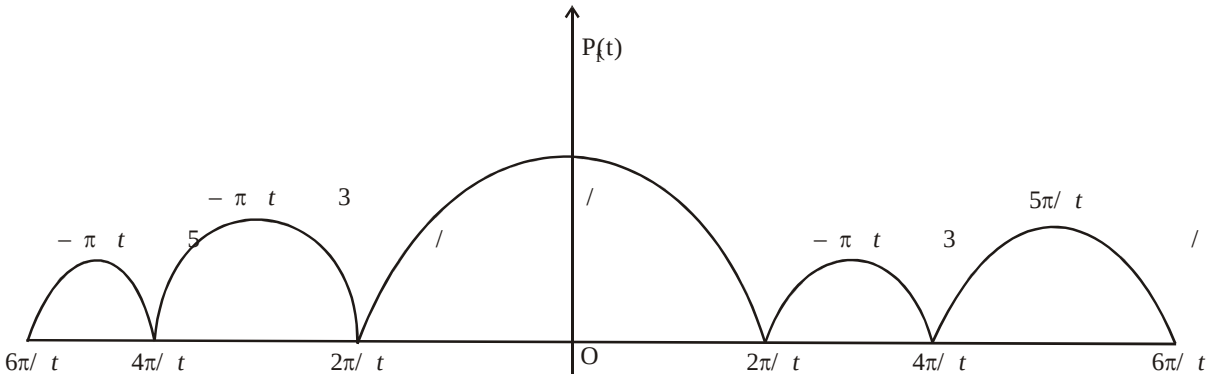
$\therefore$ equation (4) becomes

$$\int_0^t \frac{\partial C_f}{\partial t} dt = \frac{1}{i\hbar}\int_0^t V_{fi}(t)\, e^{i\omega_{fi} t}\, dt$$

$$C_f(t) = \frac{1}{i\hbar}\int_0^t V_{fi}(t)\, e^{i\omega_{fi} t}\, dt$$

This equation shows that $V_{fi}(t)$ is non- zero only when $V_{fi}(t)$ is non-zero, Thus, transitions in the first order, can take place between pair state(f,i) for which $V_{fi}(\omega \neq 0)$. Transition between any other state are forbidden in the first order. This is the first order selection rule. Even if $V_{fi}(\omega = 0)$ then, transition between the state i and f may still be possible in the higher order via an intermediate (ℓ) state. If both $V_{f\ell}(\omega \neq 0$ and $V_{\ell i}(\omega \neq 0)$, then the intermediate state ℓ will connect the initial state i and final state f. However, probability for transitions in the higher order will be smaller and will proceed at a slower rate.

If we plot the probability $P_f(t)$ as a function of the energy difference ω_f between the initial and final state of fixed t, the graph will be of the form as shown in the figure below,



The behaviour of $\sin\left(\frac{\omega_f t}{2}\right)^2 \Big/ \left(\frac{\omega_f}{2}\right)^2$ is depicted in the figure.

The main peak of the curve occurs at $\omega_f = 0$ and has a high proportional to t^2. The subsequent peaks are much smaller and occurs at $\pm 3\pi/t, \pm 5\pi$ etc. Thus, we see that the transition from the initial state 'i' to the final state 'f' occurs such that ω_f falls within the main peak.

$$|\omega_{fi}| = \frac{2\pi}{t}$$

taking only the positive value,

$$\omega_{f\ i} = \frac{2\pi}{t}$$

$$\hbar\omega_{f\ i} = \frac{2\pi\hbar}{t}$$

$$\hbar\omega_{f\ i} = h$$

which resemble uncertainty principle.

The magnitude of the energy difference between initial and final is very unlikely to be significantly to be higher than h/t. This is the energy time uncertainty relation.

6.7. LET US SUM UP

Here we have studied in detail the followings:

- Time dependent perturbation theory and its applications
- Fermi Golden rule
- Harmonic perturbation
- Constant perturbation
- Selections rules

6.8. LESSON END ACTIVITIES

Check your progress

1. Define Fermi Golden rule.
2. What do you meant by selection ruels.
3. Obtain the expression for the transition probability per unit time for first order transition under constant perturbation and show that it is proportional to the perturbation time ‘t’.

6.9. Problems

Calculate the second order energy correction for the ground state of the charge between linear harmonic oscillator subject to a constant electric field. Compare the result with the exact solution

Solution

The schrodineger's equation for the perturbed system is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}kx^2\psi+\alpha x\psi=E\psi$$

where α is the product of the charge and the magnitude of the electric field in the x-direction. Writing X = x + α / k, the above Equation becomes

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dX^2}+\frac{1}{2}kX^2\psi=\left(E+\frac{\alpha^2}{2k}\right)\psi$$

Thus $E_n=\left(n+\frac{1}{2}\right)\hbar\omega-\frac{\alpha^2}{2k}$, which is the exact result.

First order energy correction is zero.

The second order energy correction is given by

$$E_n^{(2)}=\sum_{m}\frac{\alpha^2\left|\langle n^{(0)}|x|m^{(0)}\rangle\right|^2}{\left(E_n^{(0)}-E_m^{(0)}\right)}$$

Expressing x in terms of the raising and lowering operators,

$$\langle n^{(0)}|x|m^{(0)}\rangle=\frac{1}{i}\sqrt{\frac{\hbar}{2m\omega}}\left[\langle n^{(0)}|a_-|m^{(0)}\rangle+\langle n^{(0)}|a_+|m^{(0)}\rangle\right]$$

$$=\frac{1}{i}\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{m}\delta_{n,m-1}-\sqrt{m+1}\delta_{n,m+1}\right]$$

$$=E_n^{(2)}=\frac{\alpha^2}{2m\omega^2}=\frac{\alpha^2}{2k}$$

Do it yourself

1. A hydrogen atom the energy state with n = 2 is subject to an electric field E parallel to the z – axis. Calculate the energy correction.
2. Calculate the splitting of hydrogen energy levels due to spin-orbit interaction.

6.10. References

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LESSON 7

ANGULAR MOMENTUM ALGEBRA

7.1. Aims and objectives:

In this lesson we are going to discuss the one of the most important and exciting topic of quantum mechanics namely, angular momentum algebra.

7.2. Introduction

Knowledge in angular momentum techniques is essential for quantitative study of problems in atomic physics, molecular physics, nuclear physics and solid state physics. The application of angular momentum techniques to solve physical problems has become so common. Angular momentum techniques are widely used in the study of both non relativistic and relativistic problems in physics. In this chapter, we will discuss the Quantum Mechanical definition of Angular momentum first. Then we will have a discussion on physical interpretation of Angular momentum. It is then followed by, discussion on ladder operators and coupling of two angular momenta.

7.3. Quantum Mechanical definition of Angular Momentum

In classical mechanics, the angular momentum vector is defined as the cross product of the position vector $\bar{p}$. ie

$$\vec{L} = \vec{r} \bar{p} \qquad (1)$$

Both $\vec{r}$ $\bar{p}$ change sign under the inversion of co-ordinate system and so they are called polar vector. It is easy to see that, $\vec{L}$ behaves differently and will not change sign under inversion of co-ordinate system, and hence it is known as pseudo or Axial vector.

$$\bar{L} = \vec{r} \times \bar{p}$$

$$\bar{L} = \vec{x} \begin{vmatrix} i & j & k \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

$$\vec{L} = (y\,p_z - z\,p_y)\,\hat{i} - (z\,p_x - x\,p_z)\,\hat{j} + (x\,p_y - y\,p_x)\,\hat{k}$$

$$\text{i.e. } L_x = y\,p_z - z\,p_y$$

$$L_y = z\,p_x - x\,p_z$$

$$L_z = x\,p_y - y\,p_x$$

$$[L_x, L_y] = [y\,p_z - z\,p_y\ ,\ z\,p_x - x\,p_z]$$

$$= [y\,p_z\ ,\ z\,p_x] - [y\,p_z\ ,\ x\,p_z] - [z\,p_y\ ,\ z\,p_x] + [z\,p_y\ ,\ x\,p_z]$$

$$= y\,p_x\,[p_z, z] + p_y\,x[z, p_z]$$

$$= -i\hbar\ y\,p_x + i\hbar\ p\,y_x$$

$$= i\hbar\ [x\,p_y - y\,p_x]$$

$$= i\hbar\,L_z$$

$$\text{i.e. } [L_x\ ,\ L_y] = i\hbar\,L_z \qquad (2)$$

Similarly

$$[L_y\ , \quad = \quad i\hbar\,L_x$$

$L_z]$

$$[L_z\ ,\ L_x] = i\hbar\,L_y$$

$$\text{i.e. } (\vec{L}\,x\,\vec{L}) = L_x\,L_y - L_y\,L_x$$

$$(\vec{L}\,x\,\vec{L}) = i\hbar\,L_z$$

Expressing the angular momentum in units of $\hbar$, we can write it as

$$(\vec{L}\,x\,\vec{L}) = i\ \vec{L} \qquad (3)$$

This Quantum mechanical definition must be generalized to include angular momentum of half integral values. Therefore, generalizing, we can write the definition for total angular momentum as

$$(\hat{J}\,x\,\hat{J}) = i\ \hat{J} \qquad (4)$$

$$\text{Now, } [J_x\ ,\ J_y] = i\hbar\,J_z$$

$$[J_y\ ,\ J_z] = i\hbar\,J_x \qquad (5)$$

$$[J_z\ ,\ J_x] = i\hbar\,J_y$$

7.4. Physical Interpretation of Angular Momentum Vector

Although the components of angular momentum operator do not commute among themselves, it is easy to show that, the square of angular momentum operator.

$$\vec{J}^{\,2} = J_x^2 + J_y^2 + J_z^2$$

commutes with each of its components.

$$\text{i.e. } [J^2\ ,\ J_x] = 0$$

$$[J^2, J_y] = 0 \qquad (6)$$
$$[J^2, J_z] = 0$$

Equations (5) & (6) gives simple physical interpretation. It is possible to find the simultaneous eigenvalues of $\bar{J}^2$ and one of the components, say J_z alone, but, it is impossible to find precisely the eigenvalues of J_x and J_y at the same time. Representing the operators by matrices. One can say that, $\bar{J}^2$ and J_z can be diagonolised in the same representation, but not the other components J_x and J_y. Physically this means that, one can find the magnitude of angular momentum vector and its projection on one of the axes. The projection on the other two axes cannot be determined. This is illustrated in the figure(Fig 7.1) , in which the angular momentum vector is depicted to be anywhere on the cone. If ψ_{jm} is the eigenfunction of the operators $\vec{J}^2$ and J_z, then

$$\vec{J}^2 \psi_{jm} = \eta_j \psi_{jm}$$
$$\& \quad J_z \psi_{jm} = m \psi_{jm}$$

Here j & m are Quantum Numbers used to define eigenfunctions and the corresponding eigenvalues of the operators are η_j & m.

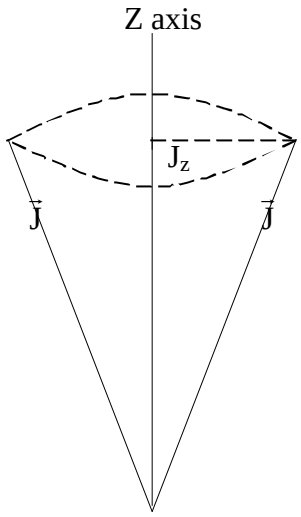

Fig: 7.1 The angular momentum vector, for which its projection on the z-axis alone is well defined, but not its projection on the x axis & y axis.

Problem 7.1

Show that $[J^2, J_x] = 0$

Solution

$$\text{We know that } J^2 = \vec{J} \times \vec{J}$$

$$= J_x^2 + J_y^2 + J_z^2$$

$$\therefore \quad [J^2, J_x] = [J_x^2 + J_y^2 + J_z^2, J_z]$$

$$= [J_x^2 + J_x] + [J_y^2 + J_x] + [J_z^2 + J_x]$$

$$= J_x [J_x, J_x] + [J_x, J_x] J_x + J_y [J_y, J_x] + [J_y, J_x] J_y + J_z [J_z, J_x] + [J_z, J_x] J_z$$

$$= -i \hbar J_y J_z - i \hbar J_z J_y + i \hbar J_z J_y + i \hbar J_y J_z$$

$$\text{i.e. } [J^2, J_x] = 0$$

$$\text{Similarly } [J^2, J_y] = 0$$

$$\& \quad [J^2, J_z] = 0$$

7.5. Ladder Operators (or) Raising and Lowering operators

We define the raising and lowering operators as J_+ and J_- given by

$$J_+ = J_x + i J_y$$

$$J_- = J_x - i J_y$$

It is to be noted that, though the angular momentum matrices are Hermitian, the ladder operators are not Hermitian.

$$\{J_+\}^\dagger = (J_+)^\dagger + (i J_y)^\dagger$$

$$= J_+ - i J_y$$

$$= J_-$$

$$\text{Similarly } \{J_-\}^\dagger = (J_+)^\dagger - (i J_y)^\dagger$$

$$= J_x + i J_y$$

$$= J_+$$

$\therefore$ J_+ & J_- are not Hermitian.

Problem 7.2

Evaluate $[J^2, J_+]$

Solution

$$\text{Now, } [J^2, J_+] = [J^2, J_x + i J_y]$$

$$= [J^2, J_x] + [J^2, i J_y]$$

$$= 0 + i (0)$$

$= 0$

Similarly $[J^2, J_-] = 0$

Also $[J_+, J^2] = 0$

and $[J_-, J^2] = 0$

Problem 7.3

Find the value of $[J_z, J_+]$ and $[J_z, J_-]$

Solution

$$\text{Now, } [J_z, J_+] = [J_z, J_x + i J_y]$$
$$= [J_z, J_x] + i [J_z, J_y]$$
$$= i \hbar J_y + i (- i \hbar J_x)$$
$$= i \hbar J_y + \hbar J_{xs}$$
$$= \hbar (J_x + i J_y)$$
$$= \hbar J_+$$
$$\text{And, } [J_z, J_-] = [J_z, J_x - i J_y]$$
$$= [J_z, J_x] - i [J_z, J_y]$$
$$= i \hbar J_y - i (- i \hbar J_x)$$
$$= i \hbar J_y - \hbar J_x$$
$$= \hbar (J_x - i J_y)$$
$$= - \hbar J_-$$

Hence we conclude that $[J_z, J_\pm] = \pm \hbar J_\pm$

Also $J^2 J_z = J_z J^2$

and $J^2 J_+ = J_+ J^2$

Problem 7.4

Find the values of $J_z J_+$ and $J_z J_-$

Solution

We Know that, $[J_z, J_+] = J_+$ in units of $\hbar$

i.e. $J_z J_+ - J_+ J_z = J_+$

or $J_z J_+ = J_+ J_z + J_+$

i.e. $J_z J_+ = J_+ (J_z + 1)$

Similarly $[Jz, J_-] = - J_-$ in units of $\hbar$

i.e. $J_z J_- - J_- J_z = - J_-$

$$J_z J_- = J_- J_z - J_-$$

$$\text{i.e.} \quad J_z J_- = J_- (J_z - 1)$$

7.6. Spectrum of eigenvalues for J^2 and J_z

Let us define $J^2 \psi_{jm} = \eta_j \psi_{jm}$

and $J_z \psi_{jm} = m \psi_{jm}$

The raising and lowering operators can be defined as

$$J_+ = J_z + iJ_y$$

$$\text{and } J_- = J_x - iJ_y$$

Let $J_+ \psi_{jm} = \varphi_+$

and $J_- \psi_{jm} = \varphi_-$

Now, Let us operate J^2 on φ_+ and φ_-

$$J^2 \varphi_+ = J^2 J_+ \psi_{jm}$$
$$= J_+ J^2 \psi_{jm}$$
$$= J_+ \eta_j \psi_{jm}$$
$$= \eta_j J_+ \psi_{jm}$$
$$= \eta_j \varphi_+$$

$$\text{i.e.} \quad J^2 \varphi_+ = \eta_j \varphi_+$$

$$\text{Similarly} \quad J^2 \varphi_- = J^2 J_- \psi_{jm}$$
$$= J_- J^2 \psi_{jm}$$
$$= J_- \eta_j \psi_{jm}$$
$$= \eta_j J_- \psi_{jm}$$
$$= \eta_j \varphi_-$$

$$\text{i.e.} \quad J^2 \varphi_- = \eta_j \varphi_-$$

Operating J_Z on φ_+ and φ_- we have,

$$J_z \varphi_+ = J_z J_+ \psi_{jm}$$
$$= J_+ J_z \psi_{jm}$$
$$= J_+ (J_z+1) \psi_{jm}$$
$$= J_+ (m+1) \psi_{jm}$$
$$= (m+1) J_+ \psi_{jm}$$

$$\text{i.e.} \quad J_z \varphi_+ = (m+1) \varphi_+$$

Similarly $J_z \varphi_- = J_z J_- \psi_{jm}$

$= J_- J_z \psi_{jm}$

$= J_- (J_z - 1) \psi_{jm}$

$= J_- (m-1) \psi_{jm}$

$= (m-1) J_- \psi_{jm}$

i.e. $J_z \varphi_- = (m-1) \varphi_-$

Thus we find that φ_+ and φ_- are eigenfunctions of J^2 operator, with the same eigenvalue η_j. However, even though we find that, φ_+ and φ_- are also eigenfunctions of J_z operator, the eigenvalues are either stepped up or stepped down by unity. It is precisely for this reason, J_+ and J_- operators are called as raising and lowering operators, respectively.

Now let us find the value of $(J^2_x + J^2_y) \psi_{jm}$

$(J_x^2 + J_y^2) \psi_{jm} = (J^2 - J_x^2) \psi_{jm}$

$= (\eta_j - m^2) \psi_{jm}$

Since the eigenvalues of square of the Hermitian matrix is always positive, we have $(\eta_j - m^2) \geq 0$. Therefore the m values are bounded. ie.. m has a spectrum of eigenvalues, the lowest being $-\sqrt{\eta_j}$ and the highest value being $+\sqrt{\eta_j}$.

Now, let us denote the lowest value of m by m_1, and the highest value of m by m_2.

Obviously $J_+ \psi_{jm_2} = 0$ (A)

and $J_- \psi_{jm_1} = 0$ (B)

Operating J_- on the left of equation (A) and J_+ on the left of equation (B), we have

$$J_- J_+ \psi_{jm_2} = 0$$

$$(J_x - iJ_y)(J_x + iJ_y) \psi_{jm_2} = 0$$

$$\left[J_x^2 + J_y^2 - i(J_y J_x - J_x J_y)\right] \psi_{jm_2} = 0$$

$$\left(J_x^2 + J_y^2 - J_z\right) \psi_{jm_2} = 0$$

$$\left(J^2 - J_z^2 - J_z\right) \psi_{jm_2} = 0$$

$$\left[J^2 - J_z(J_z+1)\right]\psi_{jm_2} = 0$$

$$\left[\eta_j - m_2(m_2+1)\right]\psi_{jm_2} = 0 \qquad \text{(C)}$$

Similarly $J_+ J_- \psi_{jm_1} = 0$

$$\Rightarrow \left[\eta_j - m_1(m_1+1)\right]\psi_{jm_1} = 0 \qquad \text{(D)}$$

From equations (C) and (D),

$$\Rightarrow \left[\eta_j - m_2(m_2+1)\right] = 0 \qquad \text{(E)}$$

$$\Rightarrow \left[\eta_j - m_1(m_1-1)\right] = 0 \qquad \text{(F)}$$

Since R.H.S of (E) and (F) are equal to zero, we can write,

$$\eta_j - m_2(m_2-1) = \eta_j - m_1(m_1-1)$$

$$\text{i.e.} \quad m_2(m_2-1) = m_1(m_1-1)$$

$$\Rightarrow m_2^2 - m_1^2 + m_2 - m_1 = 0$$

$$\Rightarrow (m_1+m_2)(m_2-m_1+1) = 0 \qquad \text{(G)}$$

Since $(m_2 - m_1)$ is always > 0, (i.e positive), the second term cannot be zero, we have

$$(m_1+m_2) = 0$$

$$\Rightarrow m_1 = -m_2$$

Taking the highest value of m_2 to be equal to j. i.e. $m_2 = j$, we have $m_1 = -j$. Thus we find that J_z has a spectrum of eigenvalues ranging from – j to + j, in steps of unity.

i.e. – j, (– j + 1) ……..(j – 1), j

We also find the value of η_j

Substituting m = j in equation (E),

$\eta_j - j(j+1) = 0$

$\Rightarrow \quad \eta_j = j(j+1)$

Thus the eigenvalue of J^2 operator is j (j +1).

Note

1. $J^2 \psi_{jm} = j(j+1)\psi_{jm}$
2. $J_z \psi_{jm} = m \psi_{jm}$

Where m = –j, –j +1,……..(j –1), j in steps of unity.

7.7. Eigen values of J_+ and J_-

Let $J_+ \psi_{jm} = \varphi_+ = \lceil_+ \psi_{j,m+1}$ (1)

$$\text{Now } \langle \varphi_+ | \varphi_+ \rangle = \langle J_+ \psi_{jm} | J_+ \psi_{jm} \rangle$$

$$= \int \psi^*_{jm} J_- J_+ \psi_{jm} \, d\tau$$

$$= \int \psi^*_{jm} (J^2 - J_z (J_z+1) \psi_{jm} \, d\tau$$

$$= \int \psi^*_{jm} [j(j+1) - m (m+1)] \psi_{jm} \, d\tau \quad (2)$$

$$\text{Now, } \langle \lceil_+ \psi_{jm+1} | \lceil_+ \psi_{jm+1} \rangle = \int \psi^*_{jm+1} \lceil^{\dagger}_{+} \{ \} \lceil_+ \psi_{jm+1} \, d\tau$$

$$= \int \psi^*_{jm+1} |\lceil_+|^2 \psi_{jm+1} \, d\tau$$

$$= |\lceil_+|^2 \int \psi^*_{jm+1} \psi_{jm+1} \, d\tau$$

$$= |\lceil_+|^2 \quad (3)$$

Using equations (1), (2) and (3) we can write,

$$|\lceil_+|^2 = j(j+1) - m(m+1)$$

or

$$\lceil_+ = \sqrt{j(j+1) - + m(m}$$

$$= \sqrt{j^2 + j - m^2 - m}$$

$$= \sqrt{(j-m)(j+m+1)}$$

In a similar fashion, we can show that,

$$\lceil_- = \sqrt{(j+m)(j-m+1)}$$

Thus the eigenvalues of J_+ and J_- operators are $\sqrt{(j-m)(j+m+1)}$ and $\sqrt{(j+m)(j-m+1)}$ respectively.

7.8. Matrix Elements

The matrix elements for J^2, J_z, $J_+ J_-$ are give below.

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

$$\langle j' m' | J_z | j m \rangle = m \delta_{jj'} \delta_{m'm}$$

$$\langle j' m' | J_+ | j m \rangle = \sqrt{(j-m)(j+m+1)} \; \delta_{jj'} \delta_{m'm+1}$$

$$\langle j' m' | J_- | j m \rangle = \sqrt{(j+m)(j-m+1)} \; \delta_{jj'} \delta_{m'm-1}$$

The above matrix elements are sufficient to construct all the angular momentum matrices.

Note

1. $J_x = \frac{1}{2}(J_+ + J_-)$
2. $J_y = \frac{1}{2}(J_+ - J_-)$
3. Since all the matrix elements defined above connect states with the same j but different m values, it is usual to construct angular momentum matrices for a given j value.
4. It is customary to label the rows by m' values (i.e. m' = j……..–j) and the columns by m values (i.e. m = j……..–j)
5. For a given j, the dimension of the angular momentum matrices are given by (2j+1) X (2j+1)

Problem 7.5

Find the angular momentum matrices of J^2, J_z, J_+ , J_- , J_x and J_y when j = ½.

Solution

Dimension of the matrix

The dimension of the matrix is (2j+1) X (2j+1) i.e. (2 X ½ +1) X (2 X ½ +1) = 2 X 2. Then, the possible values of ma are ½ and – ½.

The angular momentum matrix for J^2 is given by.

$$\begin{array}{c} m'\backslash m \\ \frac{1}{2} \\ -\frac{1}{2} \end{array} \begin{array}{c} \begin{array}{cc} \frac{1}{2} & -\frac{1}{2} \end{array} \\ \begin{bmatrix} \frac{3}{4} & 0 \\ 0 & \frac{3}{4} \end{bmatrix} \end{array}$$

$$= \frac{3}{4}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The angular momentum matrix for J_z

$$\begin{array}{c} m'\backslash m \\ \frac{1}{2} \\ -\frac{1}{2} \end{array} \begin{array}{c} \begin{array}{cc} \frac{1}{2} & -\frac{1}{2} \end{array} \\ \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{bmatrix} \end{array}$$

$$= \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \frac{1}{2}\sigma_z$$

For J_+

$m'\backslash m$	$\frac{1}{2}$	$-\frac{1}{2}$
$\frac{1}{2}$	0	1
$-\frac{1}{2}$	0	0

For J_-

$m'\backslash m$	$\frac{1}{2}$	$-\frac{1}{2}$
$\frac{1}{2}$	0	0
$-\frac{1}{2}$	1	0

Angular momentum matrix for J_x

$$J_x = \frac{1}{2}(J_+ + J_-)$$

$$= \frac{1}{2}\left\{\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}\right\}$$

$$= \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \frac{1}{2}\sigma_x$$

Similarly for J_y

$$J_y = \frac{1}{2i}(J_+ + J_-)$$

$$= \frac{1}{2i}\left\{\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}\right\}$$

$$= \frac{1}{2i}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

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

$$= \frac{1}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \frac{1}{2}\sigma_y$$

Note

$$J_x = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \frac{1}{2}\sigma_x$$

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

$$J_z = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \frac{1}{2}\sigma_z$$

are the Pauli's spin matrices for j = ½.

Problem 7.6

Obtain the angular momentum matrices J^2 , J_z , J_+ , J_- , J_x and J_y for j=1.

Solution

Dimension of the matrix (2j + 1) x (2j + 1)

= (2 x 1 + 1) x (2 x 1 + 1)

= 3 x 3 matrix

j = 1 $\Rightarrow$ possible values of m are 1, 0, –1.

Angular momentum matrix for J^2

$$\begin{array}{c} m'\backslash m \\ 1 \\ 0 \\ -1 \end{array}\begin{array}{c} \begin{array}{ccc} 1 & 0 & -1 \end{array} \\ \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} \end{array} = 2\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The angular momentum matrix for J_z

$$\begin{array}{c} m'\backslash m \\ 1 \\ 0 \\ -1 \end{array}\begin{array}{c} \begin{array}{ccc} 1 & 0 & -1 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{bmatrix} \end{array}$$

Angular momentum matrix for J_+

$$\begin{array}{c} m'\backslash m \\ 1 \\ 0 \\ -1 \end{array}\begin{array}{c} \begin{array}{ccc} 1 & 0 & -1 \end{array} \\ \begin{bmatrix} 0 & \sqrt{2} & 0 \\ 0 & 2 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix} \end{array} = \sqrt{2}\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

Angular momentum matrix for J_-

$$\begin{array}{c|ccc} m'/m & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ -1 & 0 & \sqrt{2} & 0 \end{array} = \sqrt{2} \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Angular momentum matrix for J_x

$$\begin{aligned} J_y &= \frac{1}{2}(J_+ + J_-) \\ &= \frac{1}{2}\left\{\begin{bmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{bmatrix}\right\} \\ &= \frac{1}{2}\begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix} \\ &= \frac{\sqrt{2}}{2}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \\ &= \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \end{aligned}$$

Angular momentum matrix for J_y

$$\begin{aligned} J_y &= \frac{1}{2i}(J_+ + J_-) \\ &= \frac{1}{2i}\left\{\begin{bmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{bmatrix}\right\} \\ &= \frac{1}{2i}\begin{bmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{bmatrix} \\ &= \frac{i}{\sqrt{2}}\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \end{aligned}$$

Problem 7.7

Construct the angular momentum matrices for j = 3/2.

Solution

Dimension of the matrix = $\left(2x\frac{3}{2}+1\right) x \left(2x\frac{3}{2}+1\right) = 4 \text{ x } 4$ matrix

$\therefore$ possible values of m are $\frac{3}{2}, \frac{1}{2}, \frac{-1}{2}, \frac{3}{2}$.

$$J^2 = \begin{bmatrix} \frac{15}{4} & 0 & 0 & 0 \\ 0 & \frac{15}{4} & 0 & 0 \\ 0 & 0 & \frac{15}{4} & 0 \\ 0 & 0 & 0 & \frac{15}{4} \end{bmatrix} \qquad J_z = \begin{bmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{-1}{2} & 0 \\ 0 & 0 & 0 & \frac{3}{2} \end{bmatrix}$$

$$J_+ = \begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & \sqrt{4} & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad J_- = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & \sqrt{4} & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix}$$

$$J_x = \frac{1}{2}\begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 4 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad J_y = \frac{1}{2}\begin{bmatrix} 0 & -\sqrt{3}i & 0 & 0 \\ -\sqrt{3}i & 0 & -2i & 0 \\ 0 & 2i & 0 & -\sqrt{3}i \\ 0 & 0 & \sqrt{3}i & 0 \end{bmatrix}$$

LET US SUM UP

By going through this chapter, one can easily understand the algebra of angular momentum. We can calculate the spectrum of eigenvalues for J^2 and J_z operators. One can easily construct the angular momentum matrices for a given j by studying this lesson.

LESSON END ACTIVITIES

Check your progress

1. Give the quantum mechanical definition of angular momentum.
2. Obtain the spectrum of eigen values for J^2 and J_z.
3. What are called raising and lowering operators ? Why they are called so ?

7.11. Do it Yourself

1. If $\mathbf{J} = J_1 + J_2$ show that $\mathbf{J} \times \mathbf{J} = i\hbar\mathbf{J}$.

2. Express the matrix for J_x when j = ½.
3. Find $[J_z, J_+]$
4. Show that if any operator commutes with J_x, J_y it also commutes with J_z
5. Show that J^2 and J_z form complete set of commuting observable and j can take all integral values and half integral values greater than one or equal to zero.

7.12. References

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LESSON 8

COUPLING OF TWO ANGULAR MOMENTA OR CLEBSCH – GORDON (C,G) COEFFICIENT

8.1. Aims and objectives:

Here we are going to study the coupling of two angular momenta in detail

8.2. Clebsch – Gordon (C,G) Coefficient

When we couple two angular momenta $\vec{J}_1$ and $\vec{J}_2$, the final $\vec{J}$ will be between $|J_1 - J_2|$ in steps of unity. We will have two sets of mutually commuting operator given by

Set I : $J_1^2,\ J_2^2,\ J_z,$

Set II : $J_1^2,\ J_2^2,\ J^2,\ J_z$

The state vectors or wave functions corresponding to the two sets will be

$|j_1\ j_2\ j\ m\rangle$ and $|j_1\ j_2\ m_1\ m_2\rangle$

The state vector corresponding to the first set $|j_1\ j_2\ j\ m\rangle$ is called the coupled representation. And the state vector corresponding do the second set $|j_1\ j_2\ m_1\ m_2\rangle$ is called uncoupled representation.

In order to move from coupled representation to uncoupled representation, or vice versa, we need a unitary transformation coefficient. The transition from one representation to another representation is accomplished by the following two equations.

$$|j_1\ j_2\ m_1\ m_2\rangle = \sum_{jm} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} |j_1\ j_2\ j\ m\rangle \qquad (1)$$

$$|j_1\ j_2\ j\ m\rangle = \sum_{m_1\ m_2} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} |j_1\ j_2\ m_1\ m_2\rangle \qquad (2)$$

The symbol $\begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix}$ is called the **unitary transformation coefficient** or **vector addition coefficient** or **Clebsch – Gordon (C,G) Coefficient**.

Now, taking scalar product with $\langle j_1\ j_2\ j\ \ m|'$ on both the sides of equation (1)

$$\langle j_1\ j\ \ j'\ \ m_1|'j_2\ j\ \ _1m\ \ _2m\rangle$$

$$\langle j_1\ j\ \ j'\ \ m_1|'j_2\ j\ \ _1m\ \ _2m\rangle = \sum_{j\ \ m}\begin{bmatrix} j_1 & _2j \\ m_1 & m_2 \end{bmatrix} j\ \ m\ \ \langle j_1\ j\ \ j'\ \ m_1|'j_2\ j\ \ _1m\ \ _2m\rangle$$

$$= \sum_{j\ \ m}\begin{bmatrix} j_1 & _2j \\ m_1 & m_2 \end{bmatrix} j\ \ m\ \ \delta_{j\ 'j}\delta_{m\ 'm}$$

Now, doing the summation over j and m on R.H.S, because of the presence of Kronocker delta, of all the possible values of j and m, only those terms corresponding to j = j' and m = m' will remain.

$$\langle j_1 j\ \ j\ \ m_1 j_2 j\ \ _1m\ \ _2m\rangle = \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} \qquad (3)$$

Thus we find the C.G. coefficient is the scalar product of the two state vectors in the coupled and the uncoupled representation.

In a similar manner, taking the scalar product with $|\ j_1\ j_2\ m_1'\ m_2'\ >$ on both the sides of equation (2),

$$\langle j_1 j_2 m_1\ \ m_2|\ j\ \ j_1\ \ j_2 j\ \rangle m = \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} \qquad (4)$$

Taking hermitian adjoint (Congugate transpose) of equation (4)

$$\langle j_1 j\ \ j\ \ m_1 j_2 j\ \ _1m\ \ _2m\rangle = \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} \qquad (5)$$

8.3. Orthonormal Properties of C.G. Coefficient

We know that the wave functions in the coupled representation as well as in the uncoupled representation are orthogonal.

$$\langle j_1\ j\ \ j'\ \ m_1|'j\ \ j_2\ \ j\ \ \rangle m = \delta_{j\ 'j}\delta_{m\ 'm} \qquad (1)$$

$$\langle j_1 j_2 m_1'\ \ m_2'|\ j_1\ \ j_2 m_1\ \ m_2\rangle = \delta_{m_1\ \ m_1'}\delta_{m_2' m} \qquad (2)$$

Decoupling equation (1)

$$\langle j_1 j_2 j m | = \sum_{m_1' m_2'} \begin{bmatrix} j_1 & j_2 & j' \\ m_1' & m_2' & m \end{bmatrix} \langle j_1 j_2 m_1' m_2' |$$

$$| j_1 j_2 j' m' \rangle = \sum_{m_1 m_2} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} | j_1 j_2 m_1 m_2 \rangle$$

Substituting in equation (1), we have

$$\sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \begin{bmatrix} j_1 & j_2 & j' \\ m_1' & m_2' & m \end{bmatrix} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m' \end{bmatrix} \langle j_1 j_2 m_1' m_2' | j_1 j_2 m_1 m_2 \rangle = \delta_{j'j} \delta_{m'm}$$

$$\sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \begin{bmatrix} j_1 & j_2 & j' \\ m_1' & m_2' & m \end{bmatrix} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m' \end{bmatrix} \delta_{m_1 m_1'} \delta_{m_2 m_2'} = \delta_{jj'} \delta_{mm'}$$

Now, summing over m_1' and m_2'

$$\sum_{m_1 m_2} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} \begin{bmatrix} j_1 & j_2 & j' \\ m_1 & m_2 & m' \end{bmatrix} = \delta_{j'j} \delta_{m'm} \qquad (3)$$

In a similar way, starting from equation (2), the orthogonal property for the C.G. coefficient can be written as

$$\sum_{j m} \begin{bmatrix} j_1 & j_2 & j \\ m_1' & m_2' & m \end{bmatrix} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m' \end{bmatrix} = \delta_{m_1 m_1'} \delta_{m_2 m_2'} \qquad (4)$$

8.4. Symmetry Properties of C.G. coefficients

1. $$\begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} = (-1)^{j_1 + j_2 - j} \begin{bmatrix} j_2 & j_1 & j \\ m_2 & m_1 & m \end{bmatrix}$$

2. $$\begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} = (-1)^{j_1 + j_2 - j} \begin{bmatrix} j_1 & j_2 & j \\ -m_1 & -m_2 & m \end{bmatrix}$$

3. $$= (-1)^{j_1 - m_1} \frac{[j]}{[j_2]} \begin{bmatrix} j_1 & j & j_2 \\ m_1 & -m & -m_2 \end{bmatrix}$$

4. $$= (-1^{j_2 + m_2} \frac{[j]}{[j_1]} \begin{bmatrix} j & j_2 & j_1 \\ -m & m_2 & m_1 \end{bmatrix}$$

where $[j] = (2j+1)^{1/2}$

8.5. Conditions to be satisfied to C.G. coefficient to exist

1. Triangle Rule

$\Delta (j_1\ j_2\ j)$ must be satisfied. i.e. the final j must be within the permissible limit of $|j_1 - j_2|$ to $j_1 + j_2$ (in steps of unity).

2. m sum rule must be satisfied

$m_1 + m_2 = m$

3. Projection rule must be satisfied i.e. m should be valid projection of j. i.e. m = – j, – j +1 …….(j–1), j is steps of unity.

From equations (3) and (4) we have

$$\sum_{m_1 m_2} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix}^2 = 1 \qquad (5)$$

$$\sum_{j,\ m} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix}^2 = 1 \qquad (6)$$

8.6. Some Special Types of C.G. Coefficients

1. When either j_1 or j_2 is zero, then the coupled and uncoupled representation, will become equal. In such a case, the corresponding C.G. coefficient will be equal to unity.

i.e. $$\begin{bmatrix} 0 & j & j \\ 0 & m & m \end{bmatrix} = 1$$

$$\begin{bmatrix} j & 0 & j \\ m & 0 & m \end{bmatrix} = 1$$

However it should be noted that, if the final j = 0, then

$$\begin{bmatrix} j & j & 0 \\ m & -m & 0 \end{bmatrix} \neq 1$$

8.7. LET US SUM UP

We have studied the coupling two angular momenta in detail in this chapter. Also we discussed the symmetry properties of C.G. coefficient.

8.8. LESSON END ACTIVITIES

Check your progress

1. What are C.G. Coeffifiient? Briefly explain their significance.
2. List the symmetry properties of C. G. coefficient.
3. What are the conditions to be satisfied for C.G. coefficient to exist?
4. Write down the special type of C. G. coefficient.
5. Give the orthonrmal properties of C.G. coefficient.

8.9. References

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LESSON 9

RELATIVISTIC QUANTUM MECHANICS

9.1. Aims and objectives:

In this lesson we will be studying the important aspects of relativitic quantum mechanics such as Klein Gordon equation and Dirac's relativistic wave equation. Then we will have a discussion on the free pariticle solution for Dirac's equation. Also we are going to study the properties of Dirac's matrices.

9.2. Introduction

The Quantum Mechanics developed so far, does not satisfy the requirements of special theory of relativity as it is based on a non relativistic Hamiltonian. The wave equation we used to discuss physical problems is of the first order in time and of second order in space co-ordinates. This contradicts the space-time symmetry requirement of relativity. The difficulties suggest two ways of obtaining relativistic wave equations. i) to use a relativistic Hamiltonian for a free particle is place of non-relativistic one ii) to try for a first order equation in both space and time co-ordinates. Though Schrödinger himself suggested the first possibility its implications were studied in detail by Klein and Gordon in 1926. Hence it is popularly known as Klein Gordon (K.G.) equation. It does not say anything about the spin of the particle. Hence it is used to describe spin zero particles such as in pions, kaons etc. Based on the second idea, Dirac developed his relativistic wave equation. The concept of spin has evolved automatically from Dirac's theory which is applicable to spin ½ systems.

9.3. Klein – Gordan Equation

The relativistic relation between energy and momentum is given by

$$E^2 = c^2p^2+m^2c^4$$

and the operators for the E and P are

$$E = i\hbar\frac{\partial}{\partial t} \qquad \vec{p} = -i\hbar\vec{\nabla}$$

The Schrödinger equation will be

$$H\psi = E\psi$$

$$\sqrt{c^2 p^2 + m^2 c^4}\ \psi = i\hbar \frac{\partial}{\partial t}\psi$$

But it is very difficult to give a physical meaning for the square root of an operator. Further if the square root is expanded in terms of binomial services we will have even powers of ∇ on the L.H.S. In order to avoid the difficulties Klein-Gordon proposed that the wave equation will be

$$H^2\psi = E^2\psi$$

$$\left\{c^2 \quad p^2 + \quad m^4\right\}\psi c \quad \left(\hbar \quad \frac{\partial \psi}{\partial t}\right)^2$$

$$\left\{c^2\left(-i\hbar \nabla m \quad + c \quad \hbar\right)\psi \quad ^2 - \quad \frac{\partial^2 \psi}{\partial t^2}\right.$$

$$\left\{-\hbar^2 c \quad \nabla^2 m + \quad c\hbar\right\}\psi \quad -^2 \quad \frac{\partial^2 \psi}{\partial t^2}$$

Dividing throughout by $-\hbar^2 c^2$

$$\left\{\nabla^2 \quad \frac{m^2}{\hbar^2} = \psi \quad ^2 \quad \frac{1}{c^2}\frac{\partial}{\partial t}\psi\right.$$

$$\left\{\nabla^2 \quad \frac{1}{c^2} \quad \frac{\partial m}{\partial t^2}\right\} \quad \frac{c^2}{\hbar^2} \quad \psi$$

$$\{\Box^2 - \frac{m^2 c^2}{\hbar^2}\}\ \psi = 0 \qquad (1)$$

where the D'Alemberts operator, which is relativistically invariant

$$\Box^2 = \nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}$$

Equation (1) is relativistically invariant, if ψ transform like a scalar.

9.3.1. Demerits of Klein Gordon Equation

1. Since it involves the second order time derivative $\frac{\partial^2}{\partial t^2}$, to have a future knowledge of the system we need to know not only ψ but also $\frac{\partial \psi}{\partial t}$.
2. The product $\psi^* \psi$ in KG equation does not represent the probability current density.
3. The wave function ψ in the KG equation is not orthogonal.

4. There is no way of introducing spin in to the KG equation and hence it is applicable only to spin zero particles like pions and kaons.

9.3.2. Plane Wave Solutions: Charge and Current Densities

Solutions of equation

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi + \left(\frac{mc}{\hbar}\right)^2\psi = 0 \qquad (1)$$

corresponding to particles of definite momentum $p = \hbar k$ may be obtained by substituting $\psi(x,t) = f(t)\,e^{ik.x}$. This leads to $\frac{d^2 f}{d^2 t} = [c^2 (k^2 / m^2)\hbar c^2]\, f$. Solving this we obtain, the plane wave solutions

$$\psi(x, t) = e^{i(k x - \omega t)} = e^{\frac{i}{\hbar}(p.x - Et)} \qquad (2)$$

$$E = \hbar\omega = \pm(p^2 c^2 + m^2 c^4)^{1/2} \qquad (3)$$

In contrast to the nonrelativistic case where the coefficient $(E/\hbar)$ of $(-it)$ in the exponent is the positive quantity $(p^2/2m\hbar)$, here we have solutions with -ω as well as with +ω. The appearance of the 'negative energy' solutions is typical of relativistic wave equations.

Another difference from the nonrelativistic case is that $\psi^*\psi$ cannot be interpreted as the probability density P(x,t). We expect P(x,t) to satisfy a continuity equation so that $\int P(x,t)d^3x$ is time – independent. To obtain such an equation we multiply equation (1) on the left by ψ*, its complex conjugate equation by ψ, and subtract. The resulting equation can be written as

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

This is the continuity equation with

$$P(x,t) = \frac{i\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right) \qquad (4a)$$

$$S(x,t) = \frac{i\hbar}{2m}(\psi\nabla\psi^* - \psi^*\nabla\psi) \qquad (4b)$$

A convenient choice of a common constant factor in P and S has been made here. With this choice, S coincides exactly with the corresponding nonrelativistic expression. However, P is quite different. It vanishes identically if ψ is real, and in the

case of complex wave functions, P can even be made negative by choosing $\frac{\partial \psi}{\partial t}$ appropriately. Clearly, P cannot be a probability density. One could multiply P by a charge e and then interpret it as a charge density. However, P can still have different signs at different points, and this is hardly satisfactory in the description of a single particle of given charge. It is known that equation (1) can be used to describe a system of arbitrary numbers of particles and their antiparticles by treating ψ itself as an operator function instead of a numerical – valued function. At this level, the above mentioned properties of P are no longer objectionable.

9.4. Dirac's Relativistic wave Equation

When the wave equation is of first order in time, it must be first order in space co-ordinates too. Dirac, was probably influenced by Maxwell's equation as they are first order equations in both space & time co-ordinates. In 1928 Dirac proposed a Hamiltonian that is linear in mass and energy given by

$$H = \left(\vec{\alpha}.\vec{p}\right)c + \beta mc^2$$

Dirac equation will be

$$E\psi = \left\{\vec{\alpha}.\vec{p}c + \beta mc^2\right\}\psi$$

$$\left\{E - \vec{\alpha}.\vec{p}c - \beta mc^2\right\}\psi = 0 \qquad (1)$$

Since we want this equation to be independent of space and time co-ordinates, $\vec{\alpha}$ and β must be independent of space and time co-ordinates. Otherwise this equation will give rise to space and time dependent energies and momenta.

Further we want this equation to be linear in space and time derivatives which already occur in $\vec{p}$ and E, $\vec{\alpha}$ and β must be independent of space and the time derivatives. This means that $\vec{\alpha}$ and β commute with $\vec{P}$ and E. But this does not necessarily mean that $\vec{\alpha}$ and β commute among themselves.

Premultiplying equation (1) by $\left\{E + \left(\vec{\alpha}.\vec{p}c\right) + \beta mc^2\right\}$ we get

$$\left\{E + \left(\vec{\alpha}.\vec{p}c\right) + \beta mc^2\right\}\left\{E - \left(\vec{\alpha}.\vec{p}c\right) - \beta mc^2\right\}\psi = 0$$

$$\{ E+ c (\alpha_x p_x + \alpha_y p_y + \alpha_z p_z) + \beta mc^2\} \{E - c (\alpha_x p_x + \alpha_y p_y + \alpha_z p_z) - \beta mc^2 \}\psi = 0$$

$$[E^2 - c^2 (\alpha_x^2 p_x^2 + \alpha_y^2 p_y^2 + \alpha_z^2 p_z^2) - \beta^2 m^2 c^4 - c^2 (\alpha_x \alpha_y + \alpha_y \alpha_x) p_x p_y$$

$$- c^2 (\alpha_y \alpha_z + \alpha_z \alpha_y) p_z p_y - c^2 (\alpha_z \alpha_x + \alpha_x \alpha_z) p_z p_x - mc^3 \{(\alpha_x \beta + \beta \alpha_x) p_x$$

$$+ (\alpha_y \beta + \beta \alpha_y) p_y + (\alpha_z \beta + \beta \alpha_z) p_z\}] \psi = 0$$

Comparing the above equation with the relativistic relation between energy and momentum is

$$E^2 - c^2 p^2 - m^2 c^4 = 0$$

we get

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1$$

$$\alpha_x \alpha_y = -\alpha_y \alpha_x \qquad \alpha_x \beta = -\beta \alpha_x$$

$$\alpha_y \alpha_z = -\alpha_z \alpha_y \qquad \alpha_y \beta = -\beta \alpha_y$$

$$\alpha_z \alpha_x = -\alpha_x \alpha_z \qquad \alpha_z \beta = -\beta \alpha_z$$

Thus we find that $\vec{\alpha}$ and β anticommute among themselves in pairs. Further we find that eigenvalues for all the four matrices are +1 and -1

9.4.1. Properties of $\vec{\alpha}$ and β Matrices

1. Since $\vec{\alpha}$ and β anticommute among themselves in pairs they cannot be numbers. Therefore they can be conveniently represented by matrices.
2. Since we want the Dirac Hamiltonian to be Hermitian, $\vec{\alpha}$ and β must also be Hermitian. Therefore $\vec{\alpha}$ and β must be square matrices.
3. The eigenvalues of $\vec{\alpha}$ and β matrices +1 and -1.
4. Since in a group of four anticommuting matrices in pairs, we can have only one of the matrices to be the diagonal matrix we choose β matrix to be the diagonal matrix.
5. $\alpha_x \beta = -\beta \alpha_x$

   Pre multiplying by β on both sides

   $$\beta \alpha_x \beta = -\beta^2 \alpha_x \qquad \text{Since } \beta^2 = 1$$

   $$= -\alpha_x$$

   Taking Trace on both sides

   $$T_r (\beta \alpha_x \beta) = -T_r(\alpha_x)$$

$$T_r(\beta^2\alpha_x) = -T_r(\alpha_x)$$

$$T_r(\alpha_x) = -T_r(\alpha_x)$$

$$2\,T_r(\alpha_x) = 0$$

$$T_r(\alpha_x) = 0$$

In a similar manner we can prove that

$$T_r(\alpha_y) = 0$$

$$T_r(\alpha_z) = 0$$

$$T_r(\beta) = 0$$

6. Since the traces of all these four matrices are zero, and their eigenvalues are +1 and -1, there should be same number of +1 along the diagonals as the number of -1 in β matrix. Therefore the dimension of β matrix must be even.
7. The i^{th} element of the equation

$$\alpha_x\beta + \beta\alpha_x = 0$$

i.e. $$\sum_k (\alpha_x)_{ik}\,\beta_{kl} + \sum_m (\beta)_{im}\,(\alpha_x)_{ml} = 0$$

Since β matrix is orthogonal

$$(\alpha_x)_{il} + (\beta)_{ll} + (\beta)_{ii}\,(\alpha_x)_{il} = 0$$

$$(\alpha_x)_{il}\,\{\beta_{ll} + \beta_{ii}\} = 0$$

If $\beta_{ll} = -\beta_{il}$ then $(\alpha_x)_{il} \neq 0$ for $i \neq l$ otherwise $(\alpha)_{il} = 0$ for $i = l$.

Since β matrix which is a diagonal matrix must be of even dimensions we choose β matrix to be

$$\beta = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & - & - & - \\ 0 & 1 & 0 & 0 & 0 & 0 & - & - & - \\ - & - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - & - \\ 0 & 0 & 0 & 0 & -1 & 0 & - & - & \\ 0 & - & 0 & - & 0 & - & 1 & - & - \\ 0 & - & 0 & - & & 0 & - & 1 & - \\ - & - & - & - & - & - & - & - & - \end{bmatrix}$$

From the knowledge of Pauli's spin matrices we find that there can be only three 2 X 2 matrices anticommuting among themselves in pairs. It is impossible to find a 4^{th} 2 X 2 matrix that is anticommute with the Pauli's spin matrices. But in the case we need 3 α matrices and one β matrix to anticommute among themselves in

pairs. Therefore the minimum dimension of β matrix must be 6 X 6, 8 X 8…, may be possible for β matrix, but this will not give anything new and hence we choose the minimum dimension the β matrix 4 X 4.

Therefore β matrix will be

$$\beta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

In short we write

$\beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ where each element is a sub matrix of order 2 X 2.

Since $(\alpha_x)_{il} \neq 0$ for $i \neq l$ and $(\alpha_x)_{il} = 0$ for $i = l$

We choose

$$\alpha_x = \begin{bmatrix} 0 & \alpha_{x1} \\ \alpha_{x2} & 0 \end{bmatrix}$$

Further since $\alpha_x^2 = 1$

$$\text{i.e. } \begin{bmatrix} \alpha_{x1}\alpha_{x2} & 0 \\ 0 & \alpha_{x2}\alpha_{x1} \end{bmatrix} = 1$$

ie $\alpha_{x1}\,\alpha_{x2} = 1$ and $\alpha_{x2}\,\alpha_{x1} = 1$

We choose both, α_{x1} and α_{x2} to be σ_x

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

In a similar manner we choose

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

$$\alpha_z = \begin{bmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

It is to be mentioned that the above form for $\vec{\alpha}$ and β is not unique. Any other set can also be chosen to satisfy the above commutation relations.

However these two sets will be related by the singular transformation

$$\vec{\alpha} = s^{-1}\vec{\alpha}\, s$$

$$\beta = s^{-1}\beta\, s$$

where S is a non-singular free particle solution

9.5. Free Particle Solution

The Dirac Hamiltonian is

$$E\psi = \left\{ \alpha c(\vec{} + \vec{} . \vec{\beta}\ p) \quad \psi^{2} \right\} m$$

Since α and β are 4 X 4 matrices ψ must be a 4 X 1 matrix (or) It is a column vector we choose

$$\psi_j = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \begin{bmatrix} u \\ u \\ u \\ u \end{bmatrix} \; i(\vec{k}.\vec{r}\, e^{\omega}$$

or $\psi_j = {}_j\, u \; i(\vec{k}.\vec{r}\, e^{\omega}$ where j = 1,2,3,4

$\therefore$ The Dirac equation becomes

$$i\hbar \frac{\partial}{\partial t} \left\{ uj^{\,i\,\vec{k}(\vec{r}\omega\ t)} \right\} = \left\{ -i\hbar \quad \alpha(\vec{} \vec{\nabla} \vec{\beta}+) \quad 2ij\vec{k}.r \right\} mc_{\,j}\, u^{\vec{}}\, e^{\omega}$$

$$i\hbar \;{}_j u \;\; \alpha(-i)^{i(\vec{k}\vec{e}^{\omega})} = \left\{ -\hbar \; \alpha c(i)k\beta + u \quad {}^{2} \right\} jmc^{k\,\vec{}\,r\vec{}\omega t}$$

$$\hbar\omega\, u_j = \left\{ c\,(\vec{\alpha}.\hbar k) + \beta\, mc^{2} \right\} u_j$$

Since $\hbar\omega = E\hbar$ and $\vec{k}$ we have

$E\, u_j$	=	$\left\{ c\left(\vec{\alpha}.\vec{p}\right) + \beta \quad mc^{2} \right\}_{j}$
$E\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}$	=	$c\left\{ \alpha_x p_x + \alpha_y p_y + \alpha_z p_z + \beta \right\}^{2} \begin{bmatrix} u_1 \\ u_2 \\ mc \\ u_3 \\ u_4 \end{bmatrix}$

$$E\begin{bmatrix}u_1\\u_2\\u_3\\u_4\end{bmatrix} = c\left\{\begin{bmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{bmatrix}p_x + \begin{bmatrix}0&0&0&-i\\0&0&i&0\\0&-i&0&0\\i&0&0&0\end{bmatrix}p_y + \begin{bmatrix}0&0&1&0\\0&0&0&-1\\1&0&0&0\\0&-1&0&0\end{bmatrix}p_z + \begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}mc^2\right\}\begin{bmatrix}u_1\\u_2\\u_3\\u_4\end{bmatrix}$$

Adding all the matrices

$$= \begin{bmatrix}mc^2 & 0 & cp_z & cp_- \\ 0 & mc^2 & cp_+ & -cp_z \\ cp_z & cp_- & -mc^2 & 0 \\ cp_+ & -cp_z & 0 & -mc^2\end{bmatrix}\begin{bmatrix}u_1\\u_2\\u_3\\u_4\end{bmatrix}$$

$E\,u_1$	=	$mc^2u_1 + 0.u_2 + cp_z.u_3 + cp_- u_4$
$E\,u_2$	=	$0.u_1 + mc^2u_2 + cp_+u_3 - cp_z u_4$
$E\,u_3$	=	$cp_zu_1 + cp_-u_2 - mc^2u_3 + 0.u_4$
$E\,u_4$	=	$cp_+u_1 - cp_zu_2 + 0.u_3 - mc^2u_4$

$[E-mc^2]\,u_1 - 0.u_2 - cp_zu_3 - cp_-u_4$	=	0	(A)
$0.u_1 + [E-mc^2]\,u_2 - cp_+u_3 + cp_zu_4$	=	0	(B)
$-cp_zu_1 - cp_-u_2 + [E+mc^2]\,u_3 - 0.u_4$	=	0	(C)
$-cp_+u_1 + cp_zu_2 - 0.u_3 + [E+mc^2]\,u_4$	=	0	(D)

Since the equation are homogeneous in u_j the solution will exists only if the determinant of the coefficient is zero.

$$\begin{vmatrix}E-mc^2 & 0 & -cp_z & -cp_- \\ 0 & E-mc^2 & -cp_+ & cp_z \\ -cp_z & -cp_- & E+mc^2 & 0 \\ -cp_+ & cp_z & 0 & E+mc^2\end{vmatrix} = 0$$

By expanding the determinant we can show that

$$E^2 = c^2p^2 + m^2c^4$$

$$E = \pm\sqrt{c^2p^2 + m^2c^4}$$

Thus we find that both positive and negative energy values are possible for the Dirac particle corresponding to E_+ and E_- we will have two solutions for both

Taking first $E_+ = +\sqrt{c^2p^2 + m^2c^4}$, there are two linearly independent solutions for the positive energy.

Case (i)

u_1	=	0 $\quad u_2 = 1$
From equation (C) u_3	=	$\frac{c(p_x - ip_y)}{E + mc^2}$
From equation (D) u_4	=	$\frac{-cp_z}{E + mc^2}$

$\therefore$ The wave function will be $\begin{bmatrix} 0 \\ 1 \\ c(p_x - ip_y)/(E + mc^2) \\ -cp_z/(E + mc^2) \end{bmatrix}$

Case (ii)

u_1	=	1 $\quad u_2 = 0$
From equation (C) u_3	=	$\frac{cp_z}{E + mc^2}$
From equation (D) u_4	=	$\frac{c(p_x + ip_y)}{E + mc^2}$

$\therefore$ The wave function will be $\begin{bmatrix} 1 \\ 0 \\ cp_z/(E + mc^2) \\ c(p_x + ip_y)/(E + mc^2) \end{bmatrix}$

Similarly if we choose the negative root, $E = -\sqrt{c^2p^2 + m^2c^4}$, there are two linearly independent solutions for the negative energy.

Case (iii)

u_3	=	0 $\quad u_4 = 1$
From equation (A) u_1	=	$\frac{c(p_x - ip_y)}{E - mc^2}$

From equation (B) u_2	=	$\frac{-c\,p_z}{E-m^2c}$

$\therefore$ The wave function will be $\begin{bmatrix} c\,p_x - i\,c\,p_y \\ -c\,p_z \\ E+m^2c \\ 0 \\ 1 \end{bmatrix}$

Case (iv)

u_3	=	1 $\qquad$ $u_4 = 0$
From equation (A) u_1	=	$\frac{c\,p_z}{E-m^2c}$
From equation (B) u_2	=	$\frac{c\,p_x + i\,p_y}{E-m^2c}$

$\therefore$ The wave function will be $\begin{bmatrix} c\,p_z \\ c\,p_x + i\,p_y \\ E+m^2c \\ 1 \\ 0 \end{bmatrix}$

9.5.1. Normalization Condition

We use the normalization condition that $u^+ u = 1$.

Case (i)

$$u^+ u = 1$$

$$\psi^+ \psi = (Nu)^+ Nu = N^2 u^+ u$$

$$N^2 = \begin{pmatrix} 0 & 1 & \frac{c\,p_x - i\,p_y}{E+m^2c} & \frac{c\,p_z}{E+m^2c} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ c\,p_x + i\,p_y \\ E+m^2c \\ -c\,p_z \\ E+m^2c \end{pmatrix} =$$

$$N^2 \left\{ 1 + \frac{c^2 p_x^2 + p_y^2}{(E+m^2c)^2} \right\} + \frac{c^2 p_z^2}{(E+m^2c)^2}$$

$$N^2 \left\{ 1 + \frac{c^2 p_x^2 + p_y^2}{(E+m^2c)^2} \right\} + \frac{c^2 p_z^2}{(E+m^2c)^2}$$

$$N^2 \left\{ 1 + \frac{c^2 p^2}{(E+m^2c^2)} \right\}$$

Therefore the normalized wave function will be

$$\psi_1 = \frac{1}{\sqrt{1+\frac{c^2\hat{p}^2}{(E+m)^2c^2}}} \begin{bmatrix} 0 \\ 1 \\ c\,p_x - i\,c\,p_y \\ -c\,p_z - E + mc^2 \end{bmatrix} e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

In a similar manner for the other three cases also the normalization constant can be shown to equal to

$$\psi_2 = \frac{1}{\sqrt{1+\frac{c^2p^2}{(E+mc^2)^2}}} \begin{bmatrix} 1 \\ 0 \\ cp_z/(E+mc^2) \\ cp_+/(E+mc^2) \end{bmatrix}$$

$$\psi_3 = \frac{1}{\sqrt{1+\frac{c^2\hat{p}^2}{(E-m)^2c^2}}} \begin{bmatrix} c\,p_x - i\,c\,p_y - E + mc^2 \\ -c\,p_z - E + mc^2 \\ 0 \\ 1 \end{bmatrix}$$

$$\psi_4 = \frac{1}{\sqrt{1+\frac{c^2\hat{p}^2}{(E-m)^2c^2}}} \begin{bmatrix} c\,p_z - E + mc^2 \\ c\,p_+ - E + mc^2 \\ 1 \\ 0 \end{bmatrix}$$

$$E = \pm\sqrt{c^2p^2 + m^2c^4}$$

The energy correspond to positive as well as negative states

We find that ψ_1 and ψ_2 will correspond to positive energy solutions for spin down and spin up particles

$\psi_1 = \psi_+ \downarrow$

$\psi_2 = \psi_+ \uparrow$

In a similar manner the negative energy solutions ψ_3 and ψ_4 will correspond to spin down and spin up particles respectively.

$\psi_3 = \psi_- \downarrow$

$\psi_4 = \psi_- \uparrow$

9.6. Meaning of Negative Energy States

It was found that necessary condition for the solution of Dirac equation is

$$E = \sqrt{\pm^2 cp^2 + {}^2 {}^4 n}$$

The meaning of positive energy state is clear but that of negative energy is not clear. It was at one time, suggested by Schrödinger himself as having no meaning and hence to be excluded. However there were two fundamental objections for excluding the negative energy states,

i) Mathematical and another

ii) Physical.

The exclusion of negative energy states will give rises to an incomplete set of solutions and this is mathematically not valid. On the otherhand the Dirac equation starts with positive energy states and there is a possibility of induced transition in to the negative energy states. Therefore if the negative energy states are excluded there will be contradiction, from Physicsts point of view. This has led Schrödinger into insurmountable difficulties.

In order to overcome the above difficulties, Dirac postulated that

1. The positive energy levels form a continuum from $+mc^2$ to $+\infty$ where as the negative energy states form another continuum from $-mc^2$ to $-\infty$.
2. In between $-mc^2$ and $+mc^2$ there are no available energy levels.
3. Dirac proposed that all the negative energy states are completely filled up normally.
4. The electrons in the negative energy states will not be affected by electric and magnetic fields.

9.6.1. Consequences of Dirac's Interpretation

The following consequences may arise due to Dirac's interpretation.

1. The electrons in the positive energy states will not normally make transitions to the negative energy states that are completely filled.
2. With the sea of electrons in the negative energy states, unobservable the transition of one of these electrons to the positive energy states will manifest

itself, as a hole in the negative energy states. This hole is regarded as positions and it behaves like an electron with the positive charge.

3. The fact that the negative energy states are completely filled up implies that Paulis exclusion principle is obeyed. If the Pauli's exclusion principle is not valid, the negative energy states cannot be completely filled up. Since otherwise many electrons rather than one electron will occupy level.
4. Feymann interpreted that negative energy states are electrons moving forward in time (or) positions moving backward in time.

9.7. LET US SUM UP

In this lesson we had a discussion on the two prominent relativistic wave equations namely K.G. equation and Dirac equation. Then we presented the free particle solution of Dirac's relativistic equation. Also we had a discussion on interpretation of negative energy states.

9.8. LESSON END ACTIVITIES

Check your progress

1. If you were a Dirac How would you have predicted the existence of positron? Explain
2. 'The K.G. equation has nothing to say about the spin of the particle' – Illustrate.
3. Explain how Dirac has interpreted the negative energy states.
4. Develop Dirac's relativistic wave equation for a free particle and obtain its plain wave solution.
5. Deduce relativistic Klein Gordon equation. Can we use this equation for pions and kaons. Show that its probability expression is indefinite.
6. Establish the Dirac's relativistic wave equation for an electron and calculate its magnetic moment.
7. Obtain the eigenvectors for Dirac's relativistic wave equation of a free particle.
8. Develop the relativistic wave equation for the particle of spin zero. Discuss the difficulties involved in interpreting the probability density. Derive the expression charge and current densities from the continuity equation.

9. Prove the following properties of Dirac matrices on the basis of Dirac's theory
    a. Square of matrices are unity
    b. Eigenvlues of the matrices are ±1.
    c. Trace of the matrices are zero.
    d. Dimension of the matrices are of even order.
    e. The matrices anticommuting among themselves.

9.9. References

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LESSON 10

SPIN AND SPIN MAGNETIC MOMENT OF ELECTRON

10.1. Aims and objectives:

This lesson deals with the expression for the spin of the electron and electron spin magnetic moment.

10.2. Spin of Electron

We know that the commutation relation between the z component of orbital angular momentum and the Dirac Hamiltonian is

$$[L_z,\ H] = [x,\ p_y\alpha_x - y\,.\,p_x\alpha_y + \beta m]$$

Here c is taken to be unity,

Now $$[L_z,\ H] = [x\ p_y\alpha_z + y\ p_x\alpha_z + p_z\alpha_x + p_z\alpha_y + \beta m]$$

$$= [x\ p_y\alpha_z] + [y\ p_x\alpha_z]$$

Here we have used the fact that x does not commute with p_x and y cannot commute with p_y but they commute will all other quantities.

Also $$[x,\ p_x] = [y,\ p_y] = i\hbar$$

$$[L_z,\ H] = [x,\ p_y]\alpha_z\alpha_y + [y,\ p_x]\alpha_x\alpha_z$$

$$= i\hbar[p_x\alpha_x\alpha_y + p_x\alpha_y\alpha_x] \qquad (1)$$

Here $\hbar$ is taken to be unity. But from Heisenberg's picture of time evolution,

we know that $$i\hbar\frac{dL_z}{dt} = [L_z, H] \qquad (2)$$

$$\frac{dL_z}{dt} = [p_y\alpha_x - p_x\alpha_y] \qquad (3)$$

This implies that L_z in not a constant of motion hence it is not conserved. In other words, L_z is not the complete angular momentum and there must be another part say S_z, such that (L_z + S_z) is conserved. We shall now verify that if S_z is taken

to be $\frac{1}{2}\sum_z$ where $\sum_z = \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$ (4)

Then (L_z + S_z) commutes with H

Let us first note that,

$$-i\alpha_x\alpha_y = -i\begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix},$$

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

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

$$= \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$$

$$= \sum_z \qquad (5)$$

Now $$[S_z, H] = \frac{1}{2}[\sum_z, H],$$

$$= -\frac{i}{2}[\alpha_x\alpha_y, H],$$

$$= -\frac{i}{2}[\alpha_x\alpha_y, \alpha_x p_x + \alpha_y p_y + \alpha_z p_z + \beta m],$$

$$= \frac{i}{2}\{[\alpha_x\alpha_y, \alpha_x]p_x + [\alpha_x\alpha_y, \alpha_y]p_y\},$$

$$= \frac{i}{2}\{(\alpha_x\alpha_y\alpha_x - \alpha_x\alpha_x\alpha_y)p_x + (\alpha_x\alpha_y\alpha_y - \alpha_y\alpha_x\alpha_y)p_y\},$$

$$= \frac{i}{2}\{(-\alpha_x^2\alpha_y + \alpha_x\alpha_y\alpha_x)p_x + (\alpha_x\alpha_y^2 - \alpha_y\alpha_x\alpha_y)p_y\},$$

$$= -\frac{i}{2}\{-2\alpha_y p_x + 2\alpha_x p_y\},$$

$$= -i\{-\alpha_y p_x + \alpha_x p_y\},$$

$$= i\{\alpha_x p_y - \alpha_y p_x\}, \qquad (6)$$

From (1) and (6) we find that

$$[(L_z + S_z), H] = 0 = i\frac{d}{dt}(L_z + S_z).$$

Therefore we find that the angular momentum is conserved only if we include the spin angular momentum operator

$$S_z = \frac{1}{2}\sum_z = \frac{1}{2}\begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix} \qquad (7)$$

We see that $J_z = L_z + S_z$ is a constant of motion and should be interpreted as the total angular momentum of the system.

Since ,
$$\sum_z^2 = \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix},$$
$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad (8)$$

We find that the eigenvalue of $\sum_z = \pm 1$. Therefore the eigenvalue of $S_z = \frac{1}{2}(\pm 1)$ are $+\frac{1}{2} and\ -\frac{1}{2}$.From these facts it is evident that the Dirac equation describes particles of Spin $\pm\frac{1}{2}$ such as electrons.

10.3. Spin Magnetic Moment of Electron (or) Dirac Equation in the presence of Electromagnetic Field

A familiar way of introducing electromagnetic field in the Dirac equation is to replace.

$$\vec{p} \rightarrow \vec{p} - \frac{e}{c}\vec{A} \text{ and}$$
$$E \rightarrow E - e\varphi$$

where $\vec{A}$ and φ are vector and scalar potentials respectively. Therefore, the Dirac equation becomes,

$(E - e\varphi)\,\psi$	=	$\left\{c\vec{\alpha}\left(\vec{p} - \frac{e}{c}\vec{A}\right) + \beta\right\}\psi^2 m$
$\left(i\hbar\frac{\partial}{\partial t} - e\varphi\right)\psi$	=	$\left\{c\vec{\alpha}\left(\vec{p} - \frac{e}{c}\vec{A}\right) + \beta\right\}\psi^2 m$

Assuming the vector function to be independent of time the wave function can be written as

$$\psi(\vec{r},t) = \psi(r)\, e^{\frac{-i(E_R + m^2c)}{\hbar}}$$

where E	=	$E_{N.R} + mc^2$ = Non relativistic energy + Relativistic energy
$\psi\left(\vec{r},t\right)$	=	$\psi(\vec{r})\, e^{\left\{-\frac{iE_{N.R}}{\hbar}t\right\}}\, e^{-\frac{imc^2}{\hbar}}$
	=	$\psi'\left(\vec{r},t\right), e^{-\frac{imc^2}{\hbar}}$
where $\psi'\left(\vec{r},t\right)$	=	$\psi(\vec{r})\ e^{\frac{-iE_{N.R}t}{\hbar}}$ is the non-relativistic wave form
$i\hbar\frac{\partial\psi}{\partial t}$	=	$i\hbar\left\{\frac{\partial}{\partial t}\psi'(\vec{r},t)\right\}\left(\frac{i\,m^2c}{\hbar}\right)e^{\frac{-i\,m^2c}{\hbar}t}$
	=	$\left\{i\hbar\frac{\partial}{\partial t}+mc^2\right\}e^{\frac{-imc^2}{\hbar}t}\psi'$

Substituting in the Dirac equation

$\left\{i\hbar\frac{\partial}{\partial t}+mc^2-e\varphi\right\}\psi'.e^{\frac{-imc^2}{\hbar}t}$	=	$\left\{c\vec{\alpha}.\left(\vec{p}-\frac{\vec{e}}{c}\vec{A}\right)+\beta mc^2\right\}\psi'e^{\frac{-i\,m^2c}{\hbar}t}$

Replacing the wave function ψ as a two component wave function ψ_A and ψ_B (large & small components)

$\left\{i\hbar\frac{\partial}{\partial t}+mc^2-e\varphi\right\}\begin{bmatrix}\psi_A\\ \psi_B\end{bmatrix}$	=	$\left\{c\begin{bmatrix}0 & \vec{\sigma}\\ \vec{\sigma} & 0\end{bmatrix}.\left(\vec{p}-\frac{\vec{e}}{c}\vec{A}\right)+\begin{bmatrix}0 & \\ & 0\end{bmatrix}1mc^2\right\}\begin{bmatrix}\psi_A\\ \psi_B\end{bmatrix}$
$\left\{i\hbar\frac{\partial}{\partial t}+mc^2-e\varphi\right\}\psi_A$	=	$c\vec{\sigma}.\left(\vec{p}-\frac{\vec{e}}{c}\vec{A}\right)\psi_B+\psi_A mc^2$
$i\hbar\frac{\partial\psi_A}{\partial t}$	=	$c\vec{\sigma}.\left(\vec{p}-\frac{\vec{e}}{c}\vec{A}\right)\phi_B+\psi e_A$ (1)
Similarly		
$\left\{i\hbar\frac{\partial}{\partial t}+mc^2-e\varphi\right\}\psi_B$	=	$c\vec{\sigma}.\left(\vec{p}-\frac{\vec{e}}{c}\vec{A}\right)\psi_A+\psi_B mc^2$
$\left\{i\hbar\frac{\partial}{\partial t}+2mc^2-e\varphi\right\}\psi_B$	=	$c\vec{\sigma}.\left(\vec{p}-\frac{\vec{e}}{c}\vec{A}\right)\psi_A$ (2)
Since		
$i\hbar\frac{\partial\psi_A}{\partial t}=i\hbar\frac{\partial\psi_B}{\partial t}$	=	$i\hbar\frac{\partial}{\partial t}\{\psi'(\vec{r},\}$

	=	$i\hbar \frac{\partial}{\partial t} \left\{ \psi(r)\, e^{\frac{-iE_{N.R}t}{\hbar}} \right\}$
	=	$i\hbar \left\{ -i \frac{E_{N.R}}{\hbar} \right\} \psi\, e^{\frac{-iE_{N.R}t}{\hbar}}$
Equation (2) becomes,	=	$E_{N.R}\, \psi\, e^{\frac{-iE_{N.R}t}{\hbar}}$
$\{E_{N.R} + 2mc^2 - e\varphi\}\psi_B$	=	$c\vec{\sigma}.\left(\vec{p} - \frac{e}{c}\vec{A}\right)\psi_A$
ψ_B	=	$\frac{c\vec{\sigma}.\left(\vec{p} - \frac{e}{c}\vec{A}\right)\psi_A}{\{E_{N.R} + 2mc^2 - \phi\}}$
$i\hbar \frac{\partial \psi_A}{\partial t}$	=	$c\vec{\sigma}.\left(\vec{p} - \frac{e}{c}\vec{A}\right) \frac{1}{E_{N.R} + 2mc^2 - \phi}\, \vec{A}$
		$-c\vec{\sigma}.\left(\vec{p} - \frac{e}{c}\vec{A}\right)\phi\, \psi_A$

Since $E_{N.R} <<< 2mc^2$ & assuming the magnetic field to be constant, ie $\varphi = 0$,

$$E_{N.R} + 2mc^2 \approx 2mc^2$$

$i\hbar \frac{\partial \psi_A}{\partial t}$	=	$c\vec{\sigma}.\left(\vec{p} - \frac{e}{c}\vec{A}\right) \frac{1}{2mc^2} c\vec{\sigma}.\left(\vec{p} - \frac{e}{c}\vec{A}\right)\psi_A$
	=	$\frac{1}{2m}\left[\left\{\vec{\sigma}.\left(\vec{p} - \frac{e}{c}\vec{A}\right)\right\}\left\{\vec{\sigma}.\left(\vec{p} - \frac{e}{c}\vec{A}\right)\right\}\right]$ (3)

R.H.S can be reduced by the following relation

$(\vec{\alpha}.\vec{B})(\vec{\alpha}.\vec{C})$	=	$\vec{B}.\vec{C} + i\vec{\alpha}.(\vec{B} \times \vec{C})$

where B & C commutes with $\vec{\alpha}$ but not necessarily with each other. Here

$\vec{B} = \vec{p} - \frac{e}{c}\vec{A}$ necessarily with each other. Now,

$\left\{\vec{\sigma}.\left(\vec{p} - \frac{e\vec{A}}{c}\right)\right\}\left\{\vec{\sigma}.\left(\vec{p} - \frac{e\vec{A}}{c}\right)\right\}$	=	$\left(\vec{p} - \frac{e\vec{A}}{c}\right).\left(\vec{p} - \frac{e\vec{A}}{c}\right) + i\vec{\sigma}\left\{\left(\vec{p} - \frac{e\vec{A}}{c}\right) \times \left(\vec{p} - \frac{e\vec{A}}{c}\right)\right\}$

	=	$p^2 - \frac{e}{c}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) + \frac{e^2}{c^2}A^2 + \sigma i\left(\frac{-e}{c}\left(\vec{p}\times\vec{A} + \vec{A}\times\vec{p}\right)\right)$

	=	$p^2 + \frac{e^2}{c^2}A^2 - \frac{e}{c}\left\{2\vec{A}.\vec{p} - i\hbar\vec{\nabla}.\vec{A}\right\} + i\sigma.\left\{\frac{-e}{c}(-i\hbar\vec{\nabla}\times\vec{A})\right\}$

Equation (3) becomes

$\therefore i\hbar\frac{\partial\psi_A}{\partial t}$	=	$\frac{p^2}{2m} + \frac{e^2}{2mc^2}A^2 - \frac{e}{mc}\vec{A}\cdot\vec{p} + \frac{i\hbar e}{2mc}\vec{\nabla}\cdot\vec{A} - \frac{\hbar e}{2mc}\sigma\cdot(\vec{\nabla}\times\vec{A})$

Since $\vec{\nabla}\times\vec{A} = \vec{B}$, the external magnetic field,

$\therefore i\hbar\frac{\partial\psi_A}{\partial t}$	=	$\frac{p^2}{2m} + \frac{e^2}{2mc^2}A^2 - \frac{e}{mc}\vec{A}\cdot\vec{p} + \frac{i\hbar e}{2mc}\vec{\nabla}\cdot\vec{A} - \frac{\hbar e}{2mc}\vec{B}\cdot\sigma$

This is nothing but, Schrödinger equation in N. R approximation.

The last term in the above expression gives the interaction of electron spin, with the external applied Magnetic field $\left(\vec{B}\right)$. Thus we find that the electrons behaves as a particle having a spin magnetic moment $\frac{e\hbar}{2mc}\vec{\sigma}$ where the spin of the $\vec{e}$ is

$$\vec{S} = \frac{1}{2}\hbar\vec{\sigma}$$

Now it can be shown that

$\vec{A}$	=	$\frac{1}{2}\left(\vec{B}\times\vec{r}\right)$
Then $\frac{e}{mc}\vec{A}.\vec{p}$	=	$\frac{1}{2}\frac{e}{mc}\left(\vec{B}\times\vec{r}\right)\vec{p}$
	=	$\frac{1}{2}\frac{e}{mc}\vec{B}.\vec{r}\times\vec{p}$
	=	$\frac{e}{mc}\vec{B}.\vec{L}$ (where $\vec{L} = \vec{r}\times\vec{p}$ is the orbital angular momentum)

$\therefore i\hbar \frac{\partial \psi_A}{\partial t}$	=	$\frac{p^2}{2m} + \frac{e^2}{mc^2} A^2 + \frac{e}{mc} \vec{B} \cdot \vec{L} \frac{e\hbar}{mc} \vec{A} \cdot \vec{B} \vec{\sigma}$
	=	$\frac{p^2}{2m} + \frac{e^2}{mc^2} A^2 + \frac{i\hbar e}{2mc} \vec{A} \cdot \nabla - \frac{e}{mc} \vec{B} \cdot \left(\vec{L} + \hbar \vec{\sigma} \right)$
		$\because \vec{S} = \frac{1}{2} \hbar \vec{\sigma}$
$i\hbar \frac{\partial \psi_A}{\partial t}$	=	$\frac{p^2}{2m} + \frac{e^2}{mc^2} A^2 + \frac{i\hbar e}{2mc} \vec{A} \cdot \nabla - \frac{e}{mc} \vec{B} \cdot \left(\vec{L} + 2\vec{S} \right)$

The last term gives the interaction of the orbital and spin angular momenta with the external applied magnetic field $\vec{B}$.

10.4. LET US SUM UP

This lesson deat with the expression for the spin of the electron and electron spin magnetic moment

10.5. LESSON END ACTIVITIES

Check your progress

1. Obtain an expression for spin of the electron.
2. Derive an expression electron magnetic moment

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LESSON 11

SCATTERING THEORY

11. 1 Aim and Objectives

In this lesson we are going to give an introduction to Scattering problems. First we give some simple definitions for scattering amplitude, scattering cross section. Also we will be presenting the kinematics of scattering process and the relation between the scattering amplitude and scattering cross section.

11.2. INTRODUCTION

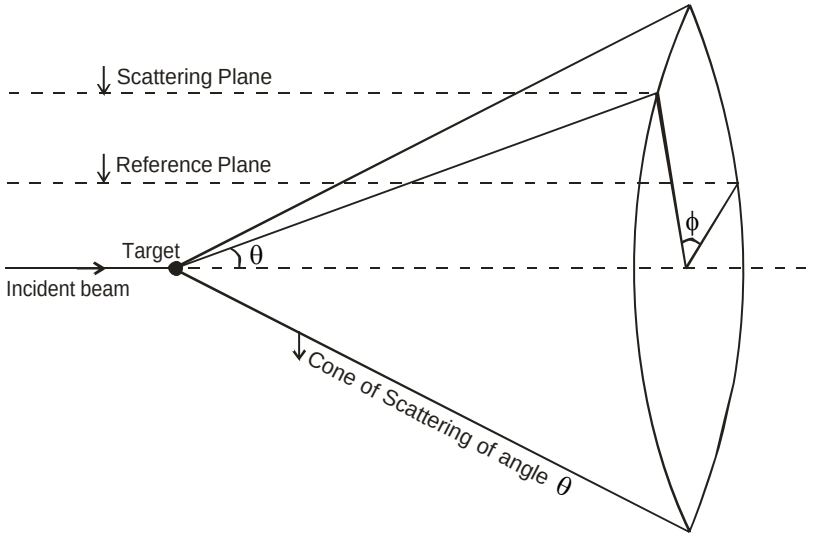
A beam of particles having a definite momentum when directed towards a target (scattering centre) will undergo scattering in all possible directions. At very large distance the scattered beam will be deflected normally outwards in the radial direction. It is usual and convenient in practice to choose a co-ordinate system, in such a way that the scattering centre as the origin and the direction of the incident beam as Z-axis. The polar angles θ and ϕ of the scattered beam which describe the scattering centre or scattering potential is chosen to be spherically symmetric. In other words the spherically symmetric potential will only have θ dependence and independent of ϕ.

11.3. SCATTERING THEORY

When a beam of particles of any kind is directed at matter the particles get deflected from their original path since it collides with particles of matter. The scattering experiments provide useful information about the nature forces, and interaction between the particles of matter. In some collisions, the energy of the incident particle does not change. Such collisions are called elastic collisions or otherwise it is called inelastic collision.

11.4. KINEMATICS OF SCATTERING PROCESS

Consider a parallel beam of particles of a definite momentum is directed towards a target. The particle gets scattered in different directions and finally diverges. At larger distance from the target the particles are subjected to a radically outward motion. Let us choose a co-ordinate system in which the origin is at the position of the target and z-axis as the direction of incident beam. The polar angles θ



and ϕ indicates the direction of scattered particle with z-axis as the polar axis. Here θ is the angle between the incident and scattered direction and is called as the angle of scattering. The azimuthal angle ϕ specifies the orientation of this scattering plane with respect to some reference plane.

11.5. INCIDENT FLUX

Incident flux is defined as the number of particles crossing per unit area per unit time, the area being normal to the incident beam. It is obtained by multiplying the square of incident wave function with velocity.

$$I = |\text{Probability density}| \times \text{Velocity}$$

$$= \frac{\text{No. of particles}}{\text{Volume}} \times \frac{\text{distance}}{\text{time}}$$

$$= \frac{\text{No. of particles}}{\text{Area}} \times \frac{1}{\text{time}}$$

11.6. DIFFERENTIAL SCATTERING CROSS SECTION

If ΔN is the number of particles scattered into a solid angle $d\Omega$ in time Δt, then naturally ΔN will be proportional to the solid angle. The tune and the incident flux.

$$\Delta N \alpha \Omega$$

$$\alpha \Delta t$$

$$\alpha I$$

$$\Delta N = \left(\frac{d\sigma}{d\Omega}\right) \Omega \; t \; \Delta \; I \qquad (1)$$

where the proportionality constant $\frac{d\sigma}{d\Omega}$ is called the differential scattering cross section. Therefore the differential scattering CROSS SECTION. is defined as the Number. of particles scattered per unit solid angle, per unit time, per unit incident flux. It has the dimension of area.

$$\therefore \frac{d\sigma}{d\Omega} = \frac{N}{d\Omega \; t \; \Delta \; I}$$

The total scattering cross section is obtained by integrating the differential cross section over all the polar angles θ and ϕ

$$\sigma = \int_0^{\pi} \int_0^{2\pi} \frac{d\sigma}{d\Omega} \sin\theta \, d\theta \, d\phi$$

For spherically symmetric potential which is independent of ϕ, the total scattering cross section becomes.

$$\sigma = \int_0^{\pi} \frac{d\sigma}{d\Omega} \sin\theta \, d\theta$$

11.7. RELATION BETWEEN DIFFERENTIAL SCATTERING CROSS SECTION AND SCATTERING AMPLITUDE

For a spherically symmetric potential, which falls of rapidly than 1/r asymptotic behaviour, the total wave function will consist of incident plane wave and out going spherical wave.

$$u(\vec{r}, \theta) \rightarrow e^{ikz} + \frac{f(\theta) e^{ikr}}{r} \qquad (1)$$

Where f(θ) is called the scattering amplitude. The incident flux is given by

$$I_{in} = |\psi_{in}|^2 \times v$$

$$= |e^{ikz}|^2 \times v$$

$$= 1 \times v$$

$$= 1 \times v$$

The outgoing flux is given by

$$I_{out} = |\psi_{out}|^2 \times v$$

$$= \frac{|f(\theta)|^2}{r^2} |e^{ikr}|^2 \times v$$

$$= \frac{|f(\theta)|^2}{r^2} \times v$$

$$= \frac{|f(\theta)|^2}{r^2} \times I_{in} \cdot v$$

$\therefore$ the Number of particles scattered in the solid angle dΩ, in time Δt is given by

ΔN = Outgoing flux x solid angle x Area x Time

$$= \frac{|f(\theta)|^2}{r^2} \times I_{inc} \times d\Omega \times r^2 \times \Delta t$$

$$= |f(\theta)|^2 I_{inc} \times d\Omega \times \Delta t \qquad \text{(A)}$$

But we find that the number of particles scattered in a solid angle dΩ,

in time Δt is given by,

$$\Delta N = \frac{d\sigma}{d\Omega} d\Omega \; t \; \Delta \; I \qquad \text{(B)}$$

Comparing equations A & B.

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

Thus we find that the differential cross section is equal to the square of scattering amplitude. Thus the scattering amplitude is related to the experimentally observable differential scattering cross section. Since $\frac{d\sigma}{d\Omega}$ has the dimension of area (m^2), f(θ) has the dimension of length (m).

11.8 LESSON END ACTIVITIES

Check your progress

1. What do you meant by incident flux?
2. Give the importance of scattering theory.
3. Define differential scattering cross section and total cross section. What is the unit in which they are measured?
4. Give the schematic diagram of the scattering event.
5. What do you meant scattering cross section?
6. Obtain the relations between scattering cross section and scattering amplitude.

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LESSON 12

SCATTERING THEORY

12.1 Aims and Objectives

In this lesson, we are going to study the various methods for analyzing scattering problems namely partial wave analysis , phase shift analysis and Born approximations. The above methods can be applied to low energy and high energy scattering problem respectively.

12.2 . PARTIAL WAVE ANALYSIS

12.2.1. INTRODUCTION

The method of partial wave is elegant procedure for the analysis of elastic scattering and low energy scattering. It is done in two steps. First wave function u(r, θ) which represents the sum of incident and scattered wave is obtained in terms of partial waves. Secondly the asymptotic value of this wave function is equated to the wave function u(r, θ) given by

$$u(\vec{r},\theta) = e^{ikz} + \frac{f(\theta)e^{ikr}}{r} \qquad (1)$$

A plane wave e^{ikz} can be expanded as a linear combination of spherical waves using Rayleigh's scattering formula.

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta) \qquad (2)$$

Here $j_l(kr)$ is a spherical Bessel function of order l. $P_\ell(\cos\theta)$ are the legendre polynomials. Each term on the R.H.S. represents a spherical wave. The plane wave is thus equivalent to a superposition of an infinite Number. of spherical waves & the individual waves are called the partial waves. The waves with $l = 0, 1, 2, 3$ are respectively called the s.wave, p-wave, d-wave and so on.

Substituting the value of $j_l(kr)$

$$j_l(Kr) = \frac{\sin(Kr - l\pi/2)}{Kr} = \frac{e^{i(Kr - l\pi/2)} - e^{-i(Kr - l\pi/2)}}{2iKr}$$

Substituting in equation (2)

$$e^{ikz} = \frac{1}{2ikr}\sum_{l=0}^{\infty}(2l+1)\left[e^{i(kr - l\pi/2)} - e^{-i(kr - l\pi/2)}\right]P_l(\cos\theta)$$

This form shows that each partial wave can be represented as the sum of incoming and outgoing spherical wave. Partial wave methods can be applied when the potential is central and of finite range. This method is really useful whenever the energy of the incident particle is low. Here the incident beam of particles are represented by a plane wave with definite linear momentum with no definite angular momentum. Hence a plane wave can be decomposed into infinite number. of components each of which corresponds to definite angular momentum (i.e) into partial waves. The process by which a plane wave is decomposed into a partial wave is called the partial wave analysis.

For a spherically symmetric potential having asymptotic behaviour, the total wave function will consist of the incident plane wave and the outgoing spherical wave.

$$u(r,\theta) = e^{ikz} + \frac{f(\theta)e^{ikr}}{r} \qquad (3)$$

Which is independent of φ. Using Rayleigh's expansion for plane wave

$$e^{ikz} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(Kr)P_l(\cos\theta) \qquad (4)$$

Where $j_l(Kr)$ is spherical Bessel function and $P_l(\cos\theta)$ is the legendre polynomial.

But $$j_l(Kr) = \frac{\sin(Kr - l\pi/2)}{Kr}$$

Expressing in terms of exponential.

$$j_l(Kr) = \frac{e^{i(Kr - l\pi/2)} - e^{-i(Kr - l\pi/2)}}{2iKr} \qquad (3)$$

$$u(r,\theta) = \sum_{l=0}^{\infty}\frac{i^l(2l+1)}{2ik}\left(e^{i(Kr - l\pi/2)} - e^{-i(Kr - l\pi/2)}\right)P_l(\cos\theta) + f(\theta)\frac{e^{ikr}}{r} \qquad (4)$$

The Schrödinger equation for the scattering problem can be written as

$$\left[\nabla^2 - \frac{2\mu}{\hbar^2}(E - V(r,\theta))\right] = 0$$

The Schrödinger equation can be separated into radial part and angular part. The angular part of the solution will be spherical harmonics., $Y_{lm}(\theta,\varphi)$ which will crumble to the legendre polynomial $P_\ell(\cos\theta)$ for spherically symmetric potential which is independent of φ.

The radial part of the solution $R_l(r)$ will involve spherical Bessel function and spherical Neumann function in the field free case. Therefore the total wave function can be written as

$$u(r,\theta) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos\theta) \qquad (5)$$

The solution of the radial Schrödinger wave equation

$$\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + K^2 - \frac{l(l+1)}{r^2} - U(r)\right] R_l(r) = 0$$

Where $K^2 = \frac{2\mu E}{\hbar^2}$, $U(r) = \frac{2\mu V}{\hbar^2}$ ——

The solution of the above equation (i.e) the radial wave function will be a linear combination of $j_l(Kr)$ and $\eta_l(Kr)$

Where $\eta_l(Kr) = \frac{-\cos(Kr - l\pi/2)}{Kr}$

However it should be noted that $j_l(Kr)$ is a well behaved function at r=0 where $\eta_l(Kr)$ is not so, since it becomes infinite at r=0. Therefore we choose the radial wave function as $R_\ell(r)$ proportional to

$$R_l(r) \propto \cos\delta_l j_l(Kr) - \sin\delta_l \eta_l(Kr)$$

In this expression if we choose $\delta_\ell = 0$ for the field free case, then at origin, only $j_l(Kr)$ will remain. At all other points both $j_l(Kr)$ and $\eta_\ell(kr)$ will be present. This is the reason why we associate $\cos\delta_\ell$ with $j_l(Kr)$ and $\sin\delta_\ell$ with $\eta_\ell(kr)$ Rewriting the above equation as

$$R_l(r) = [A_l \cos\delta_l j_l(Kr) - \sin\delta_l \eta_l(Kr)]$$

Substituting the value of $R_\ell(r)$ in equation (5) we get

$$U(r,\theta) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos\theta)$$

$$= \sum_{l=0}^{\infty} A_l [\cos\delta_l j_l(Kr) - \sin\delta_l \eta_l(Kr)] P_l(\cos\theta)$$

$$= \sum_{l=0}^{\infty} A_l \cos\delta \left[\sin(Kr - l\pi/2) + \frac{2}{K} P_l \sin\delta \, i^l e^{i(Kr - l\pi/2)} \right] P_l(\cos\theta)$$

$$= \sum_{l=0}^{\infty} \frac{1}{K} A_l \left[\cos\delta_l \sin(Kr - l\pi/2) + \sin\delta_l \cos(Kr - l\pi/2) \right] P_l(\cos\theta)$$

$$= \frac{1}{K} \sum_{l=0}^{\infty} A_l \sin(Kr - l\pi/2 + \delta_l) P_l(\cos\theta)$$

$$= \frac{1}{2iK} \sum_{l=0}^{\infty} A_l \left[e^{i(Kr - l\pi/2 + \delta_l)} - e^{-i(Kr - l\pi/2 + \delta_l)} \right] P_l(\cos\theta) \qquad (6)$$

12.2.2. SCATTERING AMPLITUDE

Comparing the co-efficient of e^{-ikr}, in equations (4) & (6), we get

$$\frac{1}{2i} \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) \frac{e^{-i(\pi/2)}}{r} = \frac{1}{2iK} \sum_{l=0}^{\infty} A_l e^{i\delta_l} P_l(\cos\theta)$$

The above equation is valid for all values of θ. Using orthogonal property of lengendre polynomial, we can easily show that $A_l = i^l (2l+1) e^{i\delta_l}$ Comparing the co-efficients of e^{ikr} in equations (4) & (6), we get

$$\frac{1}{2i} \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) \frac{e^{i(\pi/2)}}{r} + \frac{f(\theta)}{r} e^{ikr} = \frac{1}{2iK} \sum_{l=0}^{\infty} A_l e^{-i\pi l/2} e^{i\delta_l} P_l(\cos\theta)$$

Substituting the value of A_l

$$\frac{1}{2i} \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) \frac{e^{-i(\pi/2)}}{r} + \frac{f(\theta)}{r} e^{ikr} = \frac{1}{2ik} \sum_{l=0}^{\infty} i^l (2l+1) e^{i\delta_l} e^{-i\pi/2} P_l(\cos\theta)$$

$$\Rightarrow \frac{1}{2i} \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) e^{-i\pi/2} e^{ikr} + f(\theta) e^{ikr} = \frac{1}{2ik} \sum_{l=0}^{\infty} i^l (2l+1) e^{-i\pi/2} e^{2i\delta_l} P_l(\cos\theta)$$

$$\Rightarrow f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} i^l (2l+1) e^{-i\pi/2} e^{2i\delta_l} P_l(\cos\theta) - \frac{1}{2ik} \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) e^{-i\pi/2}$$

$$= \frac{1}{2ik} \sum_{l=0}^{\infty} i^l (2l+1) e^{-i\pi/2} P_l(\cos\theta) \left[e^{2i\delta_l} - 1 \right]$$

Substituting $i^l = e^{il\pi/2}$, $e^{2i\delta_l} - 1 = e^{i\delta_l} \left[e^{i\delta_l} - e^{-i\delta_l} \right]$

$$= e^{i\delta_l} \left[e^{i\delta_l} - e^{-i\delta_l} \right]$$

$$= e^{i\delta_l} \cdot 2i \sin\delta_l$$

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} e^{il\pi/2} e^{-il\pi/2} (2l+1) P_l(\cos\theta) 2i e^{i\delta_l} \sin\delta_l$$

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) e^{i\delta_l} \sin\delta_l \qquad (7)$$

12.2.3. Scattering Cross Section in Terms Of Phase Shift

The differential scattering cross section is defined as

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

$$= \frac{1}{K^2}\sum_{l'l}(2l+1)(2l'+1)e^{i(\delta_l+\delta_{l'})}\sin\delta_l \sin\delta_{l'} P_l(\cos\theta)P_{l'}(\cos\theta)$$

Total Scattering Cross Section

$$\sigma = 2\pi\int_0^{\pi}\frac{d\sigma}{d\Omega}\sin\theta\, d\theta$$

$$\sigma = \frac{2\pi}{k^2}\sum_{l'l}(2l+1)(2l'+1)e^{i(\delta_l+\delta_{l'})}\sin\delta_l \sin\delta_{l'}\int_0^{\pi} P_l(\cos\theta)P_{l'}(\cos\theta)\sin\theta\, d\theta$$

$$\sigma = \frac{2\pi}{k^2}\sum_{l'l}(2l+1)(2l'+1)e^{i(\delta_l+\delta_{l'})}\sin\delta_l \sin\delta_{l'}\frac{2}{2l+1}\delta_{ll'}$$

{by orthogonal property of legendre polynomial $\delta_{l,l'}=1 \text{ if } l=l'$ & $\delta_{l,l'}=0 \text{ if } l\neq l'$}

$$\sigma = \frac{2\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)^2\sin^2\delta_l\frac{2}{2l+1}$$

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \qquad (8)$$

This is the expression for total scattering Cross Section.

12.3. OPTICAL THEOREM

We know that the scattering amplitude is given by

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)P_l\cos\theta\, e^{i\delta_l}\sin\delta_l$$

At $\theta = 0$, $\cos\theta = 1$ and $P_l(1) = 1$ for all values of l.

$$f(0) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l$$

Equating the imaginary part of the scattering amplitude

$$\text{Im } f(0) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \qquad (1)$$

We know the total scattering cross section is given by

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$

$$= \frac{4\pi}{k}\cdot\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \qquad (2)$$

From (1) and (2)

$$\sigma = \frac{4\pi}{k}\,\mathrm{Im}f(0)$$

Thus we find that the total scattering cross section is $\frac{4\pi}{k}$ times the imaginary part of scattering amplitude for $\theta = 0$. In other words the imaginary part of forward scattering amplitude measures the intensity which the incident beam suffers because of scattering.

12.4. PHASFSHIFT ANALYSIS

12.4.1 PHASESHIFT

The effect of introducing the potential into the picture is just to change the phase angle of the normally outgoing scattered wave by an angle δ_ℓ. We have just seen that the radial wave function in the absence of potential is proportional to

$$j_\ell(Kr) = \frac{\sin(Kr - \ell\pi/2)}{kr}$$

Where as in the presence of potential it is proportional to

$$j_\ell(Kr) = \frac{\sin(Kr - \ell\pi/2 + \delta)}{kr}$$

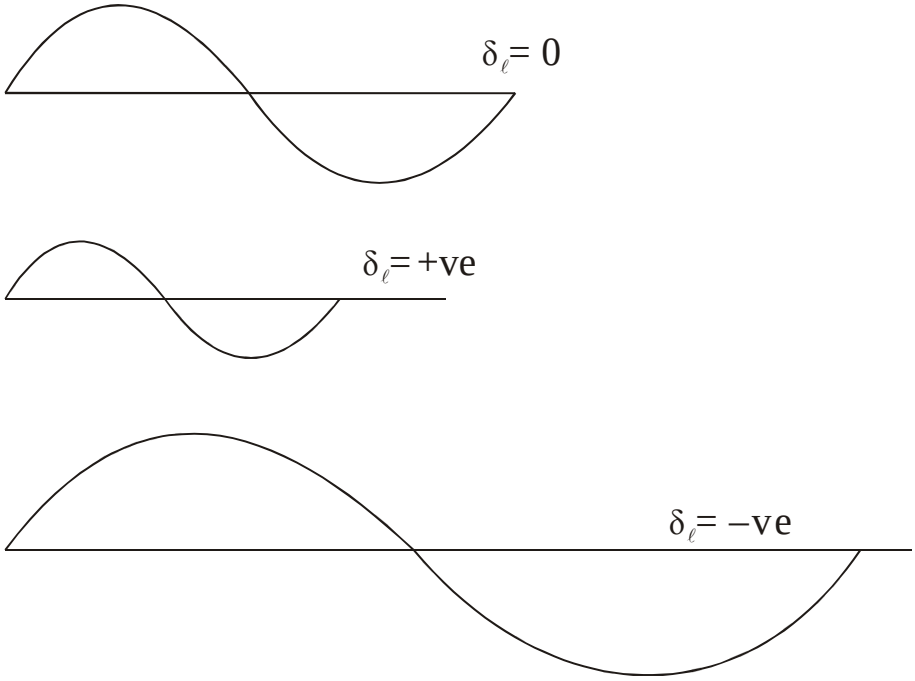
Now in the expression for local wave number the radial Schrödinger's wave equation

$$\frac{d^2}{dr^2} + \left[k^2 - \frac{2\mu}{\hbar^2}(u - u_2) - \frac{l(l+1)}{r^2}\right]r = 0$$

We find that for an attracting potential u(r) is negative and have k^2 + u(r) increases or the wavelength decreases.

For an attractive potential the waves are pulled in and for a repulsive potential u(r) is positive and the wavelength of the scattered wave increases and a repulsive potential the waves are pushed out.

It is to be noted that a phase shift will be introduced only with in the potential of will be maintained through out.



RESULTS : -

(i) The green function for the operator

$(\nabla^2 + k^2)$ is given by

$$(\nabla^2 + k^2)\, G(\vec{r} - \vec{r}') = \delta(\vec{r} - \vec{r}')$$

(ii) $(\nabla^2 + k^2)\, e^{ik\cdot r} = 0$

(iii) $$G(\vec{r} - \vec{r}') = \frac{-1}{4\pi} \frac{e^{i(k - k')\cdot \vec{r}}}{\vec{r}}$$

12.5. BORN APPROXIMATION

This method is most useful for those problems whose potential are varying rapidly. It is also used for analysing the high energy scattering problems. The Schrödinger equation for the scattering problem is given by

$$\nabla^2 u(r) + \frac{2\mu}{\hbar^2}(E - V(r))\, U(r) = 0$$

letting $\frac{2\mu E}{\hbar^2} = k^2 \quad \frac{2\mu}{\hbar^2} V(r) \quad U(r)$

$$\nabla^2 u(r) + k^2 u(r) = U(r)\, u(r)$$

$$(\nabla^2 + k^2)\, u(r) = U(r)\, u(r) \qquad (1)$$

Noting that $(\nabla^2 + k^2)\, e^{ik\cdot r}$ is zero, we can write the solution for Schrödinger equation as

$$U(r) = e^{ik\cdot r} + \int G(\vec{r} - \vec{r}')\, U(r')\, u(r')\, d\tau' \qquad (2)$$

This can be easily verified by operating $(\nabla^2 + k^2)$ on both the sides of equation (2)

$$(\nabla^2 + k^2)\, u(r) = (\nabla^2 + k^2)\, e^{ik\cdot r} + \int (\nabla^2 + k^2)\, G(\vec{r} - \vec{r}')\, U(r')\, u(r')\, d\tau'$$

$$(\nabla^2 + k^2)\, u(r) = U(r)\, u(r)$$

Thus we find that the expression for u(r) given by equation (2) is valid.

Now denoting $u_o(r) = e^{ik\cdot r}$, we have

$$u(r) = u_o(r) + \int G(\vec{r}' - \vec{r})\, U(r')\, u(r')\, d\tau' \qquad (3)$$

Here we find that right hand side contains $u(r')$ (i.e.) a function of u which we are seeking to determine. Now by replacing r by r', r' by r'', we get.

$$u(\vec{r}') = u_o(\vec{r}') + \int G(\vec{r}'' - \vec{r}')\, U(r'')\, u(r'')\, d\tau'' \qquad (4)$$

Substituting (4) in equation (2)

$$u(\vec{r}) = u_o(\vec{r}) + \int G(\vec{r}' - \vec{r})\, U(r')\, u(r')\, d\tau' + \int G(\vec{r}' - \vec{r})\, U(\vec{r}')\, G(\vec{r}' - \vec{r}')\, U(r'')\, u(r'')\, d\tau''\, d\tau'$$

The above series can be extended further by replacing r' by r'' by r''' & so on.

Equation (4) becomes

$$u(r'') = u_o(r'') + \int G(r''' - r'')\, U(r''')\, u(r''')\, d\tau'''$$

Equation (3) becomes

$$u(r) = u_o(r) + \int G(\vec{r}' - \vec{r})\, U(r')\, u(r')\, d\tau' + \int G(\vec{r}' - \vec{r})\, U(\vec{r}')\, G(\vec{r}' - \vec{r}')\, U(r'')\, u(r'')\, d\tau''\, d\tau'$$

$$+ \int \int G(\vec{r}' - \vec{r})\, U(\vec{r}')\, G(\vec{r}' - \vec{r}'')\, U(r'')\, G(\vec{r}'' - \vec{r}''')\, U(r''')\, u(r''')\, d\tau'''\, d\tau''\, d\tau'$$

Such a series is called Born series or Neumann's series. This expression is evidently a perturbation expansion of U(r) with the potential treated as perturbation. If the incident energy is very large, then the series will be converging rapidly. In such a case, only the first few terms will contribute and it will be sufficient to terminate the series after two or three terms. Thus for first Born approximation, we will have two terms.

Therefore in the first Born approximation the wave function will be.

$$u(\vec{r}) = u_0(\vec{r}) + \int G(\vec{r} - \vec{r}_0)\, U(\vec{r}')\, u(\vec{r}')\, d\vec{r}'$$

Substituting for the Green's function and for $u_o(\vec{r})$ we have,

$$u(\vec{r}) = e^{ikz} + \left(\frac{-1}{4\pi}\right)\int \frac{e^{i\vec{k}\cdot\vec{r}'}}{\vec{r}}\, U(\vec{r}')\, u(\vec{r}')\, d\vec{r}'$$

$$= e^{ikz} + \frac{1}{4\pi}\int \frac{e^{i(k-k_0)\cdot\vec{r}}}{\vec{r}}\, u(\vec{r}')\, U(\vec{r}')\, d\vec{r}'$$

Comparing the above expression with total wave function

$$U(\theta) = e^{ikz} + \frac{f_B(\theta)\, e^{ikr}}{\vec{r}}$$

$$f_B(\theta, \phi) = \frac{-1}{4\pi}\int e^{-i\vec{k}\cdot\vec{r}'}\, u(\vec{r}')\, U(\vec{r}')\, d\vec{r}'$$

Dropping the primes, we get

$$f_B(\theta, \phi) = \frac{-1}{4\pi}\int e^{-i\vec{k}\cdot\vec{r}}\, u(\vec{r})\, U(\vec{r})\, d\vec{r}$$

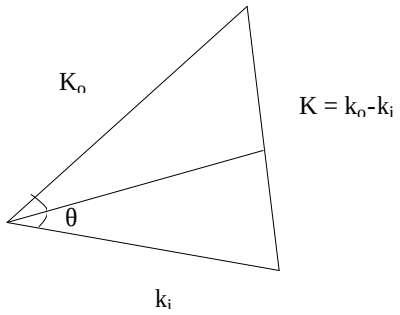
Assuming u(r) = e^{ikz}, the above equation becomes.

$$f_B(\theta, \phi) = \frac{-1}{4\pi}\int e^{-i(\vec{K}_0 - \vec{K})\cdot\vec{r}}\, U(\vec{r})\, d\vec{r}$$

Defining $\vec{K}_o - \vec{K} = \vec{K}$ the momentum transfer function.

$$f_B(\theta, \phi) = \frac{-1}{4\pi}\int e^{i\vec{K}\cdot\vec{r}}\, U(\vec{r})\, d\vec{r} \qquad (7)$$

The directions of $K_o - K_i$ are shown below



From equation (7), it is clear that for the first amplitude depends only on the momentum transfer and not on the initial and final momenta and the angle of scattering. For a spherically symmetric potential, the potential will be independent of angle ϕ and therefore.

$$f_B(\theta) = \frac{-1}{4\pi}\int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} e^{-ikr\cos\theta}\, U(r)\, r^2 \sin\theta\, dr\, d\theta\, d\phi$$

$$= \frac{-1}{2}\int_0^{\infty}\int_0^{\pi} e^{ikr\cos\theta} U(r)\, r^2 \sin\theta \, d\theta \, dr$$

$$= \frac{-1}{2}\int_0^{\infty} r^2 U(r)\, dr \int_0^{\pi} e^{ikr\cos\theta} \sin\theta \, d\theta$$

$$= \frac{-1}{2}\int_0^{\infty} r^2 U(r)\, dr \left[\frac{e^{ikr\cos\theta}}{ikr}\right]_0^{\pi}$$

$$= \frac{-1}{2}\int_0^{\infty} r^2 U(r)\, dr \left[\frac{e^{ikr} - e^{-ikr}}{ikr}\right]$$

$$f_B(\theta) = \frac{-1}{k}\int_0^{\infty} U(r) \sin kr \, dr \qquad \text{since } \sin kr = \frac{e^{ikr} - e^{-ikr}}{2i}$$

This is the Borrn amplitude for the spherically symmetric potential.

12.5.1 Validity Condition For Born Approximation

Born approximation is valid only when the total wave function is greatly different from the incident wave function.

Let $g(r) = |e^{ikz}|^2$

$$g(r)^2 < | <$$

Where g(r) is given by

$$g(r) = \frac{-1}{4\pi}\int \frac{e^{ik(r-r')}}{|r-r'|} U(r')\, e^{ikz}\, dr$$

Substituting the value of U(r), we get

$$g(r) = \frac{-1}{4\pi}\int \frac{e^{ik(r-r')}}{|r-r'|} V(r') \frac{2\mu}{\hbar^2} e^{ikz}\, dr$$

$$= \frac{-1}{2\pi}\int \frac{e^{ik(r-r')}}{|r-r'|} \frac{\mu}{\hbar^2} V(r')\, e^{ikz}\, dr$$

In several cases $|g(r)|^2 \ll 1$ the origin

$$g(r) = \frac{-\mu}{2\pi\hbar^2}\int \frac{e^{ikr'}}{r'} e^{ikz'}\, dr'$$

Dropping the primes.

$$g(r) = \frac{-\mu}{2\pi\hbar^2}\int \frac{e^{ikr}}{r} e^{ikz}\, dr$$

$$|g(r)|^2 = \left|\frac{\mu}{2\pi\hbar^2}\right| \left|\int \frac{e^{ikr}}{r} e^{ikz}\, dr\right|^2 \ll 1$$

This is the validity condition for Born approximation.

If $V(r)$ is spherically symmetric, we have,

$$|g(\theta)|^2 = \left|\frac{\mu}{2\pi\hbar^2}\right|^2 \left|\int_0^{\infty} r^2 dr \int_{-1}^{1} \frac{e^{ikr}}{r} V(r)\, d(\cos\theta)\, d\phi\right|^2$$

$$|g(\theta)|^2 = \left|\frac{\mu}{4\pi^2\hbar^4}\right|^2 \left|\int_0^{\infty} d\vec{r}\, V(r) \int_{-1}^{1} e^{ikr\cos\theta}\, d(\cos\theta)\, d\phi\right|^2$$

$$= \frac{\mu^2}{\hbar^4}\left|\int_0^{\infty} e^{i\vec{k}\cdot\vec{r}} V(\vec{r})\, d\vec{r} \int_{-1}^{1} e^{ikr\cos\theta}\, d(\cos\theta)\, d\phi\right|^2$$

$$= \frac{\mu^2}{\hbar^4}\left|\int_0^{\infty} e^{i\vec{k}\cdot\vec{r}} V(\vec{r})\, d\vec{r} \left(\frac{e^{ikr\cos\theta}}{ikr}\right)_{-1}^{1}\right|^2$$

$$= \frac{\mu^2}{\hbar^4}\left|\int_0^{\infty} e^{i\vec{k}\cdot\vec{r}} V(\vec{r})\, d\vec{r} \cdot \frac{\left(e^{ikr} - e^{-ikr}\right)}{ikr}\right|^2$$

$$= \frac{\mu^2}{k^2\hbar^4}\left|\int_0^{\infty} (e^{2ikr} - 1) V(r)\, dr\right|^2$$

$$|g(\theta)|^2 = \frac{\mu^2}{k^2\hbar^4}\left|\int_0^{\infty} (e^{2ikr} - 1) V(r)\, dr\right|^2 \qquad (1)$$

according to Born approxination.

12.6 LET US SUM UP

From this lesson one can get a clear idea on partial wave analysis , phase shift analysis and Born approximation. Also the optical theorem was presented. Once this theory are understand clearly one can extend this methods to scattering problems in atomic and nuclear physics.

12.7. LESSON END ACTIVITIES

Check your progress

1. What is called a partial wave ? Why it is called so.
2. Define the term phase shift.
3. What is called Born series.
4. Write a brief note on optical theorem.
5. Enumerate the two conditions for the validity of born approximation.

6. Obtain an expression for the Born approximation amplitude and hence derive the Rutherford formula for Coulomb scattering.
7. What do you meant by partial wave analysis? Employ this method to derive an expression for the scattering amplitude in terms of phase shift.
8. What are called Green function? How they are used in scattering theory?
9. Define phase shift and hence describe partial wave analysis in scattering theory.

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LESSON 13

APPLICATIONS OF SCATTERING THEORY

13.1 Aims and Objectives

In this lesson, we are going to discuss in the scattering by different potentials namely Coulomb , Yukawa potential. Also we will be concentrating on central field approximation methods, Thomas – Fermi Statistical Model and Hartree's Self – Consistent Fields.

13.2. Scattering By Coulomb Potential

The potential given as

$$V(r) = -\frac{ze^2}{r} \tag{1}$$

The Born Amplitude is given by

$$f(\theta) = -\frac{1}{k}\int_0^\infty r\, U(r) \sin kr \; dr$$

$$= \frac{2\mu}{\hbar^2 k} ze^2 \int_0^\infty \frac{\sin kr}{r} dr$$

$$= \frac{2\mu ze^2}{\hbar^2 k} \cdot \frac{1}{k}$$

$$= \frac{2\mu ze^2}{\hbar^2 k^2} \cdot \tag{2}$$

We know that momentum transfer $k = 2k \sin\frac{\theta}{2}$

$$\therefore f(\theta) = \frac{2\mu ze^2}{\hbar^2 4k^2 \sin^2\frac{\theta}{2}} = \frac{\mu ze^2}{2\hbar^2 k^2 \sin^2\frac{\theta}{2}} \tag{3}$$

Differential scattering cross section is given by

$$\frac{d\sigma}{d\Omega} = \left| f_k(\Omega) \right|^2 = \frac{\mu^2 z^2 e^4}{4\hbar^4 k^4 \sin^4 \frac{\theta}{2}}$$

$$= \frac{\mu^2 z^2 e^4}{4p^4 \sin^4 \frac{\theta}{2}}, \quad where \quad p = \hbar k \qquad (4)$$

This coincides with the classical Rutherford formula for coulomb scattering.

13.3. Yu kawa Potential

The potential of the form

$$V(r) = V_o \frac{e^{-\alpha r}}{r}$$

where V_o and α are constants is called yukawa potential. It is an example of a central potential. Here the potential depends only r and not on θ, ϕ. It was orginally introduced to represent the interaction between fundamental particles.

The Born amplitude is defined as

$$f_B(\theta, \phi) = \frac{-1}{4\pi} \int e^{-i \vec{k} \cdot \vec{r}} U(r) \, d\tau$$

$$= \frac{-1}{4\pi} \frac{2\mu}{\hbar^2} \int e^{-i \vec{k} \cdot \vec{r}} V(r) \, d\tau$$

$$= \frac{-1}{2\pi} \frac{\mu V_o}{\hbar^2} \int e^{-i \vec{k} \cdot \vec{r}} \frac{e^{-\alpha r}}{r} \, d\tau$$

$$= \frac{-1}{2\pi} \frac{\mu V_o}{\hbar^2} \int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} e^{-ikr\cos\theta} \frac{e^{-\alpha r}}{r} r^2 \sin\theta \, d\theta \, d\phi \, dr$$

$$= \frac{-1}{2\pi} \frac{\mu V_o}{\hbar^2} 2\pi \int_0^{\infty} e^{-\alpha r} \int_0^{\pi} e^{-ikr\cos\theta} \sin\theta \, d\theta \, dr$$

$$= \left| \left(\frac{\mu V_o}{\hbar^2} \right) \int_0^{\infty} e^{-\alpha r} \frac{e^{-ikr\cos\theta}}{-ikr} \, dr \right|_0^{\pi}$$

$$= \left(\frac{\mu V_o}{\hbar^2} \right) \int_0^{\infty} e^{-\alpha r} \frac{e^{ikr} - e^{-ikr}}{ikr} \, dr$$

$$= \left(\frac{-2\mu V_o}{\hbar^2 k} \right) \int_0^{\infty} e^{-\alpha r} \sin kr \, dr$$

Evaluating the integral and simplifying, the scattering amplitude becomes

$$= f_B(\theta, \phi) = \left(\frac{2\mu V_0}{\hbar^2} \right) \frac{1}{\alpha^2 + 4k^2 \sin^2 \theta / 2}$$

Here θ is the angle between the incident wave vector $\vec{k}$ and the unit vector $\vec{r}$ in the scattered direction. From the above expression, it is clear that, the scattering amplitude is independent of angle ϕ. This independence is a general result for elastic scattering by a central potential.

The differential scattering cross section can be written as

$$\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2$$

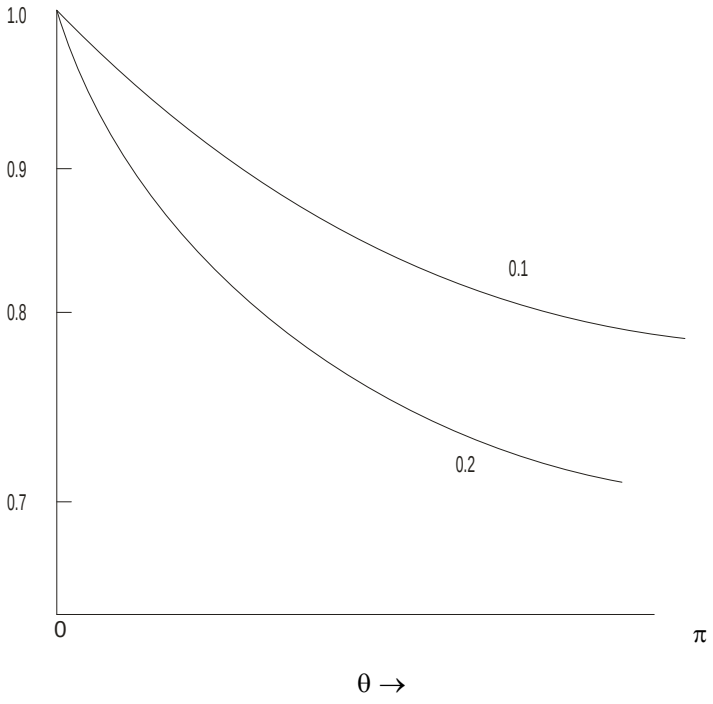
$$= \frac{4\mu^2 V_o^2}{\hbar^4} \frac{1}{(\alpha^2 + 4k^2 \sin^2\theta/2)^2}$$

Thus , we can see that, the differential scattering cross section varies with k and so it also varies with energy E. In the limit of zero energy ($k \to 0$), the differential cross section is

$$\sigma = \frac{4\mu^2 V_o^2}{\hbar^4 \alpha^4}$$

Thus the differential cross section is independent of θ as well as of ϕ. Except at zero energy, σ peaks in the forward direction ($\theta = 0$) and decreases monotonically as θ varies from 0 to π, which is shown is fig. below. It is to be noted that, with in the Born Approx, the differential cross section is independent of sign of Vo and gives the same result if the yukawa potential is attractive ($V_0 < 0$) or repulsive ($V_0 > 0$)

$\left(\sigma / 4\mu^2 V_o^2 \alpha^4 \hbar^4\right) \to$



13.4. Application to Atomic Structure : Central – Field Approximation

The starting point of calculations on all except the lightest atoms is the central – field approximation. This assumes that each of the atomic electrons moves in a spherically, symmetric potential energy V(r) that is produced by the nuclear and all the other electrons. The approximation is a good one if the deviation from the V(r) for one election produced by close passage of other electrons is relatively small. This is actually the case, since the constant nuclear potential is of the order of Z times as large as the fluctuating potential due to each nearby electron, and the latter varies quite slowly (inversely) with the separation distance. The two principal problems are the correction of the approximate results obtained from it. Before considering these problems, we discuss some general properties of the central field.

The potential energy V(r) for a neutral atom has the coulomb form $-c^2/r$ at a great distance r from the nuclear, since the removal of the electron whose potential is being measured leaves a singly charged positive ion. The electron in the hydrogen atom, for which the potential energy is $-c^2/r$ at all r has an infinite number of bound energy levels characterized by the quantum numbers n, l and m. An infinite number of energy levels is also expected for V(r), since for large n the electron wave function is small near the nucleus and only the form of V(r) of large r is significant .An important difference between the two situations is the degeneracy between states of the same n and different L that occurs in hydrogen is removed in a noncoulomb central field. This is because the electrons that have smaller angular momentum penetrate closer to the nucleus, and V(r) is stronger (more negative) than $-c^2/r$ 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, since this occurs whenever the potential is symmetric.

Because of the spin, four quantum numbers n, l, m_e and m_s are required to specify the state of an electron in a central field. The orbital quantum numbers l and m_l are the same as l and m in the hydrogen atom, $m_s = \pm \frac{1}{2}$ specifies the spin orientation and n is a natural generalization of the total quantum number that appears in hydrogen.

The equation $\lambda = n = n' + l + 1$ shows that $n - l - 1$ is the number of nodes of the radial part of the hydrogen wave function; this definition of n is carried over to the general central field, so that l does not exceed n-1.

13.5. THOMAS – FERMI STATISTICAL MODEL

Two – methods have been used for the determination of the potential energy V(r). The first of these Thomas. Fermi statistical model assumes that V(r) varies slowly enough in an electron wavelength so that many electrons can be localized within a volume over which the potential charges by a small fraction of itself. The electrons can then be treated by statistical mechanics and obey the Femi – Dirac statistics. At normal temperatures the thermal energy kT is very small in comparison with V(r) every where except at the edge of atom where the chance of finding an electron is small. In this case, the Fermi – Dirac statistics requires that the electron states fill in order of increasing energy, as assumed.

The number of electron states in a cube if edge length L at the walls of which the wave functions obey periodic boundary conditions was computed to be

$\left(\frac{L}{2\pi}\right)^3 dk_x\, dk_y\, dk_2$. This must be multiplied by 2 to take account of the two possible spin states; then the number of states for which the momentum $P = \hbar k$ is less than or equal to P_0.

$$2\left(\frac{L}{2\pi}\right)^3 d \int_0^{p_0/h} \int_0^{\pi} \int_0^{2\pi} k^2\, dk\, \sin\theta\, d\theta\, d\phi = \frac{P_o^3 L^3}{3\pi^2 h^3}$$

If all these states are occupied, the number of electrons per unit volume whose kinetic energy does not exceed $\frac{P_o^2}{2m}$ is $\frac{P_o^3}{3\pi^2 h^3}$

Now the maximum kinetic energy at any distance r form the nucleus is $-V(r)$, since otherwise the electrons would escape the atom. We thus obtain a relation between the volume density of electrons, n(r) and the pontentialenergy :

$$n(r) = \frac{[-2m\, v(r)]^{3/2}}{-3\pi^2 h^3} \qquad (1)$$

The electrostatic potential – V(r)/e is also determined by poisson's equation. in terms of the charge density – en(r) :

$$-\frac{1}{e}\nabla^2 v = \frac{-1}{er^2}\frac{d}{dr}\left(r^2\frac{dv}{dr}\right) = 4\pi\, en(r) \qquad (2)$$

Equations (1) and (2) and two simultaneous equations for n and r, the boundary condition of the solutions can be expressed in terms of v along for a neutral atom of atomic number z. as r→0, the leading term in the potential energy must be due to the nucleus, so that V(r) → - Ze^2/r. As $r \to \infty$ there must be no net charge inside the sphere for radius r, so that v falls off more rapidly than $\frac{1}{r}$ and rv (r) →0. The boundary condition at ∞ is different from that assumed earlier in this section, where v was taken to have the asymptotic form $–c^2/r$. The v discussed earlier is the potential experienced by one of the atomic electrons, where as the Thomas – Fermi potential is that experienced by an infinitesimal test charge. The diff. between the two potentials emphasizes the statistical nature of the approximation made Thomas and Fermi. The soln. for v is exact in the limit in which m becomes infinite and c becomes zero in such a way that m^3e^4 remains constant then the electron wavelength becomes zero and the density of particle becomes infinite. In this limit the potential is constant over many wavelengths and enough particles are present so that statistical mechanics can be applied

13.5.1. EVALUATION OF THE POTENTIAL

Elimination of n(r) from (1) and (5) leads to an equation. for V(r).

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

we put

$$V(r) = \frac{-z^{\ 2}e}{r}\ \chi \qquad r = b$$

$$b = \frac{1}{2}\left(\frac{3\pi}{4}\right)^{2/3} \frac{\hbar^2}{m^{\ 2}\ ^{1/3}e} \quad \frac{0.8\,8a_0}{z^{\ 1}\ ^3\ z^{/}} \qquad (4)$$

where $a_0 = h^2/me^2$ with the substitutions equation (3) becomes

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

$$\chi = 1 \text{ at } x = 0 \qquad \chi = 0 \quad \text{at } x = \infty \tag{5}$$

The most accurate solution of Equation (5) was computed by Bush and Caldwell with the help of the original differential analyzer and is expressed form of numerical table.

Equation (4) show that the radius of an atom is inversely proportional to the cube root of atomic number, if this radius is interpreted to be that of a sphere that enclose a fixed fraction of all the electrons. These equations can also be used to show that the Thomas – Fermi approximate improves with increasing z. The potential at the atomic radius is proportional to $z^{1/3}$ so that a typical electron wavelength is proportional to $z^{-2/3}$. The distance over which the potential changes by a definite fraction of itself is proportional to the atomic radices or $z^{-1/3}$. Thus the fraction change of the potential in an electron wavelength is proportional to $z^{-1/3}$ and decreases with z. Moreover since the number of electrons is equal to z, the use of the statistical method is better justified s z increases.

13.6. HARTREE'S SELF – CONSISTENT FIELDS

The second method for obtaining a central field is due to Hartree. This model assumes that each electron moves in a central field that can be calculated from the nuclear potential and the wave functions of all the other electrons, by assuming that the charge density associated with an electron is –e times its position probability density. The schrodinger equation is solved for each electron in its own central field, and the resulting wave functions made consistent with the fields from which they are calculated. Thus the k^{th} electron is described by a normalized wave function $u_k(r_k)$ that is a solution of the equation

$$\left[\frac{-h^2}{2m}\nabla_k^2 - \frac{ze^2}{r_k} + \sum_{j\neq k}\int |u_i(r_j)|^2 \frac{e^2}{r_j k} d^3 r_j\right] u_k(r_k) = \in_k u_k(r_k) \tag{1}$$

where $r_{jk} = |r_j - r_k|$. If there are z electrons in the atom, equation (1) constitutes a set of z simultaneous nonlinear integral differential equations for the z functions $u_k(r_k)$. It is therefore not feasible to solve these equations. directly, and Hartree used a method of successive approximation.

A potential energy that approximately represents the second and third terms in (1) is assumed, electron wave fns. Computed and new potentials for each electron found from these wave functions. This process is continued until the potentials are self – consistent to a high order of accuracy. The principal approximation made is the averaging of the potential energy given as the third term in (1) over the angles of r_k to make it spherically symmetric. The solutions of (1) can then be expressed as products of radial functions and spherical harmonies. A further simplification is made so that the 2 (2l +1) or fewer electrons in a shell all move in the same potential and have the same radial wave function.

It is apparent that the Hartree approximation neglects correlations between the positions of the electrons, since the entire wave function for all the electrons is assumed to be a simple product of one electron functions.

$$\psi (r_1, r_2, ..., r_2) = u_1 (r_1)\, u_2 (r_2) ..... u_2 (r_2) \qquad (2)$$

It is also clear from (2) that antisymmetrized wave functions are not employed. The antisymmetry is considered only in so far as the Quantum numbers of the one – electron states u_k are chosen in agreement with the exclusion principle.

13.6.1. CONNECTION WITH THE VARIATION METHOD

We now show that the Hartree approximation results from an optimum variation calculation with the trial function (2). The wave equation with inclusion of interelectronic interactions but neglect of spin – orbit terms is

$$H\psi = E\psi$$

$$H = \sum_k \left(\frac{\hbar}{2m} \nabla^2_k \sum_j \right) \frac{2e^2}{r_k} + \sum_k \sum_j \frac{e^2}{r} \quad — \qquad (3)$$

where j > k implies a double summation over all different pairs of indices j and k we wish to minimize the expectation value of H,

From (2) and (3) we obtain

$$\int ..... \int \psi .. H\psi .. d_1 ... r ... d_2 ... r.$$

$$= \sum_k \int u_k^* \nabla \left(r_k \frac{-\hbar^2}{2m} \right) u_k^2 \left(r \frac{z\, e}{r_k} \right) {}^3 k d) \quad {}_k r$$

$$+ \sum_{j>k} \sum \int u_j^* (r_k) u_k (r \frac{e^2}{r_j} {}^3 \mu) \; r_k (d_k^3) r_j \; d_k \; r \qquad (4)$$

since the u_k are normalized. The optimum ψ is obtained by varying each of the u_k separately to minimize equation (4). The only dependence of equation (4) on a particular one – electron function u_k is through the terms.

$$\int u_k^* \left(\left(\frac{-\hbar^2}{2m} \nabla_k^2 \right) - \frac{z e^2}{r_k} \right) u_k \, d^3 r_k + \sum_{j \neq k} \int u_j^*(r_j) u_k(r_j) \frac{e^2}{r_{jk}} u_j(r_j) u_k(r_k) \, d^3 r_j \, d^3 r_k$$

$$= \int u_k^*(r_k) \, H_k \, u_k(r_k) \, d^3 r_k \qquad (5)$$

$$H_k \equiv \frac{-\hbar^2}{2m} \nabla_k^2 - \frac{z e^2}{r_k} + \sum_{j \neq k} \int |u_j(r_j)|^2 \frac{e^2}{r_{jk}} d^3 r_j$$

The integral in equation (5) is the expectation value of the operation H_k for the function u_k. This is a minimum when u_k is an eigenfunction of H_k that corresponds to its lowest eigenvalue $\in_k$.

$$H_k \, u_k = \in_k u_k \qquad (6)$$

Since equations (1) and (6) are identical, we see that the Hartree wave functions are the best from the point of view of the variation method that can be written in the form of equation (2)

The energy associated with this wave function is just the integral in equation (4) which can be written with the help of equation (1)

$$\int \ldots\ldots\ldots\ldots\ldots \int u^* H \psi \, d^3 r_1 \ldots\ldots\ldots\ldots\ldots d^3 r_2 = \sum_k \in_k$$

$$- \sum_j > \sum_k \int \int |u_j(r_j)|^2 |u_k(r_k)|^2 \frac{e^2}{r_{jk}} \, d^3 r_j \, d^3 r_k$$

The electrostatic interaction terms between electrons are counted twice in the summation over $\in_k$ and so have to be subtracted to give (7). Thus the energy of the atom is not just the sum of the $\in_k$, although each $\in_k$. is roughly the energy of removal of the k^{th} electron. This last is not strictly true, since the removal of an electron alters the self – consistent fields and hence the wave f_r. $\in$'s for the remaining electrons. However, $\in_k$ is found to be an especially good approximation to the energy of removal in the case of an inner electron (x – ray level).

13.7. LET US SUM UP

In this unit we have discuss with the coulomb and the yukawa potentials. Also we have studied Thomas – Fermi Statistical Model, Central – Field Approximation, Hartree's Self – Consistent Fields.

13.8 LESSON END ACTIVITIES

Check your progress

1. What is the range of Coulumb potential?
2. Define yukawa potential.
3. Write down Hartree Fock equation.
4. Discuss in detail the problem of Yukawa potential.
5. Discuss in detail the problem of Coulommb potential. Obtain an expression for scattering cross section.
6. Explain the central field approximation method in detail.
7. Explain in detail Thomas Fermi Statistical model.
8. Discuss Hartree Fock self consistent model.

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LESSON 14

APPLICATION OF SCATTERING THEORY TO ATOMIC AND MOLECULAR STRUCTURES

14.1 AIMS AND OBJECTIVES

In this lesson we are going to study the application scattering theory to atomic and molecular structure physics.

14.2ALKALI ATOMS

The ground state configuration of an alkali atom consists of a series of full shells followed by a single s electron and so is 2S ½ . The inner rare–gas configuration is so stable that all but quite high excited states of the atom involve only the valence electron. Thus the alkalis can be treated to quite good approximation in terms of a model in which a single electron moves in a spherically symmetric noncoulomb potential energy V(r).

14.2.1 DOUBLET SEPARARTION

The configuration of an alkali atom can be specified by a single pair of quantum numbers *nl*. Since there is only one electron, the perturbing electrostatic term ii does not appear. In the absence of external fields the hamiltonian, including the spin orbit energy is

$$H = \frac{-\hbar^2}{2m} \nabla^2 + V(r) + \in(r)\,\vec{L}\cdot\vec{S} \qquad (1)$$

where

$$\in(r) = \frac{1}{2m^2c^2}\,\frac{1}{r}\,\frac{dV}{dr}$$

The total angular momentum J = L+S of the valence electron is a constant of the motion, so that states can be designated by jm instead of m_l m_s, where J^2 = $j(j+1)\hbar^2$ and J_z = $m\hbar$ .The states of different j have different energies, but there is still a (2j +1) fold degeneracy due to m. The removal of the m degeneracy by a magnetic field is discussed later.

The difference in energy between states of different j is due to the L.S term in (1) and can be found from its expectation value or diagonal matrix element.

$$J^2 = L(S + ^2)^2 \quad ^2 + S \quad + \quad 2 \; \vec{L}.\vec{S} \qquad (2)$$

since e, j and s are all good quantum number (s = ½). Equation (2) can be solved for the diagonal matrix element of L.S.

$$\left\langle lL\left|.Sl_j\right|\right\rangle \quad [j \quad (j1) \quad +l \quad (l1)\frac{3}{4} \qquad (3)$$

Now if L is different from o,j can be either L + ½ or L – ½ . Thus the first order perturbation arising from $\in$(r) L.S. is

$$\begin{aligned} &\tfrac{1}{2} l \in_{nl} && if \quad j = l + \frac{1}{2} \\ &\frac{-1}{2}(l+1) \in_{nl} && if \quad j = l - \frac{1}{2} \end{aligned} \qquad (4)$$

$$\in_{nl} = \hbar^2 \int_0^\infty |R_{nl}(r)|^2 \in (r)\, r^2\, dr \qquad l > 0$$

where R_{nl} (r) is the normalized radial part of the unperturbed eigenfunction associated with the *nl* configuration. Since V(r) represents an attractive potential energy, $\in(r)$ is positive and $\in_{nl}$ is positive. Thus equation (4) shows that the state with higher j has the higher energy. The pair of states is called a doublet the doublet structure characterizes all the moderately excited levels of the alkali atoms except those for which *l = 0* in which case j can only be ½.

The doublet separations can be calculated from equation (4) if radial function is known using the generating function for the associated lauguerre polynomials.

l_j

$$\in_{nl} = \frac{\hbar^2 z \; ^2 e}{2m^2 \; ^2 c} \int_0^\infty \frac{1}{r} \; R^2_{n} r(\quad d)$$

$$= \frac{e^2\hbar^2 Z^4}{2m^2c^2 a o^3 n^3 \; l\left(l+\frac{1}{2}\right)(L+1)} \qquad (5)$$

This is valid only for $l > 0$; the singularity in $\in$(r) at r – 0 makes the integral for $\in_{no}$ diverge there, so that the perturbation approximation is not valid. It follows from (4) and (5) that the doublet separation is proportional to n^{-3} and this in fair agreement with observation. The absolute value of the doublet separation and its dependence on *l* are not given at all by this simple theory, since the effective z is difficult to estimate and depends marked by on *l* because of penetration.

14.2.2 . DOUBLET INTENSITY

We now calculate the intensities of the two lines of the allowed doublet $2P\frac{3}{2} \rightarrow 2S\frac{1}{2}$ & $2P\frac{1}{2} \rightarrow 2S\frac{1}{2}$ 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. From the equation.

$$\frac{4e^2k^2w_{kn}}{3\hbar c}\;|<k\,|\,r\,|\,n>|^2 \;=\; \frac{4e^2{w_{kn}}^2}{3\hbar c^3}\;|<k\,|\,r\,|\,n>|^2$$

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 as the angular and spin co-ordinates of the electron is obtained by finding linear combination of products of the four spherical harmonics $y_{1,1}(\theta, \phi)$, $y_{1,0}(\theta, \phi)$, $y_{1,-1}(\theta, \phi)$, $y_{0,0}(\theta, \phi)$ and the two spin wave functions (+) and (-) that are eigenfunctions of J^2 and J_z. These combinations can be obtained from the Clebsch Gordan co-efficient.

$$m = \frac{3}{2} \quad y + \quad (\quad)_{1\ 1}$$

$$= \frac{1}{2} \quad + \quad 3^{\frac{-1}{2}}\left[2^{\frac{1}{-}} \quad (\quad y_{1}) - \quad (\quad y_{1}) \right]_{,\ 1}$$

$$2p_{\frac{3}{2}} = 3\frac{-1}{2^{1}} \quad 2 - y \quad (^{\frac{-1}{2}}{}_{0}\left[\frac{1}{2} + \right)_{1} \quad y(+ \quad)_{1}$$

$$= \frac{-3}{2} \quad - \quad y_{1\ ,\ 1}$$

$$m = \frac{1}{2} \quad - \quad y\ 3^{\frac{-1}{2}}\left[(\quad) + {}^{1}_{1}\ 2_{,\ 0} - (\quad)_{1} \right]_{,\ 1}$$

$$2p_{\frac{1}{2}} = 3\frac{-1}{2^{1}} \quad (- y \quad)^{\frac{-1}{2}}{}_{0}\left[-2 \quad {}_{1}{}^{2}\ y(+ \quad) \right]_{,\ 1} \quad -$$

$$2s_{\frac{1}{2}} \quad = \frac{1}{2}(m \quad +)\ y_{\ 0}$$

$$= \frac{-1}{2} \quad - \quad (\quad)y_{0\ ,\ 0}$$

The wave functions equation (6) can be used to calculate the matrix elements of x = r sinθ cosϕ y = r sinθ sinϕ and z = r cos θ. We assume that the radial functions associated with equation (6) are all the Same, so that the radial part of the matrix element integral is a common factor throughout. The angle parts of the integrals are easily evaluated by making use of the explicit expressions for the y's in terms of θ and ϕ. The products of spin fns, follows the simple rules (+) (+) = 1, (-) (+) = 0 etc., In this way we obtain the following values for the squares of the magnitudes of the indicated matrix elements, expressed in units of $\frac{1}{18}$ of the common radial factor :

$$m \quad = \frac{3}{2} \quad t \quad o\frac{1}{2} \quad - m = \quad | \ x^{2}| \quad + \ y^{2}| \quad 3 \ z^{2}| \quad | \quad 0$$

$$= \frac{3}{2} \quad t = \quad \frac{1}{2}\ o - \quad x \ + | \ {}^{2}|y \ + {}^{2} \ | z \ {}^{2}| = | \quad 0$$

$$2p_{\frac{3}{2}} \quad - 2_{1}\ s_{\ -} \ | \quad + \frac{1}{2}| \quad \frac{1}{2} - o \quad = \quad | \ x \quad {}^{2}0 = y \ {}^{2}| \quad z^{2} + \quad 4$$

$$= \frac{1}{2} \ t \quad \frac{1}{2} - o \quad | \ x \ {}^{2}| = | \ y^{2}| \quad 1 + z^{2} | \quad | \quad 0$$

$$m = \frac{1}{2} \text{ to } m = \frac{1}{2} \qquad |x|^2 = |y|^2 = 0 \quad |z|^2 = 2$$

$$= \frac{1}{2} \text{ to } \frac{-1}{2} \qquad |x|^2 = |y|^2 = 2 \quad |z|^2 = 0$$

Similar results are obtained for the transitions that start form m = $\frac{-1}{2}$ and $\frac{-3}{2}$.

It follows from equation (7) that the sum of the intensities of all the lines that originate on each of the four $2P_{3/2}$ states is equal to 6, in the above units. It is expected that these sums are equal since the four values of m differ only in the orientation of the angular momentum, and this should not affect the intensity. However the total intensity form each of the two $2P_{1/2}$ states is also equal to 6. The equality of total intensities from each state formed form a given L and S is a general property of LS coupling; this makes the absolved intensity, which is that from all the states that are degenerate with respect to m, proportional to 2J+1. In the example considered here, the two lines for the doublet have intensities in the ratio 2:1. This is observed for the lowest doublets of the alkalis, although for the higher doublets the intensity ratio exceeds 2. This is because the spin – orbit energy actually mixes different configurations (2p states with same j but different n) ; the amount of mixing is different for the two j values, so that the two radial functions are not the same. A small admixture of the low-intensity upper states in the high – intensity lowest 2p states has little effect, whereas in the opposite case there is a large effect on the doublet intensity ratio.

14.3. Application to Molecular Structure: Hydrogen Molecule

It is clear that two distinct problems arise in connection with molecular structure. The first is the solution of Schrödinger equation to obtain electronic wave functions and a potential energy function of the nuclear coordinates. The second is the solution of nuclear motion. The first problem can be solved only in the simplest cases. As an example, we now consider in outline an approximate solution for the hydrogen molecule due to Hietler and London.

14.3.1 .Heitler and London Method

The only nuclear coordinate R_j that appears in the equation

$$\left(-\frac{\hbar^2}{2m}\sum_{i=1}^{n}\nabla_i^2 + V_R\right) u_j(r)U_j(R) = u_j(r)$$ (1)

in the case of the hydrogen molecule in the magnitude R of the distance between the two hydrogen nuclei. The Hamiltonian is that given in equation

$$H = H_0 + H'$$
$$H_0 = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{r_1} - \frac{e^2}{r_2}$$ (2)
$$H' = \frac{e^2}{R} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{B1}} - \frac{e^2}{r_{A2}}$$

however, R is no longer large in comparison with $a_0 = \hbar^2/me^2$ so that the approximations implied in equation (2) are no longer useful. Nevertheless, an approximate wave function based on a simple product of two ground – state hydrogen – atom functions gives remarkably good results. The reason for this is that exchange degeneracy is taken into account; the degenerate wave functions for which electron 1 is on nucleus A and electron 2 on nucleus B, and for which electron 1 is on nucleus B and electron 2 on nucleus A are both used at once. The new feature of the work of Heitler and London was the recognition that an appropriate linear combination of unperturbed degenerate wave functions gives a significantly lower energy than the separate wave functions; it is the basis of the present – day theory of homopolar binding in molecules. This property of degeneracy is sometimes referred to as resonance. An analogous situation is that in which an interaction between two classical oscillators that are in resonance (same unperturbed frequency) gives rise to a normal mode that has a lower frequency (and also one that has a higher frequency). In a similar way, an interaction between two resonant (degenerate) state in quantum mechanics gives rise to a lower energy eigenvalue (as well as to a higher one). There may of course be more than two degenerate unperturbed states, and the degeneracy need not be of the exchange type.

14.3.2. Spin Orbit Interaction as Correction to Central field Approximation

The correction of the approximate results obtained from the central field. Two terms are omitted in the central – field approximation: the difference between the actual electrostatic interaction between electrons and the average interaction that is included in the central field, and the spin – orbit energy. The latte is an interaction energy between the spin and the orbital motion of each electron and has the form

$$\sum_k \xi(r_k)\,\bar{L}_k \cdot \bar{S} \qquad (1)$$

here, $\bar{L}_k$ is the orbital angular momentum operator $\bar{r}_k \times \vec{p}_k$ of the kth electron and has the properties of the $\bar{J}$ operator. The eigenvalues of $\bar{L}_k^2$ and L_{kz} are given in terms of the quantum numbers l and m_l for the electron as $l(l+1)\hbar^2$ and $m_l\hbar$, respectively. $\vec{S}_k$ is the spin angular momentum $\frac{1}{2}\hbar\sigma_k$ of the kth electron. The function $\xi(r)$ is given by

$$\xi(r) = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}$$

in terms of central field potential V (r).

In considering the effect of these terms, we shall assume that the perturbed eigenfucntions, which are linear combinations of various configuration wave functions, have only negligibly small amounts of all but one configuration mixed in them. From perturbation theory it is apparent that this is the case if the inter configuration matrix elements of the perturbation are small in comparison with the energy intervals between unperturbed configuration energies.

It can be shown that from equation (1) that includes electron in full shells is zero, since the function $\xi(r)$ is the same for all electrons in the shell and contributions from electrons with opposite m_l and m_s cancel. Thus the electrons in the full shell can be ignored and the summation extended only over the remaining electrons. The case in which there is just one electron outside the full shells is of interest in connection with the ground state and low excited states of alkali atoms.

14.4. LET US SUM UP

In this lesson we have applied the scattering theory to atomic and molecular structures. Also we discussed the couplings schemes and doublet separation in alkali atoms in detail. We also presented Hydrogen Molecule problem , Heitler and London Method and Spin Orbit Interaction .

14.5. LESSON END ACTIVITIES

Check your progress

1. Briefly explain the coupling schemes.
2. Write down Hartree Fock equation.
3. Explain the term spin orbit interaction.
4. Discuss the hydrogen molecular problem.
5. Explain the Heitler and London method.
6. Discuss the Spin orbit coupling. Explain how it can be treated as a Correction to central field approximation.

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LESSON 15

SEMI CLASSICAL THEORY OF RADIATION AND QUANTUM FIELD THEORY

15.1 Aims and Objectives

In this lesson, we are going to discuss the interaction atoms with radiation field. We are going to discuss spontaneous emission, induced emission , induced absorption. We are going to define the Einstein's coefficients for the above three process. Also we will be deriving an expression for transition probability. Finally we will be presenting short notes on selection rules and forbidden transition.

15.2. Introduction

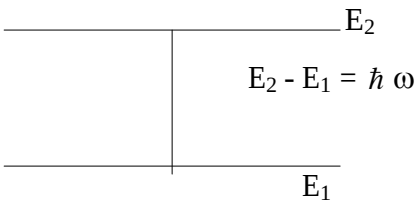
Semi classical theory is a mixture of classical & quantum picture matter i.e. atoms are assumed to exist in discrete states. But the electromagnetic radiation with which it interacts is described classically. The semi classical theory is insufficient to describe the spontaneous emission of radiation because the electromagnetic field described classically.

15.3. Interaction of Atoms with Radiation Field

An atomic system in the absence of external radiation will exist in a stationary states. However in the presence of external radiation there will be both absorption and emission. The atomic system may attain in thermal equilibrium with a external radiation. This may happen in 3 ways namely i) induced absorption ii) spontaneous emission and iii) stimulated or induced emission.

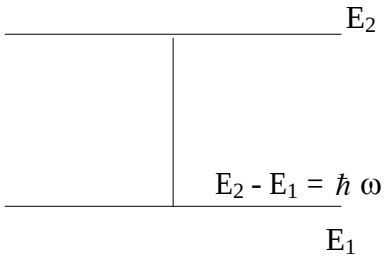
15.4. Induced Absorption

Let us suppose an atom is an low energy state E_1 by absorption of quantum of radiation it is raised to higher state E_2, then we have $E_2 - E_1 = \hbar\omega$,where ω - angular frequency of the photon. This process is known as induced absorption. The probability of occurrence per unit time of this absorption transition E_1 to E_2 depends on the properties of the state E_1 and E_2 and it is proportional to the rate at which the photon fall on the atom and therefore to the spectral energy density.



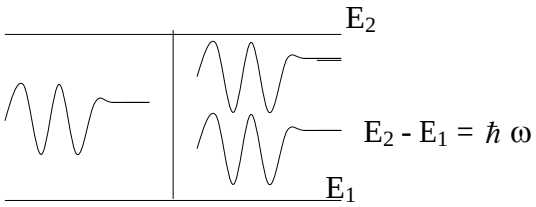
15.5. Spontaneous Emission

Let us suppose that the atom is in the highest state E_2 .Usually the life time of the exited state is very small, so the atom jumps to the lower energy state E_1 and it emits the photon of frequency υ (angular frequency ω) / $E_2 - E_1 = \hbar\,\omega$. This process is known as spontaneous emission. Its probability is determined by the properties of the state E_2 & E_1

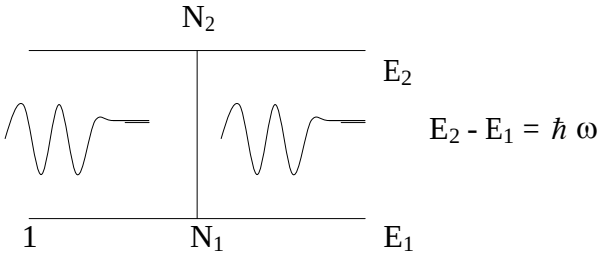


15.6. Simulated or Induced Emission

An atom is an excited energy state E_2 by the influence of electromagnetic field of a photon can come to the lower state $E_1$by emitting an additional photon of same frequency. This is known as stimulated or induced emission and its probability proportional to the properties of the state E_2 & E_1 and to the spectral energy density.



15.7. Einstein's co-efficients for Induced Absorption and Spontaneous Emission, Induced Emission



The above figure represents the two energy states of an atomic system corresponding to the energy E_1 and E_2 . Let N_1 and N_2 be the number of atoms per unit volume in the energy level 1& 2. Atom in the lower energy level can absorb radiation and get excited to the energy level 1 and 2. The excitation process occurs on by in the presence of radiation. Such a process is termed as induced absorption or stimulated absorption. The rate of absorption depend upon the energy density $u(\omega)$ associated with the radiation field corresponding to the frequency.

$$\omega = \frac{E_1 - E_2}{\hbar}$$

The energy density $u(\omega)$ is defined in such a way that $u(\omega)\, d(\omega)$ represent the number of atoms per unit volume with in the interval ω and $\omega + d\omega$. Thus the number of absorption per unit time per unit volume is proportional to $N_1\, u(\omega)$.

$$N_1\, u(\omega) = B_{12}\ N_1\, u(\omega)$$

Where B_{12} – constant of proportionality and it is called Einstein's co-efficient for induced absorption.

On the other hand when an atom, is an excited state, can make transition to the lower energy state through the emission of electromagnetic radiation. However the absorption process, emission process can occur two different ways.

The 1st refers to the spontaneous emission, in which the atom in the excited state emits radiation even in the absence of any incident radiation. It is thus not stimulated by any incident signal but occurs spontaneously. The rate of spontaneous emission is proportional to the number of atoms in the excited state. If we represent the co-efficient of proportionality by A_{21} then $N_2\ A_{21}$ would represents number of spontaneous per unit volume per unit time to the lower energy level.

The 2nd refers to the stimulated emission in which an incident signal of appropriate frequency triggers an atom is an excited state to emit radiation. The rate of transition to the lower energy level is directly proportional to the energy density of the incident radiation at the frequency ω . Thus the number of stimulated emission per unit volume per unit time is given by $N_2\, B_{21}\, u(\omega)$. The quantities $A_{21,}\, B_{12,}\, B_{21}$ are known as Einstein co-efficients and are determined by the atomic system.

15.8. Relation between Einstein Co-efficients

At thermal equilibrium the number of upper ward transition must be equal to the number of downward transition. Hence we may write

$$N_1 B_{12} u(\omega) = N_2 A_{21} + N_2 B_{21} u(\omega)$$

$$[N_1 B_{12} - N_2 B_{21}] u(\omega) = N_2 A_{21}$$

$$u(\omega) = \frac{N_2 A_{21}}{N_1 B_{12} - N_2 B_{21}}$$

$$= \frac{N_2 A_{21}}{N_2 \left[\frac{N_1}{N_2} B_{12} - B_{21} \right]}$$

Or $$u(\omega) = \frac{A_{21}}{\left[\frac{N_1}{N_2} B_{12} - B_{21} \right]} \quad (1)$$

From Boltzmann's law we have the following expression for the ratio of the population of the 2nd level at temperature T

$$\frac{N_1}{N_2} = e^{(E_2 - E_1)/K_B T}$$

$$\frac{N_1}{N_2} = e^{\hbar\omega/K_B T}$$

where K_B – Boltzmann's constant. Equation (1) becomes

$$u(\omega) = \frac{A_{21}}{e^{\hbar\omega/K_B T} B_{12} - B_{21}}$$

For most of the time $B_{12} = B_{21}$

$$u(\omega) = \frac{A_{21}}{B_{21} \left(e^{\hbar\omega/K_B T} - 1 \right)} \quad (2)$$

According Plank's law, the energy density of the radiation is given by

$$u(\omega) = \frac{\hbar\omega^3}{\pi^2 c^3} \cdot \frac{1}{e^{\hbar\omega/K_B T} - 1}$$

Using the above relation equation (2) becomes

$$\frac{\hbar\omega^3}{\pi^2 c^3}\cdot\frac{1}{e^{\hbar\omega/K_B T}-1}=\frac{A_{2\ 1}}{\left(B_{2\ 1}e^{\hbar\omega/K_B T}-1\right)}$$

$$\frac{A_{2\ 1}}{B_{2\ 1}}=\frac{\hbar\omega^3}{\pi^2 c^3}$$

$$A=B\frac{\hbar\omega^3}{\pi^2 c^3}$$

15.9. Expression for Transition Probability

The Hamiltonian of the system consisting of an atom in the presence of the radiation field is given by

$$H=\frac{p^2}{2m}V+\frac{1}{8\pi}\int\left(H^2+E^2\right)d\tau+\frac{p^2}{2m}-\frac{e}{mc}\left(\vec{A}\cdot\vec{p}+\vec{A}\cdot\vec{p}\right)+\frac{e^2}{2mc^2}A^2 \qquad (1)$$

$$H = H_1+H_2+H_{interaction} \qquad (2)$$

Where $H_1 = \frac{P^2}{2m}+V$ for the atom

$H_2 = \frac{1}{8\pi}\int\left(E^2+H^2\right)d\tau$ for the radiation field

$H_{int} = \frac{-e}{2mc}\left(\vec{p}\cdot\vec{A}+\vec{A}\cdot\vec{p}\right)$ the interaction of the Hamiltonian.

$\frac{e^2}{2mc^2}A^2$ can be neglected because the vector potential A is very small.

Now we are going to prove that $\left(\vec{p}\cdot\vec{A}\right)=\left(\vec{A}\cdot\vec{p}\right)$

In general $\left(\vec{p}\cdot\vec{A}\right)\psi=\left(\vec{A}\cdot\vec{p}\right)\psi$

$$\left(\vec{p}\cdot\vec{A}\right)\psi=-i\hbar\left(\vec{\nabla}\cdot\vec{A}\right)\psi$$

$$=-i\hbar\left[\left(\vec{A}\cdot\vec{\nabla}\right)\psi+\vec{A}\left(\vec{\nabla}\cdot\psi\right)\right]$$

For coulomb gauge $\vec{\nabla}\cdot\vec{A}=0$

$$=-i\hbar\left[\left(\vec{A}\cdot\vec{\nabla}\right)\psi\right]$$

$$=\vec{A}\left(-i\hbar\vec{\nabla}\right)\psi$$

$$= \left(\vec{A}.\vec{p}\right)\psi$$

i.e. $\frac{-e}{2m}\left(\vec{p}.\frac{\vec{A}}{c}+\frac{\vec{A}}{c}.\vec{p}\right)+\frac{e^2}{2mc^2}\vec{A}.\vec{A}\left(\vec{p}-\vec{A}\right)$

The interaction of Hamiltonian becomes

$$\Rightarrow \frac{-e}{2m}\left(\frac{2\vec{A}}{c}.\vec{p}\right)+\frac{e^2}{mc^2}\vec{A}.\left(\vec{A}.\vec{p}\right)$$

Now the vector potential $\vec{A}$ can be written as

$$\vec{A} = \hat{e}_0 A_0 \cos(\vec{k}.\vec{r}-\omega t)$$

Where $\hat{e}$ is the unit vector along the direction of propagation which is perpendicular to the vector potential $\vec{A}$.

Now expressing the vector potential in terms of the exponential function

$$\vec{A} = \hat{e}_0 A_0\left[\frac{e^{i(\vec{k}.\vec{r}-\omega t)}+e^{-i(\vec{k}.\vec{r}-\omega t)}}{2}\right]$$

From time dependent perturbation theory the probability amplitude for transition from an initial state $|n\rangle$ to final state $|s\rangle$ is given by

$$c_{sn} = \frac{1}{i\hbar}\int \langle s|V_{int}|n\rangle e^{i\omega_{sn}t}dt$$

where $\omega_{sn} = \frac{E_n - E_s}{\hbar}$

Now,

$$\langle s|V_{int}|n\rangle = \langle s|\vec{A}.\vec{p}|n\rangle$$

$$= \frac{-e}{2mc}\langle s|\vec{A}.\vec{p}|n\rangle$$

$$= \frac{-e}{2mc}\frac{\hat{e}A_0}{2}\langle s|e^{i\vec{k}.\vec{r}}.\vec{p}+e^{-i\vec{k}.\vec{r}}.\vec{p}|n\rangle\left(e^{-i\omega t}+e^{i\omega t}\right)$$

On solving the above equations the transition probability for emission become

$$|c_{sn}| = \frac{e^2}{4m^2}\frac{A_0^2}{\omega^2}\left[\langle p|e^{-i\vec{k}.\vec{r}}|n\rangle\hat{e}\right]^2 \frac{\sin^2\left(\frac{\omega+\omega_{sn}}{2}\right)t}{\left(\frac{\omega+\omega_{sn}}{2}\right)^2}$$

For atomic dimension the value of $e^{i\vec{k}\cdot\vec{r}} \approx 1$. So the transition probability for emission becomes

$$|c_s|_n = \frac{e^2}{4m^2}\frac{A_0^2}{\omega^2}\left[\langle n|\hat{e}\cdot\vec{p}|s\rangle\right]^2 \frac{\sin^2\left(\frac{(\omega+\omega_s)_n}{2}\right)t}{\left(\frac{(\omega+\omega_s)_n}{2}\right)^2}$$

15.10. Electric Dipole Transition

The transition probability for emission is given by

$$|c_s|_n = \frac{e^2}{4m^2}\frac{A_0^2}{\omega^2}\left[\langle p|e^{i\vec{k}\cdot\vec{r}}\hat{e}\cdot\vec{p}|s\rangle\right]^2 \frac{\sin^2\left(\frac{(\omega+\omega_s)_n}{2}\right)t}{\left(\frac{(\omega+\omega_s)_n}{2}\right)^2}$$

If we consider the atomic dimension the atomic radius is very small. So we can expand the exponential form as

$$e^{i\vec{k}\cdot\vec{r}} = 1 + \frac{(i\vec{k}\cdot)\vec{r}}{1!} + \frac{(i\vec{k}\cdot)^2\vec{r}}{2!} + \cdots .$$

The magnitude of the successive term are

$$1 : \frac{2\pi r}{\lambda} : \frac{1}{2}\left(\frac{2\pi r}{\lambda}\right)^2 : \frac{1}{6}\left(\frac{2\pi r}{\lambda}\right)^3$$

The magnitude of the successive term decreases by the factors of $\frac{r}{\lambda}$ but $\frac{r}{\lambda}$ is the order of 10^{-3}cm. So in this case we can approximate $e^{i\vec{k}\cdot\vec{r}} = 1$.

$$|c_s|_n = \frac{e^2}{4m^2}\frac{A_0^2}{\omega^2}\left[\langle n|\hat{e}\cdot\vec{p}|s\rangle\right]^2 \frac{\sin^2\left(\frac{(\omega+\omega_s)_n}{2}\right)t}{\left(\frac{(\omega+\omega_s)_n}{2}\right)^2}$$

Transition for which the probability can be computed using the above approximation is called electric dipole transition. Since only the matrix element of the electric dipole moment $\hat{e}\cdot\vec{p}$ of the particle is involved.

15.11. Forbidden Transition

It may happen that the matrix element $\langle s|\vec{r}|n\rangle$ is zero for particular state between S and n. In that case the approximation $e^{i\vec{k}\cdot\vec{r}}=1$ is not valid. But it should be expanded in the series of spherical harmonics.

$$e^{i\vec{k}\cdot\vec{r}} = j_0(kr) + 3j_1(kr)\cos\theta + 5j_2(kr)\cos\theta + \ldots$$

where θ is the angle between $\vec{k}$ and $\vec{r}$

The dominant factor in the nth term of the above series is proportional to the $(\vec{k}.\vec{r})^n$, if $\vec{k}.\vec{r}$ <<1. Thus if the dipole matrix element vanishes, but the next term of each series does not vanish. The transition matrix element is reduced by a factor that has the magnitude of the order of Ka where the linear dimension of the particle wave function of are of order of a. The transition of this type is called forbidden transition, since a probability is reduced by a factor $(Ka)^2$ with respect to dipole or allowed transition.

15. 12 LET US SUM UP

In this lesson, we have studied the interaction atoms with radiation field. We analysed spontaneous emission, induced emission , induced absorption. We determined the Einstein's coefficients for the above three process. Also we obtained an expression for transition probability. Finally we presented short notes on selection rules and forbidden transition.

15.13 LESSON END ACTIVITIES

Check your progress

1. Define density operator and density matrix.
2. How will you distinguish spontaneous and stimulated emission of radiation.
3. Discuss the interaction of atom with electromagnetic field and hence show that probability per unit time for induced emission and absorption are equal.
4. Distinguish induced and spontaneous emission. Define Einstein's A and B coefficients and obtain the relation between them. Write down the

expression for the transition probability per unit time for spontaneous emission.

5. Discuss in detail about the forbidden transition
6. Explain the selection rules.

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LESSON 16

QUANTUM FIELD THEORY

16.1 AIMS AND OBJECTIVES

In this lesson,we are going to studied about quantization of wave fields. We will be discussing the Legrangian , classical Hamiltonian equations and non – relativistic Schrodinger's equations. Also we will be presenting creation , destruction and number operators and anti Commutation relations.

16.2 . Quantization of Wave Fields: Introduction

A wave field is specified by its amplitudes at all points of space and the dependence of these amplitudes on the time, the same way as system of particulars is specified by the positional co-ordinates q_i and their dependence on the time. The field has an infinite number of degrees of freedom and to use the amplitudes ψ (r,t) at all points r as co-ordinates is analogous to a system that consists of an infinite number of particles and with the particles co-ordinates $q_i(t)$ respectively.

ψ can be expanded in some complete ortho – normal set of functions u_k:

$$\psi (r,t) = S_k \, a_k (t) \, u_k (r) \qquad (1)$$

where a_k is regarded as the fields co-ordinates In classical particle theory, both total and partial time derivatives were defined in connection with a function $F(q_i, p_i, t)$ of the co-ordinates, momenta and time. Also a function $F(\psi, \pi, t)$ can depend explicitly on the time as well as on the field, so that it is important to distinguish between dF/dt and ∂F/dt.

16.3. Classical Lagrangian Equation

The Lagrangian $L(q_i, q_i, t)$is a function of the time and a functional of the possible paths $q_i(t)$ of the system. The actual paths are derived from the variation principle.

$$\delta \int_{t_1}^{t_2} L.\, dt = 0, \qquad \delta q_i(t_1) = \delta q_i(t_2) = 0 \tag{1}$$

we expect the field Lagrangian to be a functional of the field amplitude $\psi(r,t)$. It can be expressed as the integral over all space of a Lagrangian density $\vec{L}$:

$$L = \int \vec{L}\,(\psi, \Delta\psi, \dot{\psi}, t) d^3 r \tag{2}$$

where $\dot{\psi}$ is $\partial\psi/\partial t$ or $d\psi/dt$

The appearance of $\nabla\psi$ as an argument of $\vec{L}$ is a result of the continuous dependence of ψ on r. The variation principle that corresponds to equation (1) is

$$\delta \int_{t_1}^{t_2} L\, dt = \delta \int_{t_1}^{t_2} \vec{L}\, dt\, d^3 r = \int_{t_1}^{t_2} \int (\delta\, \vec{L})\, dt\, d^3 r = 0 \tag{3}$$

where the variation $\delta\psi$ of ψ is subject to the restrictions,

$$\delta\psi\,(r, t_1) = \delta\psi\,(r, t_2) = 0 \tag{4}$$

The variation of $\vec{L}$ can be written as,

$$\delta L = \frac{\partial \bar{L}}{\partial \psi} \delta \vec{\psi} + \sum_{x\ y} \frac{\bar{L}}{\partial \left(\frac{\partial \psi}{\partial x} \right)} \frac{\partial}{\partial x} \delta \vec{\psi} + \left(\frac{\bar{L}}{\delta} \frac{\partial}{\partial x} \right) \vec{\psi} \quad . \tag{5}$$

where the summation over x, y, z implies the sum of three terms with y and z substituted for x we have, $\delta\dot{\psi} = \frac{\partial}{\partial t}(\delta\psi)$, $\delta \left(\frac{\partial \psi}{\partial x} \right) = \frac{\partial}{\partial x}(\delta\psi)$

Then equation (3) becomes

$$\int_{t_1}^{t_0} \left[\frac{\partial \bar{L}}{\partial \psi} \delta \vec{\psi} + \sum_{x\ y} \frac{\bar{L}}{\partial \left(\frac{\partial \psi}{\partial x} \right)} \frac{\partial}{\partial x} \delta \vec{\psi} \right] - \left(\frac{\partial \bar{L}}{\partial \dot{\psi}} \right) \frac{\partial}{\partial t} \delta \vec{\psi} = 0 \quad d\ t^3 d\ r \tag{6}$$

Then summation terms in equation (6) can be integrated by parts with respect to space co-ordinates; surface terms vanish either because ψ falls rapidly at infinite distance or because ψ obeys periodic boundary conditions. The last term in equation (6) can be integrated by parts with respect to time and the boundary terms vanish because of equation (4). Now equation (6) can be written as,

$$\int_{t_1}^{t_0} \left\{ \frac{\partial \bar{L}}{\partial \psi} - \sum_{x\,y\,z} \frac{\partial}{\partial x} \left[\frac{\bar{L}\partial}{\partial\left(\frac{\partial \psi}{\partial x}\right)} \right] t \right\} \frac{\bar{L}}{\partial} \frac{\partial}{\partial} \left(\frac{\vec{}}{\cdot} \right) = \delta \quad \psi d \quad t^3 d \quad r 0 \tag{7}$$

since equation (3) is valid for an arbitrary variation $\delta\psi$ at each point in space, equation (7) is equivalent to the differential equation,

$$\frac{\partial \bar{L}}{\partial \psi} - \sum_{x\,y\,z} \frac{\partial}{\partial x} \left[\frac{\bar{L}\partial}{\partial\left(\frac{\partial \psi}{\partial x}\right)} \right] t \quad \frac{\bar{L}}{\partial} \frac{\partial}{\partial} \left(\frac{\vec{}}{\cdot} \right) \quad 0 \tag{8}$$

Equation (8) is the classical field equation derived from the Lagrangian density $\vec{L}(\psi, \nabla\psi, \psi, t)$.

16.4. Functional Derivative

In order to peruse further the analogy with particle mechanics, it is desirable to rewrite equation (8) in terms of L rather then $\vec{L}$. For this we require derivatives of L with respect to ψ and ψ at particular points. These are called 'functional derivatives' and are denoted by $\frac{\partial L}{\partial \dot{\psi}}$ and $\frac{\partial L}{\partial \psi}$

Expressions for them can be obtained by dividing up all space into small cells and replacing volume integrals by summate over these cells. The expressions for the function derivatives are as follows.

$$\frac{\partial L}{\partial \psi} = L_{\delta_r \tau \to 0} t \frac{\partial L \delta}{\delta \quad \psi \quad \delta} \quad \frac{\partial \bar{L}}{\partial \quad \psi} \quad \sum_{x\,y\,z} \frac{\partial \bar{L}}{x} \left[\frac{}{\partial\left(\frac{\partial \psi}{\partial x}\right)} \right] \tag{9}$$

Here all the $\delta\psi_i$ and $\delta\psi_i$ are zero except for particular $\delta\psi_j$, and $\delta\tau_i$ is the volume of the cell. Similarly, the functional derivative of L w.r.t ψ is defined by setting all the $\delta\psi_i$ and $\delta\psi_i$ zero except for $\delta\psi_i$

$$\frac{\partial L}{\partial \psi} = L_{\delta \tau \to 0} \frac{L \quad \delta}{t \psi \quad \partial \delta \quad _j \tau} \frac{}{\cdot \quad \psi} \tag{10}$$

Here again at point r at which the functional derivative is evaluated is in the j^{th} cell. Substituting equations (9) & (10) in (8) gives,

$$\frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{\psi}} - \frac{\partial L}{\partial \psi} = 0 \qquad (11)$$

which closely resembles the Legrangian equations

$$\frac{d}{d}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0 \text{ for a system of particle.}$$

16.5. Classical Hamiltonian Equations

The momentum canonically conjugate to ψ_j can be defined as in particle mechanics to be the ratio of δL to the infinitesimal change $\delta\psi_j$ when all the other $\delta\dot{\psi}_j$ and all $\delta\psi_i$ are zero we thus obtain.

$$P_j = \frac{\delta L}{\delta \dot{\psi}_j} = \delta\tau_j \left(\frac{\partial L}{\partial \psi}\right)_j \qquad (1)$$

It follows that

$$P_j = \delta\tau_j \left(\frac{\partial L}{\partial \dot{\psi}}\right)_j \qquad (2)$$

The Hamiltonian $H = \sum_i P_i \dot{\psi}_i - L = \sum_i \left(\frac{\partial L}{\partial \dot{\psi}}\right)_i \dot{\psi}_i \, \delta\tau_i - L$ (3)

H is written as the volume integral of a Hamiltonian density $\vec{H}$ and assume that the cells are small enough so that the difference between a volume integral and the corresponding cell summation can be ignored; we than have,

$$H = \int \vec{H}\, d^3 r \qquad \vec{H} = \pi\dot{\psi} - L \qquad \pi \equiv \frac{\partial L}{\partial \dot{\psi}} = \frac{\partial \vec{L}}{\partial \dot{\psi}} \qquad (4)$$

The true field Hamiltonian H given in equation (4) which is a functional of ψ and π from which $\dot{\psi}$ has been eliminated. The classical Hamiltonian equations of motion will be derived without further recourse to the cell a approximation. The variation of L produced by variations of ψ and $\dot{\psi}$ can be written using equation (4) and

$$\frac{\partial}{\partial t}\frac{\partial L/}{\partial \dot{\psi}/} - \frac{\partial L/}{\partial \psi/} = 0$$

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

$$= \int [\delta(\pi\dot{\psi}) - \pi\dot{\delta\psi} - \dot{\psi}\delta\pi] d^3 r$$

$$= \delta H + \delta L + \int (\dot{\pi}\delta\psi - \dot{\psi}\delta\pi) d^3 r \qquad (5)$$

The variation of H produced by corresponding variations of ψ and π can be written,

$$\delta H = \int \left(\frac{\partial H}{\partial \psi} \delta\psi + \frac{\partial H}{\partial \pi} \delta\pi \right) d^3 r \qquad (6)$$

It follows from the earlier discussion of functional derivatives that.

$$\left.\begin{aligned} \frac{\partial H}{\partial \psi} &= \frac{\delta H}{\delta \psi} - \sum_{x,y,z} \frac{\partial}{\partial x} \frac{\partial H}{\partial \left(\frac{\partial \psi}{\partial x} \right)} \\ \frac{\partial H}{\partial \pi} &= \frac{\delta H}{\delta \pi} - \sum_{x,y,z} \frac{\partial}{\partial x} \frac{\partial H}{\partial \left(\frac{\partial \pi}{\partial x} \right)} \end{aligned}\right\} \qquad (7)$$

Comparison of equations (5) & (6) for arbitrary variations $\delta\psi$ and $\delta\pi$ then gives the classical field equations is Hamiltonian form.

$$\dot{\psi} = \frac{\partial H}{\partial \pi} \qquad \dot{\pi} = -\frac{\partial H}{\partial \psi} \qquad (8)$$

The Hamiltonian equation for the time rate of change of a functional F of ψ and π can now be found. We express F as volume integral of the corresponding functional density $\vec{F}(\psi, \pi, t)$, which for simplicity is assumed not to depend explicitly on time or on gradients of ψ or π. Hence,

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \int \left(\frac{\partial \vec{F}}{\partial \psi} \dot{\psi} + \frac{\partial \vec{F}}{\partial \pi} \dot{\pi} \right) d^3 r$$

$$= \frac{\partial F}{\partial t} + \int \left(\frac{\partial \vec{F}}{\partial \psi} \frac{\partial H}{\partial \pi} - \frac{\partial \vec{F}}{\partial \pi} \frac{\partial H}{\partial \psi} \right) d^3 r$$

$$= \frac{\partial F}{\partial t} + \{F, H\} \qquad (9)$$

The above equation also serves to define poisson bracket expression for two function as of the field variables. The RHS of equation (9) is not changed if F also depends on $\nabla\psi$ or $\nabla\pi$. It is clear from equation (9) that H is a constant of the motion if it does not depend explicitly on time; in this case H is the total energy of the field.

16.6. Field Quantization of the non – Relativistic Schrödinger Equation

Consider the Schrödinger wave equation,

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

Schrödinger equation. For this reason, As a first example of the application of the field quantization technique, we consider here the quantization of the non relativistic Schrödinger equation. The application implies treating (1) as though it were a classical equation that describes the motion of some kind of material fluid. The resulting quantized field theory is equivalent to a many – particle field quantization is often called 'second quantization', and the transaction from classical particles mechanics to equation (1) constitutes the 'first quantization.'

Classical Lagrangian and Hamiltonian equations,

The Lagrangian density may be taken to be

$$\bar{L} = \frac{i\hbar}{2}(\psi^*\dot{\psi} - \dot{\psi}^*\psi) - \frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi - V\psi^*\psi \qquad (2)$$

ψ and ψ^* can be varied separately to obtain the Lagrangian equations of motion.

The equation of the form that results from variation of ψ is

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

Which is the complex conjugate of (a) variation of ψ^* gives

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \qquad (3)$$

The momentum canonically conjugate to ψ is

$$\pi = \frac{\partial\bar{L}}{\partial\dot{\psi}} = \frac{i\hbar}{2}\psi^* \qquad (4)$$

However ψ^* does not appear in the Lagrangian density so that π is identically zero. It is therefore impossible to satisfy the corresponding classical poission bracket relation, so that ψ^*, π cannot be regarded as a pair of canonically conjugate variables. π is the second momentum.

The Hamiltonian density is,

$$H = \pi\dot{\psi} - L = \frac{-i\hbar}{2m}\pi\nabla^2\psi + \frac{i}{\hbar}V\pi\psi \qquad (5)$$

The Hamiltonian equations of motion obtained from the classical field equations with the help of functional derivates are,

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

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

We have thus shown, from the point of view of classical field theory, that the Lagrangian density and the canonical variables and hamiltonian derived from it are in agreement with the wave equation.

16.7. Creation, Destruction, and Number Operations

Consider the commutation relations

$$\left[a_k(t), a_l^\dagger(t')\right] = \int u_k^*(r,t)u_l(r,t')d^3r = \delta_{kl}\delta(t-t') \qquad (1)$$

for the operations a_k and a_k^+ were solved in connection with the harmonic oscillator. It was found that the solution of $aa^+ - a^+a = 1$ in the representation in which a^+a is diagonal, consists of the matrices.

$$a = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 2^{1/2} & 0 \\ 0 & 0 & 0 & 3^{1/2} \end{bmatrix} \qquad a^+ = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 2^{1/2} & 0 & 0 \\ 0 & 0 & 3^{1/2} & 0 \end{bmatrix} \qquad (2)$$

Let N be Hermitian, its eigenvalues are real.

$$N = \sum_k N_k \qquad where \qquad N_k = a_k^+ a_k \qquad (3)$$

The states of the quantized field, in the representation in which each N_k is diagonal, are the kets

$$|n_1, n_2 \ldots n \ldots n_k, \ldots\ldots\rangle. \qquad (4)$$

Where each n_k is an eigen value of N_k and must be a +ve integer or zero. We also have the relations.

$$\left.\begin{aligned} a_k|n_1, \ldots n \ldots n_k \ldots n_1, \ldots n_k\rangle &= n_k^{1/2}|n_1, \ldots n \ldots n_k - 1, \ldots\ldots\rangle \\ a_k^\dagger|n_1, \ldots n \ldots n_k \ldots n_1, \ldots\rangle &= (n_k+1)^{1/2}|n_1, \ldots n \ldots n_k + 1, \ldots\ldots\rangle \end{aligned}\right\} \qquad (5)$$

These a_k^+ and a_k are called 'creation' and 'destruction' operators for the state k of the field.

The 'number operation' N_k need not be a constant of the motion, that $N = \sum N_k$ is a constant The rate of change of N_k is given by,

$$i\hbar \dot{N}_k = [a_k^\dagger a_k, H]$$

where $H = \sum_{j\,l} a_j^\dagger\, {}_l a \int \left(\frac{\hbar^2}{2m} \nabla \quad . \nabla^*_j \right) u + \quad u^3 \quad d \quad r$

$$= \sum_{j\,l} a_j^\dagger \; {}_l \, c \int_j \; {}^* \left(u \frac{-\hbar^2}{2m} V_l^2 \nabla \right) u + \; {}^3 d \quad r \qquad (6)$$

diagonal, N_k is constant only if all the volume integrals in equation(6) are zero for which either j or l is equal to k. These integrals are just matrix elements of the one particle Hamiltonian. The integrals in equation (6) are than $E_l \, \delta_{jl}$, and the field Hamiltonian becomes,

$$H = \sum_k a_k^+ a_k E_k = \sum_k N_k E_k$$

This particular N representation is the one in which H is also the ket $|n_1, \ldots\ldots n_k, \ldots\ldots>$ has the eigen value $\sum_k n_k E_k$ for the total energy operator H. It is apparent that all the N_k are constant in this case.

16.8. Anti Commutation Relations

The commutation relations are

$$\left.\begin{array}{l} [\psi(r) \psi_{\cdot} r(\,)] = \psi[\,) r^+(\,) \psi^+ \,] = (\quad ' \quad) \; 0 \\ [\psi(\,), (') \psi^+ r] \quad \mathrm{r}\delta = {}^3 \left(- \quad ' \quad \right) \mathrm{r} \end{array}\right\} \qquad (1)$$

It is necessary to modify the above equations if we are obtain a theory of particles that obey the exclusion principle. It is reasonable to require that this modification be made in such a way that The quantum equation of motion of ψ is the wave equation,

$$i\hbar \dot{\psi} = V \frac{\hbar^2}{2m} \psi \nabla r \quad - (\psi \; , \quad)$$

when the Hamiltonian has the form,

$$H = \int \left(\frac{\hbar^2}{2m} \nabla\psi^{+}.\nabla\psi \right) + \psi V \quad \psi d \quad {}^{3}r$$

It was found by Jordon and Wigner that the descried modification consists in the replacement of the commutator brackets,

$$[A,B] \equiv AB - BA$$

By anticommutator brackets

$$[A,B]_{+} \equiv AB + BA$$

This means that equations (1) are replaced by,

$$\left.\begin{array}{l} \left[\psi(r)\ \psi,\ r(\right]_{+}\ 'ψ=)r(\ ψ)\ r(+'ψ)r(\ ψ=r)\ (\ )\ 0 \\ \left[\psi^{+}(r\ )\psi\right],\ r(\ \ _{+}'ψ^{+}=)r(\ ψ^{+})\ r(+'ψ^{+})r(\ ψ'=r)\ (\ )\ 0 \\ \left[\psi(r\ )\ \psi^{+}\right]r(\ \ _{+}'ψ=)^{+}\ (\ ψ)r\ -(^{+}\ 'ψr\ )\ (=ψ'\ )\ rδ(-)^{3}\ (r\ ' \end{array}\right\} \qquad (2)$$

It then follows that

$$\left.\begin{array}{l} [a_k, a_L]_{+} = a_k a_l + a_l a_k = 0 \\ [a_k^{+}, a_L^{+}]_{+} = a_k^{+} a_l^{+} + a_l^{+} a_k^{+} = 0 \\ [a_k , a_L^{+}]_{+} = a_k a_l^{+} + a_l^{+} a_k = \delta_{kl} \end{array}\right\} \qquad (3)$$

We define $N_k = a_k^{+} a_k$ as before and notice first that each N_k commutes with all the others, so that they can be diagonalized simultaneously. The eigen values of N_k can be obtained from the matrix equation,

$$N_k^{2} = a_k^{+} a_k \ \ a_k^{+} a_k = a_k^{+} (1-a_k^{+} a_k)\ a_k = a_k^{+} a_k = N_k \qquad (4)$$

If N_k is in diagonal form and has eigen values n_k^{1}, n_k^{11}....., it is clear that N_k^{2} is also in diagonal form and has eigen values n_k^{12}, n_k^{112}, ... Thus the matrix equation is equivalent to the algebraic equations.

$$n_k^{1\ 2} = n_k^{1} \qquad n_k^{11\ 2} = n_k^{11} .....$$

For the eigen values. These are quadratic equations that have two roots 0 and 1. Thus the eigen values of each N_k are 0 and 1, and the particles obey the exclusion principle. The eigen values of $N = \sum N_k$ are the +ve integers and zero as before. The earlier expressions for the Hamiltonian in creation, destruction and number operators are unchanged, and the energy eigen values are $\sum n_k E_k$.

16.9 LET US SUM UP

In this lesson, we have discussed about quantization of wave fields. We studied the Legrangian , classical Hamiltonian equations and non – relativistic Schrodinger's equations, in detail. Also we presented creation , destruction and number operators and anti Commutation relations.

16.10 LESSON END ACTIVITIES

Check your progress

1. Define density operator and density matrix.
2. Obtain the Legrangian equations of motion.
3. Obtain the classical Hamiltonian equation.
4. Arrive at the non – relativistic Schrodinger's equation.
5. Explain the creations, destruction and number operators.

16.11 References

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M.Sc. DEGREE EXAMINATION, APRIL 2008

Model Question

Physics

QUANTUM MECHANICS

Time : Three hours **Maximum :** 100 marks

Answer any five questions

Each question carries 20 marks. (5 x 20 = 100)

1. Give the matrix theory of harmonic oscillator and obtain the energy eigenvalue spectrum. Write down the physical meaning of matrix elements.
2. Explain the main stages involved in the WKB approximation. Use the technique to obtain the asymptotic solution of the one dimensional Schrödinger equation. Also arrive at the solution near a turning point.
3. Develop the relativistic wave equation for the particle of spin zero. Discuss the difficulties involved in interpreting the probability density. Derive the expression charge and current densities from the continuity equation.
4. Prove the following properties of Dirac matrices on the basis of Dirac's theory :
    a) Square of matrices are unity
    b) Eigenvalues of the matrices are ±1.
    c) Trace of the matrices is zero.
    d) Dimension of the matrices are of even order.
    e) The matrices anticommuting among themselves.
5. Obtain an expression for the Born approximation amplitude and hence derive the Rutherford formula for Coulomb scattering. Enumerate the two conditions for the validity of born approximation.
6. Discuss the Thomas Fermi Model and Hartree's Self Consistent Model in detail. Briefly explain Heitler and London method.
7. Distinguish induced and spontaneous emission. Define Einstein's A and B coefficients and obtain the relation between them. Write down the expression for the transition probability per unit time for spontaneous emission.
8. Obtain classical Lagrangian equation. Write notes on Creation, Destruction and Number Operators. Also discuss their anti commutation relations.

M.Sc. DEGREE EXAMINATION, APRIL 2008

Model Question

Physics

QUANTUM MECHANICS

Time : Three hours **Maximum :** 100 marks

Answer any five questions

Each question carries 20 marks. (5 x 20 = 100)

1. What do you understand by equation of motion? Obtain the equation of motion in the Heisenberg picture and state the distinction between Schrödinger picture and Heisenberg picture.
2. Give the matrix theory of harmonic oscillator and obtain the energy eigenvalue spectrum. Discuss the significance of zero point energy.
3. Obtain Perturbation theory for non degenerate states. Show that the first order perturbation energy for a non degenerate state of a system is just the perturbation for average over the corresponding unperturbed state of the system. Distinguish stationary and time dependent perturbation theory.
4. Explain how the ground state energy could be evaluated using the variation method and hence find the ground state energy of hydrogen atom.
5. Obtain the spectrum of eigenvalues for J^2 and J_z. Hence calculate the angular momentum matrices for j = ½. What are C.G. Coeffifiient? Briefly explain their significance.
6. Develop Dirac's relativistic wave equation for a free particle and obtain its plain wave solution. Give the significance of negative energy states. What are the consequences of Dirac's interpretation?
7. What do you meant by partial wave analysis? Employ this method to derive an expression for the scattering amplitude in terms of phase shift. Obtain an expression for scattering cross section for Coulomb potential.
8. Discuss the interaction of atom with electromagnetic field and hence show that probability per unit time for induced emission and absorption are equal. Obtain classical Hamiltonian equation.

M.Sc. DEGREE EXAMINATION, APRIL 2008

Model Question

Physics

QUANTUM MECHANICS

Time : Three hours **Maximum :** 100 marks

Answer any five questions

Each question carries 20 marks. (5 x 20 = 100)

1. What are the conditions under which an operator can be represented by a diagonal matrix. Write down the physical meaning of matrix elements. Explain Kronig penny model.
2. 'There is no first order stark effect in the ground state of an atom' – Illustrate. Define the degeneracy of an energy eigenvalue and illustrate its removal by considering the stark effect in the n = 2 level of the hydrogen atom.
3. Obtain the expressions for the first order corrections to the energy and wavefunction making the use of the non-degenerate stationary perturbation theory. Obtain an expression for harmonic perturbation.
4. Give the quantum mechanical definition of angular momentum. Find the angular momentum matrices for j = 1. List the symmetry properties of C. G. coefficient.
5. Show that the angular momentum of electron is a constant of motion only if we include the spin. Establish the Dirac's relativistic wave equation for an electron and calculate its magnetic moment.
6. Define the terms "scattering amplitude" and "phase shift'. Obtain an expression for scattering amplitude in terms of phase shift. State and explain optical theorem. Discuss in detail the problem of Yukawa potential.
7. Explain the terms doublet separation and doublet intensity. Explain how the spin orbit interaction can be accounted as correction to central field approximation.
8. Distinguish induced and spontaneous emission. Define Einstein's A and B coefficients and obtain the relation between them. Write down the expression for the transition probability per unit time for spontaneous emission.