

**KARPAGAM ACADEMY OF HIGHER EDUCATION**

(Deemed to be University)

(Established Under Section 3 of UGC Act 1956)

Coimbatore - 641021.

(For the candidates admitted from 2017 onwards)

DEPARTMENT OF PHYSICS

SUBJECT : QUANTUM MECHANICS – II**SEMESTER : III****SUBJECT CODE: 17PHP301****CLASS : II M.Sc Physics**

Scope: This is a continuation of Quantum Mechanics – I. More detailed study of problems like scattering problem, relativistic quantum mechanics, quantum electrodynamics etc. are added in this paper.

Objectives: To make the students capable of analyzing theoretical problems like interaction of particles, scattering of particles etc.

UNIT - I

Angular momentum: Angular momentum operators – Angular momentum commutation relations – Eigen values and Eigen functions of L^2 and L_z – General angular momentum – Eigen values of J^2 and J_z – Ladder operators (J_+ and J_-) – Angular momentum matrices – Matrices for J^2 , J_z , J_+ , J_- , J_x and J_y – Spin angular momentum – Spin $\frac{1}{2}$ systems – Spin vectors for spin $\frac{1}{2}$ systems – Addition of angular momentum – Clebsh-Gordan coefficients.

UNIT -II

Scattering: Scattering cross-section – Scattering amplitude – Partial waves – Scattering by a central potential: partial wave analysis – Significant number of partial waves – Scattering by an attractive square-well potential – Briet-Wigner formula – Scattering length – Expression for phase shift – Integral equation – The Born approximation – Scattering by screened coulomb potential – Validity of Born approximation - Laboratory and center of mass co- ordinate systems.

UNIT - III

Many Electron Problem: Indistinguishable particles, Pauli principle – Inclusion of spin – Spin functions for two electrons – Spin functions for three electrons – The Helium atom – Central field approximation – Thomas-Fermi model of the atom – Hartree equation – Hartree-Fock equation – Molecular orbital theory: Hydrogen molecule ion H_2^+ - Valence bond theory

UNIT - IV

Relativistic quantum mechanics: Klein-Gordan equation – Interpretation of the Klein- Gordan equation – Particle in a coulomb field – Dirac's equation for a free particle – Dirac matrices – Covariant form of Dirac equation – Probability density – Negative energy states – Spin of the Dirac particle – Magnetic moment of the electron – Spin-orbit interaction – Radial equation for an electron in a central potential – Hydrogen atom – Lamb shift.

UNIT - V

Field theory: Introduction – Classical approach to field theory – Relativistic Lagrangian and Hamiltonian of a charged particle in an electromagnetic field – Field: Lagrangian and Hamiltonian formulations – Quantum equation for the field – Second quantisation – Quantisation of non-relativistic Schroedinger equation – Creation, annihilation and number operators

Text Book

1. Aruldas. G, 2008, Quantum Mechanics, 2nd Edition, Prentice-Hall of India, NewDelhi.

REFERENCES

1. Gupta, Kumar and Sharma, 2002, Quantum Mechanics, 22nd Edition, Jai Prakash Nath & Co, Meerut.
2. Satya Prakash, 2003, Quantum Mechanics, New Edition Kedar Nath & Ram Nath & Co, Meerut.
3. Leonard Schiff, 2006, Quantum Mechanics, 3rd Edition, McGraw Hill International, Auckland.
4. Engen Merzbacher, 2014, Quantum Mechanics, 3rd Edition, Wiley, Weinheim.
5. Mathews. P.M. and K. Venkatesan, 2nd edition 2013, Textbook of Quantum Mechanics, McGraw Hill International, Weinheim.

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DEPARTMENT OF PHYSICS**SUBJECT : QUANTUM MECHANICS II****SEMESTER : III****SUBJECT CODE: 17PHP301****CLASS : II M.Sc. PHYSICS**

LECTURE PLAN
DEPARTMENT OF PHYSICS

S.No	Lecture Duration Hour	Topics to be covered	Support materials/page no
		UNIT - I	
1	1	Angular momentum: Angular momentum operators - Angular momentum commutation relations	T1-170-171
2	1	Eigen values and Eigen functions of L^2 and L_z General angular momentum	T1-172-173
3	1	Eigen values of J^2 and J_z - Ladder operators (J_+ and J_-)	T1-173-176
4	1	Angular momentum matrices - Matrices for J^2 , J_z , J_+ , J_- , J_x and J_y	T1-176-179
5	1	Spin angular momentum, Spin $\frac{1}{2}$ systems	T1-179
6	1	Spin vectors for spin $\frac{1}{2}$ systems - Addition of angular momentum	T1-179-180
7	1	Clebsch-Gordan coefficients.	T1-180-182
8	1	Revision	
		Total no of hours planned for unit I = 8	

S.No	Lecture Duration Hour	Topics to be covered	Support materials/ page no
UNIT - II			
1	1	Scattering: Scattering cross-section- Scattering amplitude , Partial waves - Scattering by a central potential:	T1 - 283-290
2	1	partial wave analysis - Significant number of partial waves	T1 - 290-291
3	1	Scattering by an attractive square-well potential	T1 – 291
4	1	Briet-Wigner formula, Scattering length	T1 - 292-294
5	1	Expression for phase shift - Integral equation	T1 - 295-298
6	1	The Born approximation - Scattering by screened coulomb potential	T1 – 298-300
7	1	Validity of Born approximation - Laboratory and center of mass co-ordinate systems	T1- 300-303
8	1	Revision	
Total no of hours planned for unit II = 8			

S.No	Lecture Duration Hour	Topics to be covered	Support materials/ page no
UNIT - III			
1	1	Many Electron Problem: Indistinguishable particles, Pauli principle ,Inclusion of spin - Spin functions for three electrons	T1-260-265
2	1	Spin functions for three electrons - The Helium atom	T1-266-269
3	2	Central field approximation	T1-269- 270
4	1	Thomas-Fermi model of the atom -	T1-270- 272
5	1	Hartree equation , Hartree-Fock equation	T1-272- 276
6	1	Molecular orbital theory: Hydrogen molecule ion H ₂ ⁺	R2-433- 444
7	1	Valence bond theory , Heitler-London theory of hydrogen molecule.	R2-457

8	1	Revision	
	Total no of hours planned for unit III = 9		

S.No	Lecture Duration Hour	Topics to be covered	Support materials/ page no
		UNIT - IV	
1	1	Relativistic quantum mechanics: Klein-Gordan equation	T1 -310-311
2	1	Interpretation of the Klein-Gordan equation	T1-311-318
3	2	Particle in a coulomb field - Dirac's equation for a free particle -	T1-312-316
4	1	Dirac matrices , Covariant form of Dirac equation	T1-316-318
5	1	Probability density ,Negative energy states	T1-318-321
6	1	Spin of the Dirac particle, Magnetic moment of the electron	T1 322-336
7	1	Spin-orbit interaction - Radial equation for an electron in a central potential	T1 326-331
8	1	Hydrogen atom , Lamb shift	T1-331-333
9	1	Revision	
	Total no of hours planned for unit IV = 10		

S.No	Lecture Duration Hour	Topics to be covered	Support materials/ page no
		UNIT - V	
1	1	Field theory: Introduction , Classical approach to field theory	R2-410
2	2	Relativistic Lagrangian and Hamiltonian of a charged particle in an electromagnetic field	R2-412
3	1	Lagrangian - Hamiltonian formulations	R2-413-414
4	1	Quantum equation for the field	R2-414-416
5	1	Second quantisation	R2-416-418
6	1	Quantisation of non-relativistic Schroedinger equation	R2-419-420
7	2	Creation, annihilation and number operators.	R2-420-422
8	1	Revision	
9	1	Old question paper discussion	
10	1	Old question paper discussion	
11	1	Old question paper discussion	
		Total no of hours planned for unit IV = 13	

Text Book

1. Aruldas. G, 2008, Quantum Mechanics, 2nd Edition, Prentice-Hall of India, NewDelhi.

Reference Book

1. Gupta, Kumar and sharma ,2002,Quantum Mechanics, 22nd edition, Jaiprakash nath & Co, Meerut
2. Satya Prakash, 2003, Quantum Mechanics, New Edition Kedar Nath & Ram Nath & Co, Meerut.

UNIT- I

SYLLABUS

Angular momentum: Angular momentum operators – Angular momentum commutation relations – Eigen values and Eigen functions of L^2 and L_z – General angular momentum – Eigen values of J^2 and J_z – Ladder operators (J_+ and J_-) – Angular momentum matrices – Matrices for J^2 , J_z , J_+ , J_- , J_x and J_y – Spin angular momentum – Spin $\frac{1}{2}$ systems – Spin vectors for spin $\frac{1}{2}$ systems – Addition of angular momentum – Clebsh-Gordan coefficients.

ANGULAR MOMENTUM OPERATORS

The Angular Momentum Operator:

In classical physics the angular momentum of a particle with momentum p and position r is defined by

$$L = r \times p = (y p_z - z p_y) i + (z p_x - x p_z) j + (x p_y - y p_x) k$$

The orbital angular momentum operator L can be obtained at once by replacing r and p by the corresponding operators in the position representation, R and $P = -i\hbar \nabla$ where q is the coordinate expression for the operators of L_x, L_y, L_z .

The Cartesian components of L are

$$L_x = -i\hbar (y \frac{d}{dz} - z \frac{d}{dy})$$

$$L_y = -i\hbar (z \frac{d}{dx} - x \frac{d}{dz})$$

$$L_z = -i\hbar (x \frac{d}{dy} - y \frac{d}{dx})$$

Clearly, angular momentum does not exist in a one-dimensional space. We should mention that the components

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

ANGULAR MONENTEUM COMMUTATION RELATION:

The commutation relation of the component of L can easily be obtained in Cartesian coordinates

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

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

in these commutations p_z stands for $-i \hbar \frac{d}{dz}$. In the second and third terms on the right side of the equation all the variables involved commute with each other. Hence both of them vanish. Since y and p_x commute with z and p_z

$$[\hbar y p_z, \hbar z p_x] = \hbar y p_x [p_z, z] = -i \hbar y p_x$$

based on similar arguments, we get

$$[\hbar z p_y, \hbar x p_z] = \hbar p_y x [z, p_z] = -i \hbar x p_y$$

Hence

$$[L_x, L_y] = i \hbar (x p_y - y p_x) = i \hbar L_z$$

the commutators $[L_y, L_z]$ and $[L_z, L_x]$ can be obtained in the same way and we have

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

that is the components of angular momentum do not commute with one another and therefore they are not measurable simultaneously. In other words if the system is an eigenstate of one angular momentum component, it will not be simultaneously in an eigenstate of either of the others. These commutations relation hold for the components of total angular momentum $L = L_i$ of a system of particle also. The commutation relation in can be written in a compact form as

$$\mathbf{L} \times \mathbf{L} = i \hbar \mathbf{L}$$

In the usual sense the vector product of a vector with itself is zero. Hence we have to consider \mathbf{L} as a vector operator and not as a usual vector. The left hand side to be considered as a determinant and has to be expanded before the term by term comparison with the commutator of L^2 with the component of \mathbf{L} .

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

Hence we conclude that

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

The square of the angular momentum commutes with its components. That is the total angular momentum can be measured simultaneously with any one component. As the components among themselves are noncommuting one cannot measure L^2, L_x, L_y, L_z simultaneously. Therefore we cannot have a representation in which all the four are diagonal.

$$L_+ = L_x + iL_y, \quad L_- = L_x - iL_y$$

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

The reason for the names would be clear in section.

$$[L^2, L_+] = 0, \quad [L^2, L_-] = 0$$

and

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

The other commutators can also be evaluated in the same way and we have the relations

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

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

we also have

$$[L_x, L_z] = 0$$

and

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

EIGENVALUES AND EIGENFUNCTIONS OF L^2 AND L_z :

The eigen value equation for L^2 in spherical polar coordinates can be written as

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

where λ is the eigen value of L^2 and Y is the corresponding eigen function rearranging we get

$$\left[\frac{1}{\sin \theta} \left(\frac{d}{d\theta} \sin \theta \frac{d}{d\theta} \right) + \frac{1}{\sin^2 \theta} \frac{d^2}{d\phi^2} \right] Y + \lambda Y = 0$$

which is the same as the angular part of the schrodinger equation of a system moving in a potential $V(r)$. The solution gives $\lambda = l(l+1)\hbar^2$ with eigenfunction

$$Y = Y_{lm}(\theta, \phi) = \left[\frac{(2l+1)!}{4(l-lm)!(l+lm)!} \right]^{1/2} P_l^{lm}(\cos \theta) e^{im\phi}$$

where

$$l=0,1,2,3,\dots \text{ and } m=0,\pm 1,\pm 2,\pm 3,\dots,\pm l$$

$$\text{and } (-1)^m \text{ for } m > 0 \text{ and } = 1 \text{ for } m = 0.$$

The form of L_z , immediately gives

$$L_z Y_{lm} = -i\hbar \frac{d}{d\phi} Y_{lm}(\theta, \phi)$$

$$= m\hbar Y_{lm}(\theta, \phi)$$

thus the spherical harmonic $Y_{lm}(\theta, \phi)$ are eigenfunction of L^2 and L_z with eigen value $l(l+1)\hbar^2$ and $m\hbar$ respectively

GENERAL ANGULAR MOMENTUM:

Number of experimental result such as spectra of alkali metals anomalous

zeeman effect , stern gerlach experiment ,etc,...could be explained only by invoking the concept that the electron in an atom possesses an additional intrinsic angular momentum involving half integral quantum numbers. However the definition of angular momentum based on classical physics let to the $2l+1$ integral values

$m, m=0, \pm 1, \pm 2, \dots, \pm l$ for the z component of angular momentum . In other words the difinision of angular momentum $\mathbf{L}=\mathbf{r}\times\mathbf{p}$ is not general enough to include half integral quantum number and therefore one may take the definition of general angular momentum as the commutation relation given by

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

where the J symbol is used for the general angular momentum.

EIGEN VALUES OF J^2 AND J_z ,

The square of the general angular momentum J commutes with its components J_x, J_y, J_z

.However the components among themselves are noncommutting. Therefore J^2 and one component, say J_z can have simultaneous eigenkets at a time. Denoting the simultaneous eigenkets by $|l, m\rangle$ the eigenvalue equation for J^2 is given by

$$J^2 |l, m\rangle = l(l+1) |l, m\rangle$$

and

equation 1 can be written as

$$J_x^2 + J_z^2 |l, m\rangle + m^2 |l, m\rangle = l(l+1) |l, m\rangle$$

multiplying from left by bra $\langle l, m|$ and rearranging

$$\langle l, m| J^2 |l, m\rangle + \langle l, m| J_z^2 |l, m\rangle = l(l+1) \langle l, m| |l, m\rangle$$

since J_x and J_y are hermitian their eigenvalues must be real and therefore the left side of must be positive. Hence

$$-m^2 \leq 0 \text{ or } m^2$$

operating eq 1 from left by J_+ , we get

$$J_+ J^2 |m\rangle = J_+ |m\rangle$$

that is $|m\rangle$ and $J_+ |m\rangle$ are eigenkets of J^2 with the same eigenvalues premultiplying by J_+ we have

$$J_+ J_z |m\rangle = m J_+ |m\rangle$$

but $[J_z, J_+] = J_+$ or $J_+ J_z = J_z J_+ - J_+$. replacing $J_+ J_z$ in the above equation

we get

$$(J_z J_+ - J_+) |m\rangle = m J_+ |m\rangle$$

or

$$J_z J_+ |m\rangle = (m+1) J_+ |m\rangle$$

thus $J_+ |m\rangle$ is an eigenkets of J_z with the eigenvalue $(m+1)$ and of J^2 with the same eigenvalue. Since operation by J_+ generates a state with the same magnitude of angular momentum but with z component higher by 1, it is called raising operator.

Repeated operation by J_+ increases the eigenvalue of J_z in steps. This has to be stopped at some point otherwise the condition eq 4 be μ . Then

$$J_z |1 \mu\rangle = \mu |1 \mu\rangle$$

operation by J_+ from left gives

$$J_z J_+ |1 \mu\rangle = (\mu+1) J_+ |1 \mu\rangle$$

eigenvalue of $(\mu+1)$ is not possible since μ is the highest eigenvalue. Hence,

$$J_+ |1 \mu\rangle = 0$$

premultiplying by J_- and using the result

$$J_- J_+ = J^2 - J_z^2 - J_z$$

we get

$$J_- J_+ |1 \mu\rangle = 0 \text{ or } (J^2 - J_z^2 - J_z) |1 \mu\rangle = 0$$

therefore

$$(-\mu^2 - \mu) |1 \mu\rangle = 0$$

as

$$(-\mu - \mu) = 0 \text{ so}$$

$$= \mu(\mu + 1)$$

operating eq $J_z | \mu \rangle = \mu | \mu \rangle$ from left by J_- , we get

$$J_- J_z | \mu \rangle = \mu J_- | \mu \rangle$$

or

$$J_z J_- | \mu \rangle = (\mu - 1) J_- | \mu \rangle$$

For the maximum eigenvalue μ we have

$$J_-^2 | \mu \rangle = 0$$

that is $J_- | \mu \rangle$ eigenkets of J^2 and J_z with the eigenvalues μ^2 and $\mu - 1$ respectively.

Hence J_- is called a lowering operator. J_+ and J_- together is often referred to as ladder operator. repeating the lowering operation by J_- , n times we get

$$J_z J_-^{n+1} | \mu \rangle = (\mu - (n+1)) J_-^{n+1} | \mu \rangle = 0$$

again there must be a cut off value of m without violating the condition $m^2 \leq \mu^2$ be $\mu - n$ then

$$J_z J_-^{n+1} | \mu \rangle = [\mu - (n+1)] J_-^{n+1} | \mu \rangle = 0$$

since $[\mu - (n+1)] \neq 0$

$$J_-^{n+1} | \mu \rangle = 0$$

or

$$J_- J_-^n | \mu \rangle = 0$$

or

$$J_+ J_-^n | \mu \rangle = 0$$

Replacing $J_+ J_-$, we have

$$(J^2 - J_z^2 + J_z) J_-^n | \mu \rangle = 0$$

or

$$[-(\mu - n)^2 + (\mu - n)] J_-^n | \mu \rangle = 0$$

As $J_-^n | \mu \rangle \neq 0$, $-(\mu - n)^2 + (\mu - n) = 0$, substituting the value of n from

we find

since $(n+1)0$

$$(n+1)(2\mu - n) = 0$$

$$2\mu - n = 0 \text{ or } \mu = n/2$$

where n is the number of steps from the maximum eigenvalue μ to the minimum eigenvalue $\mu - n$. The number of steps n is always an integer including zero. Writing j for $n/2$ the maximum and minimum eigenvalues of J_z are j and $-j$ respectively. In other words for a given value of j the integer possible values of j are $0, 1/2, 1, 3/2, \dots$ thus half integral quantum numbers have emerged automatically from the general treatment of angular momentum. A result we have been looking for denoting the simultaneous eigenvector of the operator J^2 and J_z with eigenvalues $j(j+1)\hbar^2$ and $m\hbar$ by $|j, m\rangle$ we get

$$J^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle$$

and

$$J_z |j, m\rangle = m\hbar |j, m\rangle$$

where $j = 0, 1/2, 1, 3/2, \dots$ and $m = -j, -j+1, \dots, j$

ANGULAR MOMENTUM MATRICES:

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

Matrices for J^2 and J_z :

As J^2 commutes with J_z the matrices for J^2 and J_z will be diagonal. In that representation J_x and J_y . Multiplication of eq $J^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle$ and $J_z |j, m\rangle = m\hbar |j, m\rangle$ from left by $\langle j', m' |$ gives

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

and

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

the presence of the factor $\delta_{jj'} \delta_{mm'}$ indicate that the matrices are given they are of infinite dimentionions

Matrices for J_+ , J_- , J_x and J_y :

$$J_z J_+ |jm\rangle = (m+1) J_+ |jm\rangle$$

this implies that $J_+ |jm\rangle$ is an eigenvalue of J_z , the eigen vectores can differ at the most by a multiplicative constant say a_m

$$J_+ |jm\rangle = a_m |j, m+1\rangle$$

similar we get

$$J_- |jm\rangle = b_m |j, m-1\rangle$$

where

$$a_m = \langle j, m+1 | J_+ | jm \rangle \quad \text{or} \quad a_m^* = \langle jm | J_- | j, m+1 \rangle$$

$$b_m = \langle j, m-1 | J_- | jm \rangle \quad \text{or} \quad b_{m+1}^* = \langle jm | J_+ | j, m+1 \rangle$$

compare the two equations gives

$$a_m^* = b_{m+1}$$

operating of eq from left by J_- , we have

$$J_- J_+ |jm\rangle = a_m J_- |j, m+1\rangle$$

replacing $J_- J_+$ we get

$$(J^2 - J_z^2 - J_z) |jm\rangle = a_m b_{m+1} |jm\rangle$$

or

$$[j(j+1) - m^2 - m] |jm\rangle = a_m b_{m+1} |jm\rangle$$

or

$$a_m = [j(j+1) - m(m+1)]^{1/2}$$

with the value of a_m

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

or

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

similarly

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

last two give equation give the matrix element for J_+ and J_- they are infinte dimentisional

matrices like the j^2 and J_z matrices. The nature of the kronecker deltas in last two equation indicates that all nonvanishing element occure in bloiges along the diagonal corresponding to $j'=j$. The block matrices corresponding to $j=0, 1/2$ and are given below .The rows are labelled by the value of m' and the columns by the values of m .the nonvanishing matrixes for J_x and J_y are evaluated using the relation

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

for $j=0$

$$J_+ = 0, \quad J_- = 0, \quad J_x = 0, \quad J_y = 0$$

for $j=1/2$

$$J_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad J_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

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

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

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

$$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

for $j=1$

$$J_+ = \begin{pmatrix} 0 & 2 & 0 \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix}$$

$$J_- = \begin{pmatrix} 0 & 0 & 0 \\ 2 & 0 & 0 \\ 0 & 2 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \end{pmatrix}$$

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

$$\begin{pmatrix} 0 & 2 & 0 \end{pmatrix}$$

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

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

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

$$\begin{pmatrix} i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

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

$$\begin{pmatrix} 0 & i & -i \end{pmatrix}$$

without a word about the eigenvector the discussion would not be complete. The eigenvector with respect to the $|jm\rangle$ basis will be the column vector would be used for particular cases: $j=0, j=1/2, j=1, \dots$

SPIN ANGULAR MOMENTUM:

To account for the multiplicity of atomic states uhlebeck and goudsmit proposed in 1925 that an electron in an atom possesses an intrinsic angular momentum in addition to orbital angular momentum. This intrinsic angular momentum S is called the spin angular momentum whose projection on the z axis can have the value

$s_z = m_s \hbar$, $m_s = \pm 1/2$. the maximum measurable component of spin angular momentum in units of \hbar is called the spin of the particle and is usually denoted by s . They also suggested that the spin angular momentum gives rise to an intrinsic magnetic moment μ_s gives by

$$\mu_s = - \frac{e\hbar}{2m} S$$

assuming that all the stable and unstable particles to have spin angular momentum

S , we expect its components S_x , S_y and S_z to obey the general commutation relation and S^2 and S_z to have the eigen values $s(s+1) \hbar^2$ and $m_s \hbar$, $m_s = -s, -s+1, \dots, s$ respectively

spin $-(1/2)$ systems

most of the stable elementary particles, electrons, protons, neutrons, etc., come under this category. The matrices representing S_x , S_y and S_z are obtained from the J_x , J_y , and J_z matrices by taking the part corresponding to $j=1/2$, hence

$$S_x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

often it is convenient to work with a matrix defined by

$$S = \frac{1}{2}$$

where

$$x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

the x , y and z matrices are called the Pauli's spin matrices. From the definition it is obvious that their eigenvalues are ± 1 . These matrices satisfy the relation

$$x^2 = y^2 = z^2 = I$$

$$x y = i z, \quad y z = i x, \quad x z = i y$$

$$x y + y x = y z + z y = z x + x z = 0$$

Pauli was the first to recognize the necessity of two component state vectors to explain certain observed features to atomic spectra.

spin vectors for spin $-(1/2)$ system:

Including spin the spin $-(1/2)$ system has how four degree of freedom, the three position coordinates (x, y, z) and another observable pertaining to spin. Taking the z component S_z as the fourth observable the electron wave function can be written as $\psi(r, S_z)$

or (r, m_s) the coordinate m takes the values $+1/2$ or $-1/2$. When the interaction between the spin and space parts is negligible the wave function

$$(r, m_s) = (r) (m_s)$$

where (r) represented that depends on the space coordinates and (m_s) the part that depends on the spin coordinates

The eigenvectors of the spin matrices S_x , S_y and S_z , can easily be obtained by writing the eigenvalue equation. Since the matrices are 2×2 the eigenvectors must be column vector with two components. the eigenvalue equation for S_z with eigenvalue $\hbar/2$ is

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

$$\begin{pmatrix} 0 & -1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

it is evident that $a_2 = 0$ the normalization condition gives

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

the eigenvector of the matrix S_z corresponding to eigenvalue $\hbar/2$ is then

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

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

processing on similar lines the eigenvector for the eigenvalue $-\hbar/2$ is

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

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

these eigenvectors are denoted by χ_+ and χ_- and are usually called the spin up and spin down states respectively

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

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

the two component eigenvectors of spin $-(1/2)$ particles are sometimes called spinors. Eigenvectors of S_x and S_y can also be found in the same way. the spin matrices of a spin $-(1/2)$ system along with eigenvalue and eigenvectors.

Addition of Angular momentum

The operators, J^1 , J^2 , J^3 which satisfy the “standard angular momentum commutation relations”

$$J^j, J^k = i \epsilon_{jkl} J^l, \quad j, k, l = 1, 2, 3 \text{ or } x, y, z,$$

and all results will be equally valid in which J^3 points is called the “quantization axis”, and its choice is arbitrary. This ‘axis’ makes sense as a direction in the usual space only if \hat{J} is an actual angular momentum vector operator—orbital, spin or a combination.

Clebsch – Gordon Coefficient

Clebsch–Gordan (CG) coefficients are numbers that arise in angular momentum coupling in quantum mechanics. They appear as the expansion coefficients of total angular momentum eigenstates in an uncoupled tensor product basis. In more mathematical terms, the CG coefficients are used in representation theory, particularly of compact Lie groups, to perform the explicit direct sum decomposition of the tensor product of two irreducible representations (i.e., a reducible representation) into irreducible representations, in cases where the numbers and types of irreducible components.

From a vector calculus perspective, the CG coefficients associated with the $SO(3)$ group can be defined simply in terms of integrals of products of spherical harmonics and their complex conjugates. The addition of spins in quantum-mechanical terms can be read directly from this approach as spherical harmonics are eigenfunctions of total angular momentum and projection thereof onto an axis, and the integrals correspond to the Hilbert space inner product. From the formal definition of angular momentum, recursion relations for the Clebsch–Gordan coefficients can be found. There also exist complicated explicit formulas for their direct calculation.

For the total angular momentum vector $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$,

$$\mathbf{J} \times \mathbf{J} = i\hbar \mathbf{J}$$

Also, it follows that

$$[J^2, J_z] = 0, [J^2, J_1^2] = [J^2, J_2^2] = 0$$

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

$$|jm\rangle = \sum_{m_1, m_2} C_{jm m_1 m_2} |m_1 m_2\rangle$$

The coefficient of this linear combination are called Clebsh- Gordon coefficient or Wigner coefficients or vector coupling coefficients.

$$\langle m_1 m_2 | jm \rangle = C_{jm m_1 m_2}$$

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

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

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

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

And

$$\langle j m | m_1 m_2 \rangle = \langle m_1 m_2 | jm \rangle^*$$

Second rules

Operating eq from left by J_z , we have

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

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

replacing $|jm\rangle$ using eq and rearranging, we get

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

which is valid only if the coefficient of each term vanishes separately. This leads to one of the rules of vector atom model, that is,

$$m = m_1 + m_2$$

the various m and j values arise from the values of m_1 and m_2 . For given values of j_1 and j_2 , can have values from j_1 to $-j_1$ and j_2 to $-j_2$ m_1 in integral step.

The smallest value w of j occurs for

$$j_1 - k = -j_1 \text{ or } j_2 - k = -j_2$$

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

which is the triangle rule of the vector atom model.

Possible Questions

PART B (4 Marks each)

1. State the commutation relations obeyed by the components of angular momentum and express them in vector notation.
2. What are ladder operators and why are they so called?
3. The definition of angular momentum given by $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is not a general one. Why? Define a general angular momentum operator.
4. Explain spin-up and spin-down states. What are spinors?
5. What are Clebsh-Gordon coefficients? Explain their significance.
6. Write a short note spin of an electron
7. if J_1 and J_2 are angular momentum operators, are $J_1 + J_2$ and $J_1 - J_2$ angular momenta? Explain.
8. State the eigen value-eigen vector relations for the operators J^2 and J_z . Hence obtain the matrices for J^2 and J_z .
9. Show that the raising and lowering operators J_+ and J_- operators are Hermitian conjugates.
10. Prove that the spin matrices S_x and S_y are $\pm \hbar/2$ eigen values.

Part C (10 marks each)

1. What are angular momentum operators? Derive the commutation relations between the different components of the angular momentum.
2. a. Explain the difference between the orbital angular momentum \mathbf{L} and general angular momentum \mathbf{J} . Write down the commutation relations between the components of general angular momentum. (5 Marks)
b. Derive the eigen values of J^2 and J_z . (5 Marks)
3. Explain the matrix formulation of angular momenta. Derive the matrix forms of J_+ , J_- ,

J_x and J_y

4. Explain how concept of spin was introduced and how spin angular momenta contributes to the total angular momentum of the atom. Obtain the spin angular momenta in terms of matrices. What are Pauli matrices?
5. Discuss the various aspects of addition of angular momenta. What are Clebsh-Gordon coefficients and how are they determined?

KARPAGAM ACADEMY OF HIGHER EDUCATION

CLASS: II M.Sc PHYSICS COURSE NAME: QUANTUM MECHANICS II

COURSE CODE: 17PHP301 UNIT I (Angular momentum) BATCH-2017-2019

S.NO	Question	option 1	option 2	option 3	option 4	Answer
1	Equation of Linear momentum	$P = mv$	$P = dv$	$P = md$	$P = m^2v$	$P = mv$
2	Torque	$r \times F$	$r^2 \times F$	$r^2 \times$	$r \times F^2$	$r \times F$
3	Angular momentum is defined as	moment of inertia x angular velocity	torque x velocity	acceleration x force	force x mass	moment of inertia x angular velocity
4	Total angular momentum is equal to	orbital angular momentum + spin angular momentum	. spin angular momentum	linear angular momentum	torque	orbital angular momentum + spin angular momentum
5	Angular momentum =.....	$\hbar(r \times \hat{r})$	$\hbar I r \times$	$\hbar(r^2 \times \hat{r})$	$\hbar I r \times$	$\hbar I r \times$
6	$L \times L = \dots\dots\dots$	$i\hbar L$	$i L$	$i L^2$	$i^2 L$	$i L$
7	Total angular momentum is defined by	$J^2 = J_x^2 + J_y^2 + J_z^2$	$J^3 = J_x^3 + J_y^3 + J_z^3$	$J^2 = J_x + J_y + J_z$	$J = J_x^2 + J_y^2 + J_z^2$	$J^2 = J_x^2 + J_y^2 + J_z^2$
8	Commutative law $[J_x, J_y]$ is equal to	$i J_z$	$i J_z$	$i J_y$	$i J_{z+x+y}$	$i J_z$

9	$[J^2, J_y]$ =.....	1	2	0	3	0
10	$J_+ =$	$J_x + iJ_y$	$J_x - iJ_y$	$J_x^2 + iJ_y^2$	$J_x^2 - iJ_y^2$	$J_x + iJ_y$
11	$J_- =$	$J_x + iJ_y$	$J_x - iJ_y$	$J_x^2 + iJ_y^2$	$J_x^2 - iJ_y^2$	$J_x - iJ_y$
12	$[J_x^2, J_x] =$	$J_x [J_x J_x] + J_x$	J_x	$J_x [J_x J_x] + [J_x J_x] J_x$	J_x^2	$J_x [J_x J_x] + [J_x J_x] J_x$
13	$[J_z, J_+]$ =.....	J_+	J_x	J_z	$J_x J_y$	J_+
14	$[J^2, J_+]$ is equal to	1	2	4	0	0
15	$[J_+, J_-]$ is equal to	J	J_z	J^2	$\hbar J$	J
16	Torque is defined as	moment of force	moment of inertia	rate of change of force	rate of change of distance	moment of force
17	Momentum is a	vector	scalar	dimensionless	product of vector and scalar	vector
18	In quantum mechanics operator associated with linear momentum is	$\hbar \mathbf{r} \times$	$\hbar \mathbf{i}$	$\hbar \mathbf{r}$	$\hbar (\mathbf{r} \times)^2$	$\hbar \mathbf{r} \times$

19	The operator that increases or decreases eigen value another operator is called	. Hamilton operator	Ladder operator	Hermitian operator	angular momentum operator	Ladder operator
20	$[J_x^2, J_x] = \dots\dots\dots$	1	2	4	0	0
21	The operator for energy is _____	i / t	$-i / t$	i / x	$-i v$	i / t
22	Operation on a ket vector from left with an operator A produces	Another ket vector	A bra vector	Another operator	Phase vector	Another ket vector
23	Operation on a bra vector from right with an operator A produces	A ket vector	Another operator	Another bra vector	Phase vector	Another bra vector
24	When an eigen function is not normalizable in a free domain, we can resort to _____	box normalization	plane normalisation	total normalisation	any of the above	box normalization
25	The orbital corresponding to $l = 0$ is called	s orbital	p orbital	d orbital	f orbital	s orbital
26	The orbital corresponding to $l = 1$ is called	s orbital	p orbital	d orbital	f orbital	p orbital
27	The orbital corresponding to $l = 2$ is called	s orbital	p orbital	d orbital	f orbital	d orbital

28	The orbital corresponding to $l = 3$ is called	s orbital	p orbital	d orbital	f orbital	f orbital
29	The quantum numbers required to explain the position of an electron in hydrogen atom are ____	n and l	l and m	n, l and m	n and m	n, l and m
30	The value of the magnetic quantum number can be	0,1,2,3, ...	1,2,3,4, ...	$\pm 1, \pm 2, \pm 3, \pm 4, \pm 5 \dots$	0, $\pm 1, \pm 2, \pm 3, \pm 4 \dots$	0, $\pm 1, \pm 2, \pm 3, \pm 4 \dots$
31	Which of the following statements is correct?	A linear combination of degenerate eigenfunctions of a degenerate level is not an eigen function	A linear combination of degenerate eigenfunctions of a degenerate level is also an eigen function, with the same eigen value.	A linear combination of degenerate eigen functions of a degenerate level is also an eigen function but with different eigen value	A linear combination of degenerate eigen functions of a degenerate level is not an eigen function, but the eigen values are the same.	A linear combination of degenerate eigenfunctions of a degenerate level is also an eigen function, with the same eigen value.
32	The correct form of the angular momentum for quantum number l is ____	lh	l	$[l(l+1)]$	$[l(l+1)]^{1/2}$	$[l(l+1)]^{1/2}$

33	The quantum number l is referred to as _____	angular momentum quantum number	spin angular momentum quantum number	orbital angular momentum quantum number	any of the above	orbital angular momentum quantum number
34	An energy level with orbital angular momentum quantum number l , is _____ fold degenerate.	2-fold	3-fold	$(2l+1)$ fold	1-fold	$(2l+1)$ fold
35	The potential involved outside the nucleus is _____	gravitational	electromagnetic	nuclear	Coulombic	Coulombic
36	The probability of finding the electron of the hydrogen atom at a distance r from the nucleus is called as _____	probability function	probability density	radial probability density	any of the above	radial probability density
37	For the ground state of the hydrogen atom, a maximum probability density P_{10} exists at a radial position given by _____	$P_{10} = 2a$, where a is the radius of the first shell	$dP_{10}/dr = 0$	$dP_{10}/dr = a$ constant	none of the above	$dP_{10}/dr = 0$

38	For the ground state of the hydrogen atom, a maximum probability density occurs at a radial distance from the origin, equal to ____	the Bohr radius	twice the Bohr radius	half the Bohr radius	No relation with Bohr radius.	the Bohr radius
39	The binding energy of deuteron is ____	2.226 MeV	2.226 eV	2.226 keV	Zero	2.226 MeV
40	The eigen value of ground state of helium atom is $Z^2 E_H / n^2$ in which E_H is	13.5 eV	2.75 eV	12.75 eV	3.5 eV	13.5 eV
41	The energy value of two electrons relative to axes with the nucleus at the origin, in ground state of helium atom is	$2Z^2 E_H$	$2Z E_H$	$- 2Z E_H$	$- 2Z^2 E_H$	$- 2Z^2 E_H$
42	For $n = 1, l = 0, m = 0$, the wave function for He atom becomes	$(Z/a_0)^{1/2} e^{-Z/a_0}$	$(Z^3/a_0^3)^{1/2} e^{-Z/a_0}$	$(Z/a_0)^{3/2} e^{-Z/a_0}$	$(Z/a_0^3)^{1/2} e^{-Z/a_0}$	$(Z^3/a_0^3)^{1/2} e^{-Z/a_0}$
43	The secular equation in which all the elements are zero, except	principal diagonal	lower diagonal	upper diagonal	lower and upper diagonal	principal diagonal

44	The perturbation $H^{(1)}$ which is the extra energy of nucleus and electron due to external field in H atom is	$eEr \cos$	$er \cos$	$- eEr \cos$	$- er \cos$	$- eEr \cos$
45	The ground state for H atom is non-degenerate state, the wave function ψ_{100} is given by	$(1/a_0^3)^{1/2} \exp(-r/a_0)$	$(1/a_0^3)^{1/2} \exp(r/a_0)$	$(1/a_0^3)^{3/2} \exp(-r/a_0)$	$(1/a_0^3)^{3/2} \exp(r/a_0)$	$(1/a_0^3)^{1/2} \exp(-r/a_0)$
46	The behaviour of hydrogen atom in first excited state is like a	electric quadrupole moment	electric dipole moment	Zeeman effect	Magnetic dipole moment	electric dipole moment
47	The Bohr radius of the first orbit is	5.267 \AA	0.05267 \AA	0.5267 \AA	52.67 \AA	0.5267 \AA
48	By expansion theorem ψ_{100} may be expanded in terms of a complete set of ortho-normal functions $\psi_{00}, \psi_{10}, \psi_{20}, \dots$ if	$= 1$	$= 0$	$= 0$	0	0
49	The orientation of the splitting of energy levels in first excited state of hydrogen atoms, with external electric field is	parallel	perpendicular	anti-parallel	none of the above	anti-parallel

Scattering: Scattering cross-section – Scattering amplitude – Partial waves – Scattering by a central potential: partial wave analysis – Significant number of partial waves – Scattering by an attractive square-well potential – Briet-Wigner formula – Scattering length – Expression for phase shift – Integral equation – The Born approximation – Scattering by screened coulomb potential – Validity of Born approximation - Laboratory and center of mass co-ordinate systems.

Scattering cross-section

When two particles interact, their mutual cross section is the area transverse to their relative motion within which they must meet in order to scatter from each other. If the particles are hard inelastic spheres that interact only upon contact, their scattering cross section is related to their geometric size. If the particles interact through some action-at-a-distance force, such as electromagnetism or gravity, their scattering cross section is generally larger than their geometric size. When a cross section is specified as a function of some final-state variable, such as particle angle or energy, it is called a differential cross section. When a cross section is integrated over all scattering angles (and possibly other variables), it is called a total cross section. Cross sections are typically denoted σ (sigma) and measured in units of area.

Scattering cross sections may be defined in nuclear, atomic, and particle physics for collisions of accelerated beams of one type of particle with targets (either stationary or moving) of a second type of particle. The probability for any given reaction to occur is in proportion to its cross section. Thus, specifying the cross section for a given reaction is a proxy for stating the probability that a given scattering process will occur. The measured reaction rate of a given process depends strongly on experimental variables such as the density of the target material, the intensity of the beam, the detection efficiency of the apparatus, or the angle setting of the detection apparatus. However, these quantities can be factored away, allowing measurement of the underlying two-particle collisional cross section.

Differential and total scattering cross sections are among the most important measurable quantities in nuclear, atomic, and particle physics.

Scattering amplitude

The differential cross section, $d\sigma/d\Omega$, can be written in terms of a scattering amplitude,

$f(\theta)$. If the interaction is spherically symmetric, then there is no dependence for f . So

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

where $f(\theta)$ is a complex number with units of length. In our application, $f(\theta)$ will have units of fm^2 . For non-relativistic energies, $f(\theta)$ can be determined from the Schrodinger equation with the appropriate scattering boundary conditions at $r \rightarrow \infty$. If the interaction is spherically symmetric, i.e. $V(\vec{r}) = V(r)$, then the Schrodinger equation can be separated into the different orbital angular momentum quantum numbers l .

$$-\frac{\hbar^2}{2m} \left(\frac{d^2 u(r)}{dr^2} - \frac{l(l+1)}{r^2} u(r) \right) + V(r)u(r) = Eu(r)$$

with an equation for each value of l . The same separation holds for scattering problems. One will obtain a scattering amplitude for each value of orbital angular momentum l , which we label as f_l . The complete scattering solution will have a $Y_{lm}(\theta, \phi)$ added on for each l . For spherical symmetry, where there is no ϕ dependence, so the Y_{lm} reduce to Legendre polynomials in $\cos(\theta)$, $P_l(\cos(\theta))$. The scattering amplitude therefore becomes

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) f_l P_l(\cos(\theta))$$

The scattering amplitude $f(\theta)$ and the f_l are complex numbers, with a real and an imaginary part. The sum over orbital angular momentum l in the expression for the scattering amplitude goes to infinity. The contribution from large l goes to zero, and one only needs to sum over a few values of l . The maximum value needed for l is roughly Rp , where R is the size of the target and p is the momentum of the projectile.

Partial waves

Partial wave refers to a technique for solving scattering problems by decomposing each wave into its constituent angular momentum components and solving using boundary conditions.

Scattering by a central potential, partial wave analysis

Partial wave expansion the scattering amplitude is represented as a sum over the partial waves,

$$f = \sum_{\ell=0}^{\infty} (2\ell + 1) f_{\ell} P_{\ell}(\cos \theta)$$

where f is the partial scattering amplitude and P are the Legendre polynomials.

The partial amplitude can be expressed via the partial wave S-matrix element

$$f_{\ell} = \frac{S_{\ell} - 1}{2ik} = \frac{e^{2i\delta_{\ell}} - 1}{2ik} = \frac{e^{i\delta_{\ell}} \sin \delta_{\ell}}{k}$$

Then the differential cross section is given by

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{1}{k^2} \left| \sum_{\ell=0}^{\infty} (2\ell + 1) e^{i\delta_{\ell}} \sin \delta_{\ell} P_{\ell}(\cos \theta) \right|^2$$

and the total elastic cross section becomes

$$\sigma = 2\pi \int_0^{\pi} \frac{d\sigma}{d\Omega} \sin \theta d\theta = \frac{4\pi}{k} \text{Im } f(0)$$

where $\text{Im } f(0)$ is the imaginary part of $f(0)$.

Scattering by an attractive square well potential

The Schrodinger equation for the perturbed system can be written as

$$(\hat{H}_0 + \hat{H}_p) | \mathbf{i} \rangle = E | \mathbf{i} \rangle \quad (1)$$

where \hat{H}_0 is the Hamiltonian of the unperturbed system whose solution is known,

and \hat{H}_p is due to the small perturbation where ϵ is a small parameter. Here, \hat{H}_0 can be the Hamiltonian of the infinite potential well, for instance. In the above equation,

$| \mathbf{i} \rangle$ and E are both

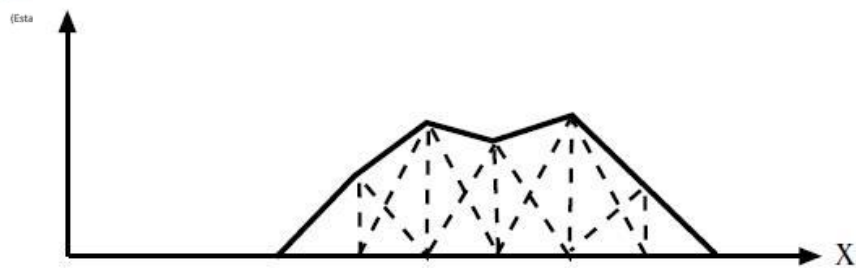


Figure 1: The triangle functions for a piecewise linear approximation of a function. This is a basis that is not orthogonal but yet can be used to seek approximate solutions .

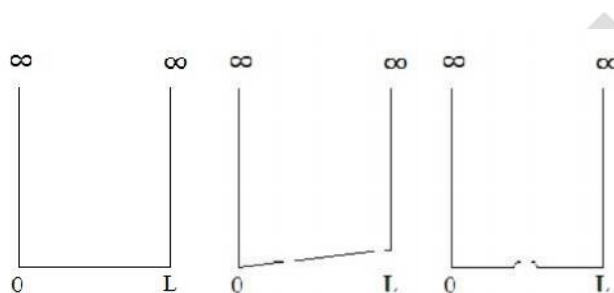


Figure 2: The infinite potential well on the left represents the unperturbed problem. The middle figure represents a perturbation due to a tiny electric field. The right figure represents a perturbation due to imperfection in fabrication or impurities.

unknowns, but we can write them in a perturbation series or expansion, namely

$$|\psi\rangle = |\psi^{(0)}\rangle + |\psi^{(1)}\rangle + |\psi^{(2)}\rangle + \dots \quad (2)$$

$$E = E^{(0)} + E^{(1)} + E^{(2)} + \dots \quad (3), (4)$$

Upon substituting the above series into (1), we obtain The left-hand side of (4) can be expanded and rewritten on a power series in

These two power series in are equal only if $a_i = b_i$, $i = 0, 1, \dots, \infty$.²

Equating the coefficients of the power series on both sides of (4) we have the following equations:

Zeroth Order:

$$\hat{H}_0 |^{(2)}i + \hat{H}_p |^{(1)}i = E^{(0)} |^{(2)}i + E^{(1)} |^{(1)}i + E^{(2)} |^{(0)}i$$

assume that the zeroth order equation is known in terms of an eigenstate $|m\rangle$ with energy

E_m . In other words

$$|^{(0)}i = |m\rangle, \quad E^{(0)} = E_m \quad (7)$$

note is in order regarding the uniqueness of the eigenvalue problem (1). An eigenvector is known only within a multiplicative factor. Hence, its length is indeterminate. This non-uniqueness in its length manifests in the non-uniqueness of the value of the perturbation series (2). To achieve uniqueness, it is best to pin down the length of the total eigenvector given by (2). length of the eigenvector $|i\rangle$ by requiring that

$$\langle m | i \rangle = 1 \quad (8)$$

With this requirement, we substitute (2) into the above. Since $\langle m | ^{(0)}i \rangle = 1$,

because

$|^{(0)}i = |m\rangle$, it is easy to show that $\langle m | ^{(i)}i \rangle = 0, i > 0$. As a consequence, $|^{(i)}i$ is orthogonal to $|m\rangle$. The perturbation series is not necessarily normalized, but it can be normalized later after the series has been calculated. Next, to find the first order corrections to the eigenvalue and the eigenvector, we move the unknowns $|^{(1)}i$ to the left of (8). We then have

$$\hat{H}_0 - E_m |^{(1)}i = E^{(1)} |m\rangle - \hat{H}_p |m\rangle \quad (9)$$

since the operator $\hat{H}_0 - E_m$ has a null space with a null space vector $|m\rangle$.

$$\langle m | \hat{H}_0 - E_m |^{(1)}i = E^{(1)} - \langle m | \hat{H}_p$$

(10)

the first order correction to the energy of the perturbed system.

First, testing the equation (10) with $\langle i |$, we have

$$\langle i | \hat{H}_0 - E_m |^{(1)} i \rangle = E^{(1)} \langle i | i \rangle - \langle i | \hat{H}_p | i \rangle \quad (11)$$

Upon substituting (11) into the above, the left-hand side evaluate

choose $a^{(1)} = 0$ for a number of m reasons: It makes the correction term unique since $|^{(1)} i \rangle$ is orthogonal to $|^{(0)} i \rangle$. It makes the normalization of the eigenvector $| i \rangle$ accurate to second order even though the correction is first order. It will also make the second order corrections much simpler to find.

To find the second order corrections, we rewrite (9) with the unknown $|^{(2)} i \rangle$ on the left hand side. Then (9) becomes

$$\hat{H}_0 - E_m |^{(2)} i \rangle = E^{(1)} |^{(1)} i \rangle + E^{(2)} | i \rangle - \hat{H}_p |^{(1)} i \rangle \quad (12)$$

Testing the above with $\langle m |$, the left hand side becomes zero as before.³ Since we have made $|^{(1)} i \rangle$ orthogonal to $| m \rangle$, on the right-hand side, only the last two terms remain.

Consequently,

$$0 = E^{(2)} - \langle m | \hat{H}_p |^{(1)} i \rangle \quad (13)$$

$$E^{(2)} = \langle m | \hat{H}_p |^{(1)} i \rangle \quad (14)$$

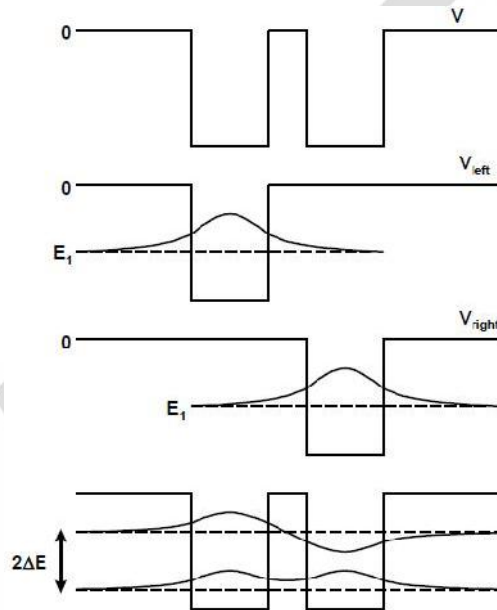
The above procedure can be generalized to arbitrary order. By induction, we notice that the equivalence of to p -th order is

$$\hat{H}_0 | (p) i + \hat{H}_p | (p-1) i = E^{(0)} | (p) i + E^{(1)} | (p-1) i + E^{(p)} | (0) i \quad (15)$$

The above can be rewritten as

$$\hat{H}_0 - E^{(0)} | (p) i = E^{(1)} | (p-1) i + E^{(p)} | (0) i - \hat{H}_p | (p-1) i \quad (16)$$

It is to be noted that with modern advent of computer technology, and given the availability of numerical methods, the calculation of perturbation theory to very high order is laborious and not necessary. However, a perturbation correction can give us insight on how a small change in the Hamiltonian can change the solution.



The tight binding model can be used to find the approximate eigenstates of two quantum wells that are weakly coupled to each other.

Breit-Wigner formula

The condition is equivalent to the condition that a spherical well of depth possesses a *bound state* at zero energy. Thus, for a potential well which satisfies, the energy of the scattering system is essentially the same as the energy of the bound state. In this situation, an incident particle would like to form a bound state in the potential well. However, the bound state is not stable, since the system has a small positive energy. Nevertheless, this sort of resonance scattering is best understood as the capture of an incident particle to form a metastable bound

state, and the subsequent decay of the bound state and release of the particle. The cross-section for resonance scattering is generally much larger than that for non- resonance scattering.

The **relativistic Breit–Wigner distribution** (after the 1936 nuclear resonance formula of Gregory Breit and Eugene Wigner) is a continuous probability distribution with the following probability density function

$$f(E) = \frac{k}{(E^2 - M^2)^2 + M^2\Gamma^2}$$

where k is a constant of proportionality, equal to

$$k = \frac{2\sqrt{2}M\Gamma\gamma}{\pi\sqrt{M^2 + \gamma}}$$

$$\gamma = \sqrt{M^2 (M^2 + \Gamma^2)}.$$

The form of the relativistic Breit–Wigner distribution arises from the propagator of an unstable particle,^[4] which has a denominator of the form $p^2 - M^2 + iM$. (Here, p^2 is the square of the four-momentum carried by that particle in the tree Feynman diagram involved.) The propagator in its rest frame then is proportional to the quantum-mechanical amplitude for the decay utilized to reconstruct that resonance,

$$\frac{\sqrt{k}}{(E^2 - M^2) + iM\Gamma}$$

The resulting probability distribution is proportional to the absolute square of the amplitude, so then the above relativistic Breit–Wigner distribution for the probability density function.

The form of this distribution is similar to the amplitude of the solution of the classical equation of motion for a driven harmonic oscillator damped and driven by a sinusoidal external force. It

has the standard resonance form of the Lorentz, or Cauchy distribution, but involves relativistic variables $s=p^2$, here $=E^2$. The distribution is the solution of the differential equation for the amplitude squared w.r.t. the energy (frequency), in such a classical forced oscillator,

$$f'(E) \left((E^2 - M^2)^2 + \Gamma^2 M^2 \right) - 4Ef(E)(M - E)(E + M) = 0$$

$$f(M) = \frac{k}{\Gamma^2 M^2}$$

This is the famous Breit-Wigner formula. The variation of the partial cross-section with the incident energy has the form of a classical resonance curve.

THE BORN APPROXIMATION:

The wave function (r') required to evaluate the equation. Born used an iterative procedure for its evaluation. In the first Born approximation (r') in the integral equation is replaced by the incoming plane wave $\exp(iK.r')$. This leads to an improved value for the wave function (r) which is used in the integral in the second Born approximation. This iterative procedure is continued till both the input and output r' s are almost equal. As higher order approximations are complicated we shall restrict our discussion only to first Born approximation.

Replacing (r') in the integral equation by $\exp(iK.r')$, we get

$$f(\theta) = -1/4 \int \exp[i(k-k').r'] U(r') d^3r' \quad (1)$$

where k and k' are the wave vectors in the incident and scattered directions respectively. The quantity $(k-k') = q$ is then the momentum transfer from the incident particle to the scattering potential. In other words the change in momentum q due to collision is given by

$$q = (k-k') \quad \text{or} \quad q = 2k \sin \theta/2 \quad (2)$$

Replacing $(k-k')$ by q in eq 1 we get

$$f(\theta) = -1/4 \int \exp(iq.r') U(r') d^3r' \quad (3)$$

the angular integration in equation 3 can easily be carried out by taking the direction of q

and r' by θ as the polar axis. Denoting the angle between q and r' by ϕ

$$f(\theta) = -\frac{1}{4} \int_0^\infty \int_0^{2\pi} \exp(iq r' \cos \phi) U(r') r'^2 \sin \phi d\phi dr' \quad (4)$$

integration over ϕ gives 2π . The integral can easily be evaluated by writing

$$-\cos \phi = x \text{ or } -\sin \phi d\phi = dx$$

we get

$$\int_0^{2\pi} \exp(iq r' \cos \phi) \sin \phi d\phi = \int_{-1}^1 \exp(iq r' x) dx \\ = \exp(iq r') - \exp(-iq r') \quad (5)$$

substituting the value of the angular part in equ (4)

$$f(\theta) = -2\mu^2 \int_0^\infty \sin(qr')/qr' V(r') r'^2 dr'$$

from which $f(\theta)$ can be calculated. It may be noted from eq (5) that the only variable parameter in $f(\theta)$ is magnitude of the momentum transfer q where q is given by eq (2) thus the scattering cross section depends on the momentum of the incident particle k and the scattering angle θ through the combination $q = 2k \sin(\theta/2)$

Scattering by screened coulomb potential

The cross section $\sigma(\theta)$ for the scattering of protons by a screened Coulomb potential is evaluated using the numerical solution of the classical equations of motion.

Let the potential energy of a screened Coulomb potential interacting with a positive charge be given by

$$V(r) = k Ze^2 \exp(-\mu r)/r \quad (1-a)$$

$$= C \exp(-\mu r)/r \quad (1-b)$$

where $C = k Ze^2$.

In SI units, $k = 9.00 \times 10^9 \text{ Nm}^2/\text{C}^2$, Z is the atomic number of the nuclei, $e = 1.602 \times 10^{-19} \text{ C}$, $\mu \sim 1/\text{length} \sim \text{m}^{-1}$

the equations of motion and find θ for a varying set of impact parameters.

An approximation to $\sigma(\theta)$ would be

$$\sigma(\theta) \sim \left(\frac{1}{\sin(\theta/2)} - \frac{1}{\sin(\theta/2 - \theta_0)} \right)^2 \sim m^2 \quad (2)$$

Using eq (1-b) we have

$$d^2 x/dt^2 = (1/m) \{-V/x\} \quad (3)$$

$$d^2 y/dt^2 = (1/m) \{-V/y\} \quad (4)$$

The finite difference solution are

$$x_n = 2x_{n-1} - x_{n-2} + ((\hbar^2/m) C \exp(-\mu r_{n-1}) x_{n-1} \{\mu^2/r_{n-1}^2 + 1/r_{n-1}^3\}) \quad (5)$$

and

$$y_n = 2y_{n-1} - y_{n-2} + ((\hbar^2/m) C \exp(-\mu r_{n-1}) y_{n-1} \{\mu^2/r_{n-1}^2 + 1/r_{n-1}^3\}) \quad (6)$$

Validity of Born approximation

Born approximation replaces ψ by ϕ in Lippmann–Schwinger equation, which is integrated together with the potential. Therefore, in order for Born approximation to be good, the difference between ψ and ϕ must be small where the potential exists. The self-consistency requires that

$$|\psi(\vec{x}) - \phi(\vec{x})| \ll |\phi(\vec{x})|$$

where $V(\vec{x})$ is sizable, and the l.h.s. can be evaluated within Born approximation itself. From Lippmann–Schwinger equation

$$\left| \frac{2m}{\hbar^2} \int d\vec{x}' \frac{e^{ik|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|} V(\vec{x}') e^{i\vec{k}\cdot\vec{x}'} \right| \ll 1$$

we require this condition at $x = 0$ where the potential is the strongest presumably.

For a smooth central potential, with a magnitude of order V and a range of order a , we can qualitatively work out the validity constraint. Taking

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k along the z axis, and looking at $x' = 0$ where the potential is most important presumably (and relabeling $x = 0$ as $\sim x$), the condition is

$$\frac{2m}{\hbar^2} \left| \int d\vec{x} \frac{e^{ikr}}{4\pi r} V(\vec{x}) e^{ikz} \right| \ll 1$$

When $k \ll a-1$, we can ignore the phases in the integral, and it is given roughly by

$$\frac{2m}{\hbar^2} |V_0| a^2 \frac{1}{2} \ll 1 \quad (k \ll a^{-1})$$

Numerical coefficients are not to be trusted. On the other hand, when $k \gg a-1$, the phase factor oscillates rapidly and we can use stationary phase approximation. The exponent is $ikr + ikz$, and it is stationary only along the negative z -axis $z = -r$. Expanding around this point, it is $ikr + ikz = ik(x^2 + y^2)/r + O(x^3, y^3)$. The Gaussian integral over x, y then gives a factor of r/k , while z is integrated along the stationary phase direction from $-a$ to 0. Therefore, the validity condition is given roughly by

$$\frac{2m}{\hbar^2} \frac{a}{4k} |V_0| \ll 1 \quad (k \gg a^{-1})$$

On the other hand, we can estimate the total cross section in both limits.

$$\begin{aligned} f^{(1)}(\vec{k}', \vec{k}) &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d\vec{x} V(\vec{x}) e^{i\vec{q} \cdot \vec{x}} \\ &\sim -\frac{1}{4\pi} \frac{2m}{\hbar^2} V_0 \frac{4\pi}{3} a^3 \quad (q \ll a^{-1}) \end{aligned}$$

For a large momentum transfer, say along the x axis, y and z integral each gives a factor of a because of no phase variation, while x integral oscillates rapidly and cancels mostly; it leaves only $\sim 1/q$ contribution from non-precise cancellation. Therefore,

$$f^{(1)}(\vec{k}', \vec{k}) \sim -\frac{1}{4\pi} \frac{2m}{\hbar^2} V_0 \frac{\pi a^2}{q} \quad (q \gg a^{-1})$$

Because the momentum transfer q is of the order of k (except the very forward region which we neglect from this discussion), the total cross sections are roughly

$$\sigma \sim \begin{cases} \frac{1}{4\pi} \left(\frac{2m}{\hbar^2} V_0 \frac{4\pi}{3} a^3 \right)^2 & (k \ll a^{-1}) \\ \frac{1}{4\pi} \left(\frac{2m}{\hbar^2} V_0 \frac{\pi a^2}{q} \right)^2 & (k \gg a^{-1}). \end{cases}$$

It is interesting to note that, once the validity condition is satisfied, the total cross section is always smaller than the geometric cross section $4a^2$

$$\sigma \ll \frac{16}{9}\pi a^2 \quad (k \ll a^{-1})$$

$$\sigma \ll 4\pi a^2 \quad (k \gg a^{-1})$$

Laboratory and centre of Mass co-ordinate system

Unlike the two-body case, there is no gain in simplicity if we use relative coordinates for the N body system in general. For two bodies, there is only one set of relative coordinates, while there are two sets of particle coordinates, one for each particle. For three bodies, there are three combinations of separations between individual particles, just as there are three sets of particle coordinates. For all higher values of, the number of relative separations is always larger than the number of particles. In conclusion, from onward, it makes more sense to define the positions and velocities with respect to a given coordinate system. Although not necessary, it is often convenient to use the center of mass system for our orbit calculations. The center of mass is defined in any coordinate system.

In a one-dimensional system of weights hanging from a beam in the Earth's gravitational field, the left and right parts of the beam will be in equilibrium if we support the beam exactly at the center of mass. The same is true for a two-dimensional plank with masses. With three dimensions, we have no room left in an extra dimension for external support, but an analogous result still holds: the motion of the center of mass is the same as if the entire mass of the system was concentrated there and acted upon by the resultant of all external forces.

Possible Questions

Part B (4 Marks each)

1. Write a note on Scattering Amplitude.
2. Briefly explain Neutron Proton scattering with relevant expression.
3. Describe scattering cross section.
4. What is the difference between differential scattering cross section and total scattering cross section? Explain.
5. Write a short note on partial waves.
6. Define scattering length. How is related to zero energy cross-section?
7. Discuss the validity conditions for Born approximation.
8. What is phase shift? Explain the nature of phase shift in the case of repulsive and attractive potentials.
9. Discuss about the scattering by screened Coulomb potential.
10. Write a short note on laboratory coordinate system and centre of mass coordinate system.

Part C (10 marks each)

1. Explain scattering amplitude and scattering cross section. Derive expressions for them.
2. Discuss in detail about the scattering by a central field, using partial wave analysis and obtain equations for scattering cross section and scattering amplitude.
3. Deduce optical theorem
4. What is meant by Ramsauer-Townsend effect?
5. Discuss the theory of scattering by an attractive square well potential well.
6. Derive Breit-Wigner formula for resonant cross sections.

7. Explain phase shift during a scattering. Obtain relation for Born approximation for phase shift.
9. Discuss the validity of Born Approximation.
10. Explain the difference between laboratory coordinate system and centre of mass coordinate system.

S.No	Questions	Opition 1	Opition 2	Opition 3	Opition 4	Answer
1	In _____ a beam of particle is allowed to pass close to a scattering material	scattering	target	energy	wave	scattering
2	Scattering material is called _____	dicrete	particles	frquency	energy	target
3	In bound states the energy of eigen values are _____	positive	negative	infinty	zero	negative
4	The angular distribution of the scattered particles are related to _____	light	energy	particle	wave function	wave function
5	The study of scattering is important in studying the properties of _____ atom		energy	spectral line	material	atom
6	The angle between the initial and final straight line paths ia called _____ scattering angle		polarization	spectral line	scattering	scattering angle
7	Cross- sections are usually measured in _____	barn	cm	mm	ampere	barn
8	The probability that a particle will be scattered as it traverses a given thickness of matter can be expresses in terms of a quantity called the _____.	Total scattering cross-section	Differential scattering cross-section	Scattering cross-section	scattering	Scattering cross-section
9	If the energy of the incident particles does not change, then such scattering are called _____.	elastic scattering	inelastic scattering	Compton scattering	differential scattering	elastic scattering

10	If the energy of the incident particles changes after collision, then such scattering are called _____.	elastic scattering	inelastic scattering	Compton scattering	b and c	b and c
11	In wave mechanics, an incident beam of particles is represented by a _____ wave.	normal	Longitudinal	Stationary wave	ordinary	Longitudinal
12	The scattering of a particle of mass m by a central potential V(r), such that V(r) tends to zero when r tends to _____.	zero	constant value	infinity	finite value	Infinity
13	The complete time dependent solution of the schroedinger equation for central potential V(r) is _____.	$y(r,t) = y(r) e^{iEt/\hbar}$	$y(r,t) = -y(r) e^{-iEt/\hbar}$	$y(r,t) = -y(r) e^{iEt/\hbar}$	$y(r,t) = y(r) e^{-iEt/\hbar}$	$y(r,t) = y(r) e^{iEt/\hbar}$
14	The Schroedinger equation for central potential V(r) is written as _____.	$[-(\hbar^2/2m)\nabla^2 + V(r)]y = Ey$	$[-(\hbar^2/2m)\nabla^2 + V(r)]y = Ey$	$[-(\hbar^2/2m)\nabla^2 - V(r)]y = Ey$	$[-(\hbar^2/2m)\nabla^2 - V(r)]y = Ey$	$[-(\hbar^2/2m)\nabla^2 - V(r)]y = Ey$
15	_____ is a solution of the scattering problem for a source of unit strength at point r'.	Bessel's function	Green's function	Legendre's function	Hermite's function	$[-(\hbar^2/2m)\nabla^2 + V(r)]y = Ey$
16	The delta function of Green's function is _____ everywhere except at r=0.	zero	finite	infinite	constant	Bessel's function
17	Green's function has proper _____ form.	differential	integral	asymptotic	none of the above	asymptotic
18	The scattering amplitude f(q,f) for the scattering problem of stationary wave is given by _____.	$(m/2\pi\hbar^2)\int_0^\infty V(r) Y(r) dr e^{-ik.r}$	$(m/2\pi\hbar^2)\int_0^\infty V(r) Y(r) dr e^{ik.r}$	$(m/4\pi\hbar^2)\int_0^\infty V(r) Y(r) dr e^{-ik.r}$	$(m/4\pi\hbar^2)\int_0^\infty V(r) Y(r) dr e^{-ik.r}$	$(m/4\pi\hbar^2)\int_0^\infty V(r) Y(r) dr e^{-ik.r}$

19	Born approximation is applicable for the scattering centres which are _____.	strong	Weak	moderate	none of the above	Weak
20	In the equation $Y(r) = e^{ikr} + f(q) e^{ikr}/r$, the first term represents the _____.	scattered wave function	re-scattered wave function	incident wave function	recoiled wave function	incident wave function
21	The first Born approximation is given by	$Y = e^{ikr} - (m/2p^2) \oint G(r,r') V(r') e^{ik.r'} d\mathbf{r}'$	$Y = -e^{ikr} - (m/2p^2) \oint G(r,r') V(r') e^{ik.r'} d\mathbf{r}'$	$Y = e^{ikr} + (m/2p^2) \oint G(r,r') V(r') e^{ik.r'} d\mathbf{r}'$	$Y = -e^{ikr} + (m/2p^2) \oint G(r,r') V(r') e^{ik.r'} d\mathbf{r}'$	$Y = -e^{ikr} - (m/2p^2) \oint G(r,r') V(r') e^{ik.r'} d\mathbf{r}'$
22	The first Born approximation scattering amplitude is _____.	$f(q,f) = (m/2p^2) \oint e^{i(k-k')r'} V(r') d\mathbf{r}'$	$f(q,f) = (m/2p^2) \oint e^{i(k-k')r'} V(r') d\mathbf{r}'$	$f(q,f) = - (m/2p^2) \oint e^{i(k-k')r'} V(r') d\mathbf{r}'$	$f(q,f) = - (m/2p^2) \oint e^{i(k-k')r'} V(r') d\mathbf{r}'$	$f(q,f) = - (m/2p^2) \oint e^{i(k-k')r'} V(r') d\mathbf{r}'$
23	The scattering of high energy particle by the square well potential well of radius 'a' and V_0 , $V_0 \ll E$, this condition gives _____.	$(m/2p^2 E) V_0$ $a \gg 1$	$(m/2p^2 E) V_0$ $a = 0$	$(m/2p^2 E) V_0$ $a \ll 1$	$(m/2p^2 E) V_0$ $a = a$	$(m/2p^2 E) V_0$ $a \ll 1$
24	The ordinary coulomb potential is $V(r) =$ _____.	$(1/4pe_0) (Zze^2/r)$	$-(1/4pe_0) (Zze^2/r)$	$(1/4pe_0) (Z^2 ze^2/r)$	$(1/4pe_0) (Zz^2 e^2/r)$	$-(1/4pe_0) (Zze^2/r)$
25	The screened coulomb potential is _____.	$(-Zze^2/4pe_0) e^{-r/r_0}$	$Zze^2/4pe_0) e^{-r/r_0}$	$(-Zze^2/4pe_0) e^{r/r_0}$	$(Zze^2/4pe_0) e^{r/r_0}$	$Zze^2/4pe_0) e^{-r/r_0}$
26	The method of partial waves is mainly applicable to _____.	Coulomb potential	Screened coulomb potential	Weak potential	Spherically symmetric potential	Spherically symmetric potential
27	In higher perturbation theory, a plane wave is equivalent to _____.	transverse waves	longitudinal waves	number of spherical waves	radial waves	number of spherical waves

28	In the case of scattering problem having high scattering potential will have the solution for Y as _____.	$R(r) \ddot{A}(q) j(f)$	$r q f$	e^{ikr}	e^{ikz}	$R(r) \ddot{A}(q) j(f)$
29	If the incident wave travels along Z-axis, the value of $j(f) =$ _____.	differentiable	infinite	finite	constant	constant
30	In the method of partial wave, the Legendre polynomial is _____.	$-P_1(\cos q)$	$P_1(\cos q)$	$P_1(\sin q)$	$P_1(\sin q)$	$P_1(\cos q)$
31	A plane wave is equivalent to the superposition of a number of _____.	Stationary	Transverse	Spherical	Longitudinal	Spherical
32	The phase between the asymptotic form of the actual radial function $R(r)$ and the radial function $j_l(kr)$ in the absence of scattering potential $v=0$ will be _____.	minimum	Constant	infinite	maximum	maximum
33	The Green's function has a singularity at $r =$ _____	finite	infinity	0	none of the above	0
34	The Born approximation simply accounts neglecting the rescattering wave of the scattered waves provided the scattered wave is _____ compared with the incident wave.	large	small	damped	none of the above	small
35	If V_1 and V_2 are spherically symmetric, the distorted Born approximation of the phase shift d_l that are associated with _____.	V_1 and V_2	V_2	V_1	None of the above	V_1

36	Born approximation is poor for the _____.	alkali	c and d	lighter	heavier	heavier
37	Green's function is _____ in nature.	asymptotic	differentiable	symmetrical	antisymmetrical	asymptotic
38	If r represents the number of particles present in unit volume and v represents the velocity of the incident particles, then $J =$ _____.	$-rv$	$-rv^2$	rv	rv^2	rv
39	The plane wave term e^{ikr} represents a wave unit density and of current density _____.	k/m	$-k/m$	k/m^2	$-k^2/m$	k/m
40	$d(r)$ satisfies the first requirement of a delta function i.e., it is zero everywhere except at $r =$ _____.	1	-1	infinity	0	0
41	The born approximation will be good only when the scattered wave function is not much different from _____ wave function.	recoiled	incident	rescattered	none of the above	incident
42	If the high energy particles are scattered by the spherical potential well of radius a and depth V_0 then it means that V_0 _____ E .	\ll	\gg	\geq	\leq	\ll
43	Green's function is a solution of the scattering problem for a source of _____ strength at point r .	maximum	minimum	unit	none of the above	unit
44	_____ has proper asymptotic form.	Legendre's function	Green's function	Hermite's function	Bessel's function	Green's function

45	The method of _____ waves is mainly applicable to spherically symmetric potential.	polarized	unpolarised	circular	partial	partial
46	In _____ perturbation theory, a plane wave is equivalent to number of spherical waves.	Higher	Lower	Linear	Spherical	Higher
47	_____ approximation is poor for heavier atoms.	Maclaurin's	Rolle's	Born's	Lagrangian's	Born's
48	An angular momentum is also called _____	spin	half spin	eigen value	momentum	spin
49	In study of angular momentum the commutation relations obeyed by the _____	operator	spin	momentum	spin	operator
50	The classical particle do not get scattered if _____	$l > k r_0$	$l = 0$	$l > k$	$l < k$	$l > k r_0$
51	If the cross-section of the scattering reaches the value is called _____	absorbance	phase shift	function	resonance	resonance
52	The concept of scattering length is extensively used in the investigations relating to the scattering of thermal _____	positrons	electrons	neutrons	protons	neutrons
53	The scattering cross-section depends on the momentum of the incident _____	particle	wave	light	energy	particle

UNIT-III SYLLABUS

Many Electron Problem: Indistinguishable particles, Pauli principle – Inclusion of spin – Spin functions for two electrons – Spin functions for three electrons – The Helium atom – Central field approximation – Thomas-Fermi model of the atom – Hartree equation – Hartree-Fock equation – Molecular orbital theory: Hydrogen molecule ion H_2^+ - Valence bond theory

Indistinguishable Particles

These basis functions does not solve the Schrodinger equation yet, but they have to satisfy certain symmetry conditions depending on the kind of particles they represent.

1. Non-identical Particle Case:

Let us assume that we have N particles, and M modes to fit this N particles. We can construct a state for non-identical particles that looks like

$$| \text{diff } i = |1, a_i | 2, b_i | 3, c_i \dots | N, n_i$$

In terms of basis function, we may express the above as

$$| a b \dots n i = |1, a_i | 2, b_i | 3, c_i \dots | N, n_i \quad (1)$$

Or

$$a b \dots n (r_1, r_2, \dots, r_N) = a(r_1) b(r_2) \dots n(r_N) \quad (2)$$

We can fit the N particles in n modes, and these n modes can be repeating or non-repeating. For non-repeating case, it is necessary for $M > N$.

However, the above wavefunction cannot be used for bosons and fermions, as we will get a new wavefunction when we swap the positions of two particles. But bosons and fermions are indistinguishable particles. We will consider them separately.

2. Boson Case:

For the N boson particle case, we can write the legitimate wavefunction, which can be used as a basis function, as

| identical-bosons $i \propto$ | identical-bosons $i \propto$

$$\hat{P}|1, a|2, b|3, c| \cdots |N, n| \quad (3)$$

where \hat{P} is a permutation operator, and the above summation is over all possible per

mutations of the coordinate \mathbf{r}_i over the one-particle eigenstates a, b, c, \cdots, n . The

above

wavefunction remains unchanged when we permute the positions of two particles, because for every $|1, a| \cdots |i, l| \cdots |j, p| \cdots |N, n|$, there is a $|1, a| \cdots |j, l| \cdots |i, p| \cdots |N, n|$ in

above summation. Hence, swapping of i and j will not change the sign of the above wavefunction. The above can also be written as a basis function as

$$| a b \cdots n | \propto \hat{P} | 1, a | 2, b | 3, c | \cdots | N, n | \quad (4)$$

3. Fermion Case:

For the N fermion case, we can write the wavefunction, which can be used as a basis function, as

where the “+” sign is chosen for even permutation while the “-” sign is chosen for odd

permutation. A permutation involves a unique pairwise exchange of two particles. The permutation is even or odd depending on the number of pairwise exchanges that have taken place.

Therefore, given a term $|1, a| \cdots |i, l| \cdots |j, p| \cdots |N, n|$, there always exists another term:

$-|1, a| \cdots |j, l| \cdots |i, p| \cdots |N, n|$ in the above summation since they differ by one permutation. If $i = j$, the two terms cancel each other implying that they cannot be in the

same position. Likewise all the terms in the sum cancel each other since every term that

contains i and j can be paired up with every other terms in the sum. Moreover, If $l = p$, all terms in the summation above cancel as well implying that they cannot be in the same mode or state. Therefore, the above is a legitimate basis function that represents the fermions as it obeys Pauli's exclusion principle. Also, there is a sign change when the position of two particles are swapped.

Pauli exclusion principle

The interactions between electrons and only consider their Coulomb repulsion by empirical rules.

Consider two identical particle system (e.g., two electrons in a Helium atom). Suppose their wavefunction is (x_1, x_2) , where x_i is the coordinate of the i th particle, e.g., $x = (r, \sigma)$ with r the spatial position and $\sigma = \pm \frac{1}{2}$, the spin of the particle, etc.

Consider the exchange operation \hat{P}_{12} : exchanging the coordinates of the two particles,

$$\hat{P}_{12} (x_1, x_2) = (x_2, x_1).$$

If we choose (x_1, x_2) as an eigenstate of \hat{P}_{12} with eigenvalue p , then the eigen equation is

$$\hat{P}_{12} (x_1, x_2) = p (x_1, x_2).$$

Acting \hat{P}_{12} second time we get back to the original state,

$$p^2 (x_1, x_2) = (x_1, x_2), \quad \text{or } p^2 = 1$$

Therefore, p can only has two values

$$p = \pm 1.$$

The quantum particles with $p = 1$ are referred to as Boson particles, or simply Bosons; The quantum particles with $p = -1$ are referred to as Fermion particles, or simply Fermions. A more general analysis shows that with integer spin are always

Bosons, and particles with half-odd-integer spins are always Fermions. For example, electrons and protons are Fermions, and photons (light quanta) are Bosons; Helium-4 is Boson because its spin is zero, but Helium-3 atom is Fermion with spin 1/2.

For a general quantum many-body wavefunction, the exchange operation is

$$\hat{P}_{nm}(\dots, x_n, \dots, x_m, \dots) = \pm (\dots, x_m, \dots, x_n, \dots),$$

where + corresponds to Boson system, and – to Fermion system. This is an exact property of a quantum many-body system.

Spin function for two electrons

Spin is a special property of atomic or subatomic particles that has no classical analogue. Electron has spin. We can think of it as being due to the self spinning of the electron, but we should not let our imagination run further than that. Spin of an electron gives it a spin angular momentum in addition to the orbital angular momentum it possesses. The spin also endows an electron with a magnetic dipole moment that causes it to interact with a magnetic field.

The spin of some particles is found to have binary values of “spin up” and “spin down” experimentally by the famous Stern-Gerlach experiment. This binary nature, as we shall see, fits nicely in the mathematical structure of angular momentum in quantum mechanics, but it cannot be described by a wavefunction or wave mechanics. Instead, it can be represented by matrix mechanics.

Spin functions for three electrons

The z component of the orbital angular momentum, represented by the operator L_z , is quantized to be $m\hbar$ where $-l \leq m \leq l$, l being an integer related to the total

angular momentum square operator L^2 with eigenvalue $l(l+1)\hbar^2$.

It can be shown that the relationship between the total angular momentum number l and the z-component of the angular number m is not restricted to orbital angular momenta. It can be established for all quantum mechanical angular momenta, as is

shown in Appendix A. A more general framework for angular momentum is that for $J^2 = J_x^2 + J_y^2 + J_z^2$, an operator J^2 that represents the square of the total angular momentum, and J_x, J_y, J_z , operators that represent the x, y, and z components of angular momenta, then

$$J^2 |L, M\rangle = L(L+1)\hbar^2 |L, M\rangle \quad (1)$$

$$J_z |L, M\rangle = M\hbar |L, M\rangle, \quad -L \leq M \leq L \quad (2)$$

The above results for orbital angular momentum by using wave mechanics and wavefunctions, but they can be proven for general angular momentum by using rotational symmetry of 3D coordinate space, and mathematics of raising and lowering operators. Spin angular momentum operators also fit under the framework of general angular momentum operator, and can be thought of as a special case of the above framework. For spins, we let \hat{S} represent the total angular momentum operator, while \hat{S}_z represents the z component of the spin angular momentum. As a result, the corresponding z component of the spin angular momentum, represented by the operator \hat{S}_z , has only two eigenvalues and two eigenstates: an up state with angular momentum

The corresponding x and y components of the spin angular momentum can be represented by operators \hat{S}_x and \hat{S}_y . Together with \hat{S}_z , they satisfy the following commutation relations

$$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z, \quad [\hat{S}_z, \hat{S}_x] = i\hbar \hat{S}_y, \quad [\hat{S}_z, \hat{S}_y] = -i\hbar \hat{S}_x$$

The above is similar to the commutation relations satisfied by \hat{L}_x, \hat{L}_y , and \hat{L}_z , where they have been motivated by wave mechanics. That if an operator is to represent an angular momentum, then their x, y, and z components have to satisfy the above commutation relations by rotational symmetry of the 3D coordinate space.

The Helium atom

The essence of this approximation is to keep the quantum nature of particles

but ignoring their dynamic interactions due to Coulomb repulsion by empirical Hund's rule, Single-particle Schrodinger equation,

$$\hat{H} \psi_k(x_1) = E_k \psi_k(x_1)$$

the total wavefunction may be written as

$$\psi(x_1, x_2, \dots, x_N) \propto \psi_{k_1}(x_1) \psi_{k_2}(x_2) \dots \psi_{k_N}(x_N)$$

not taking the exchange symmetry into account. In order to include this important quantum symmetry, consider first a 2-particle system, $N = 2$,

$$\psi_B(x_1, x_2) = [\psi_{n_1}(x_1) \psi_{n_2}(x_2) + \psi_{n_1}(x_2) \psi_{n_2}(x_1)] \quad \text{for Boson}$$

or $[\psi_{n_1}(x_1) \psi_{n_1}(x_2) \dots]$ so that $\psi_B(x_1, x_2) = \psi_B(x_2, x_1)$ for Bosons

$\psi_F(x_2, x_1)$ for Fermions. One can also construct a symmetric wavefunction for two Bosons by a single wavefunction as $\psi_B(x_1, x_2) = \psi_{n_1}(x_1) \psi_{n_1}(x_2)$, or $\psi_{n_2}(x_1) \psi_{n_2}(x_2)$.

Notice that if $k_1 = k_2$, $\psi_F(x_1, x_2) = 0$, but not $\psi_B(x_1, x_2)$. This indicates that two Fermions cannot occupy the same state, but it two bosons are allowed to occupy the same state.

A state can only be occupied by at most a single Fermion; But it can be occupied by any number of Bosons.

The first above statement is Pauli exclusion principle. The second statement is the property that leads to the so-called Bose-Einstein condensation of bosons at low temperature. As active ingredients in atoms and molecules are electrons which are fermions, we will mainly use Pauli principle. It is obvious that in the independent-particle approximation (e.g., ignoring particle interactions), the ground state of an N -electrons system is given by the Slater determinant constructed from the lowest N single particle states. For atoms, these single particles states are naturally the eigenstates of hydrogenlike atoms as we discussed previously. For molecules, these single particle states are constructed by a linear combinations of atomic different nuclear states at configurations.

$$(x_1, \dots, x_N) = (r_1, \dots, r_N) (1, \dots, N).$$

Hence, if spin wavefunction is antisymmetric, the spatial wavefunction must be symmetric in order for the total wavefunction to be antisymmetric, vice versa.

Now we apply this simple analysis to atoms, the elements on the periodical table, where the identical fermions are electrons with spin-1/2. We will qualitatively discuss the ground states of the atoms. In the next section, we will attempt to calculate the ground-state energy value of the two electron system, helium atom. By solving the Schrödinger equation of hydrogenlike atoms in the previous section, we know the electron's states in an atom can be characterized by four quantum numbers (n, l, m, m_s): n - principle quantum number specified main energy levels (shells), l - (orbital) angular momentum quantum number, and m - (orbital) magnetic quantum number and m_s - spin magnetic quantum number. We extend this to many-electron's state ignoring the interactions, spin-orbit couplings, etc., by using the independent-particle approximation. Using notation

$$l = 0 \text{ s state, } l = 1 \text{ p state, } l = 2 \text{ d state } \dots$$

and noticing m and m_s are degenerate quantum numbers, we conclude that s shell can take up to two electrons (single orbital with $m = 0$ but one electron with spin up $m_s = 1/2$, the other electron with spin down $m_s = -1/2$); p shell can take up to 6 electrons (three states specified by $m = 1, 0, -1$, each can take one electron with spin up and one electron with spin down); d shell can take up to 10 electrons (5 states with $m = 2, 1, 0, -1, -2$, each can take two electrons), etc. These energy levels are ordered as total possible maximal number of electrons.

In this independent-particle picture, the way each electron of an atom occupies a particular hydrogen state is called electron configuration. In the ground state, the electron configuration of an atom is given by filling these hydrogen orbitals from the lowest, in the ordered series as

$$(1s)(2s)(2p)(3s)(3p)(4s)(3d)(4p)(5s) \dots$$

ies (such as total angular momentum, spins etc.) of the corresponding atom. More information can be specified by using the so called atomic spectral term (or atomic term) to represent states of an atoms. Some correction to independent-particle approximation for the ground-state atomic term due to Coulomb repulsion will be considered by the empirical rules.

Atomic spectral terms. We use notation $(2S+1)LJ$ to denote a particular atomic state where S is its total spin, L its total orbital angular momentum and J the total angular momentum (spins and orbitals). We use capital Latin letters for each value of orbital quantum number as

$L =$	0	1	2	3	4	5	6	7	8	9	10	...
	S	P	D	F	G	H	I	K	L	M	N	...

For example, $2P_{3/2}$ denotes levels with $L = 1$, $S = 1/2$ and $J = 3/2$. The difference in energy between atomic levels having different L and S but the same electron configuration is due repulsive Coulomb interaction between electrons. These energy differences are small. We have the following empirical Hund's rules (F.Hund, 1925) concerning relative position of levels with the same configuration but different L and S :

(i) For a given shell (configuration), the term with greatest possible value of S gives the lowest energy;

(ii) The greatest possible value of L (for this S) has the lowest energy;

(iii) For half or less than half filling shell, $J = |L - S|$ gives lowest energy; For more than half-filling shell, $J = L + S$ gives lowest energy.

The origin of the first rule is obvious: the largest total spin corresponds to symmetric

(parallel) spin wavefunction and antisymmetric orbital wavefunction, the later reduces electron-electron repulsive interaction energy.

Example. Helium ($Z = 2$) has a simple configuration $(1s)^2$. Hence $S = 0$ and

$L = 0$. The ground state term is $1S_0$ with $J = 0$. We will use this term to construct an approximate wavefunction to calculate its ground-state energy in the next section.

Example. Carbon ($Z = 6$) has electron configuration as $(1s)^2(2s)^2(2p)^2$. There are three p orbitals with $m = 1, 0, -1$ as $l = 1$. Two electrons with both spin equal to $1/2$ (corresponding to total largest spin $S = 1$) are in orbital $m = 1, 0$ with total maximal $M = 1 + 0 = 1$, corresponding to $L = 1$. Hence the ground state term is $3P_0$. It is less than half-filling, $J = |L - S| = 0$. The other two possible terms are $1S$ and $1D$. They correspond to higher energies.

Example. Nitrogen ($Z = 7$): $He(2s)^2(2p)^3$. Three electrons with total spin $S = 3/2$ are in states $m = 1, 0, -1$ with total maximal $M = 0$ corresponding to $L = 0$. Ground state term is therefore $4S_{3/2}$. Other terms are $2P$ and $2D$.

Example. Oxygen ($Z = 8$): $He(2s)^2(2p)^4$. Equivalent to two holes (two missing electrons for filled shell) in $2p$ orbitals. Its ground state term is therefore same as carbon, $3P$. However, as it is more than half-filling, $J = L + S = 2$. So we have $3P_2$ for its ground state.

Example. Boron ($Z = 5$) and fluorine ($Z = 9$) have similar term but different J values, due to electron-hole symmetry.

Thomas-Fermi model of the atom

The theory for the electronic structure of many-body systems developed semiclassically shortly after the introduction of the Schrödinger equation. It stands separate from wave function theory as being formulated in terms of the electronic density alone and as such is viewed as a precursor to modern density functional theory. The TF model is correct only in the limit of an infinite nuclear charge. Using the approximation for realistic systems yields poor quantitative predictions, even failing to reproduce some general features of the density such as shell structure in atoms and Friedel oscillations in solids. It has, however, found modern applications in many fields through the ability to extract qualitative trends analytically and with the ease at which the model can be solved. The kinetic energy expression of Thomas-Fermi

theory is also used as a component in more sophisticated density approximation to the kinetic energy within modern orbital-free density functional theory. The electrons are distributed nonuniformly in an atom, an approximation was made that the electrons are distributed uniformly in each small volume element but the electron density can still vary from one small volume element.

Hydrogen molecule ion H^{2+}

The electronic Schrödinger wave equation for the hydrogen molecular ion H^{2+} with two fixed nuclear centers, labeled A and B , and one electron can be written as

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi = E\psi$$

where V is the electron-nuclear Coulomb potential energy function

$$V = -\frac{e^2}{4\pi\epsilon_0} \left(\frac{1}{r_a} + \frac{1}{r_b} \right)$$

and E is the (electronic) energy of a given quantum mechanical state (eigenstate), with the electronic state function $\psi = \psi(r)$ depending on the spatial coordinates of the electron. An additive term $1/R$, which is constant for fixed internuclear distance R , has been omitted from the potential V , since it merely shifts the eigenvalue.

The Hartree-Fock method

The kinetic energy term and the nucleus-electron interaction term are sums of single-particle operators, each of which act on a single electronic coordinate. The electron-electron interaction term on the other hand is a pair interaction and acts on pairs of electrons.

The Hartree-Fock method is a variational, wavefunction-based approach. Although it is a many-body technique, the

approach followed is that of a single-particle picture, i.e. the electrons are considered as occupying single-particle orbitals making up the wavefunction. Each electron feels the presence of the other electrons indirectly through an effective potential.

Each orbital, thus, is affected by the presence of electrons in other orbitals.

The starting point of the Hartree-Fock method is to write a variational wavefunction, which is built from these single-particle orbitals. Once we make a suitable ansatz to the wavefunction, all that is left is the application of the variational principle.

The simplest wavefunction that can be formed from these orbitals is their direct product

$$(\psi_1, \dots, \psi_N) = \frac{1}{\sqrt{N!}} \psi_1(\mathbf{r}_1) \psi_2(\mathbf{r}_2) \dots \psi_N(\mathbf{r}_N) \quad (1)$$

This is the Hartree approximation and it is a straightforward task to calculate the variational lowest energy from Eq. 1

However, the Hartree wavefunction has a very important shortcoming, which is that it fails to satisfy antisymmetry, which states that a fermion wavefunction changes sign under odd permutations of the electronic variables. The permutation

operator is defined by its action on the wavefunction

$$\hat{P}_{ij} \psi(\mathbf{r}_1, \dots, \mathbf{r}_i, \dots, \mathbf{r}_j, \dots, \mathbf{r}_N) = \psi(\mathbf{r}_1, \dots, \mathbf{r}_j, \dots, \mathbf{r}_i, \dots, \mathbf{r}_N) = -\psi(\mathbf{r}_1, \dots, \mathbf{r}_i, \dots, \mathbf{r}_j, \dots, \mathbf{r}_N) \quad (2)$$

If an odd number of such permutation operators are applied to the wavefunction, it picks up a minus sign while no change

in sign occurs under an even number of permutations. In order to satisfy the antisymmetry condition, a more sophisticated form than that of the Hartree wavefunction is needed.

II. THE SLATER DETERMINANT

If, for example, we have a two-electron system with orbitals $\psi_1(\mathbf{r}_1)$ and $\psi_2(\mathbf{r}_2)$, the following variational wavefunction satisfies the antisymmetry condition, at the same time preserving the single-particle picture

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = c [\psi_1(\mathbf{r}_1) \psi_2(\mathbf{r}_2) - \psi_1(\mathbf{r}_2) \psi_2(\mathbf{r}_1)] \quad (3)$$

where c is the normalization constant. For three electrons, the equivalent

antisymmetrized wavefunction would be

$$\begin{aligned} (\sim x_1, \sim x_2, \sim x_3) = & \frac{1}{\sqrt{6}} \left[\psi_1(\sim x_1) \psi_2(\sim x_2) \psi_3(\sim x_3) - \psi_1(\sim x_1) \psi_2(\sim x_3) \psi_3(\sim x_2) + \right. \\ & \left. \psi_1(\sim x_3) \psi_2(\sim x_1) \psi_3(\sim x_2) - \psi_1(\sim x_2) \psi_2(\sim x_1) \psi_3(\sim x_3) + \right. \\ & \left. \psi_1(\sim x_3) \psi_2(\sim x_2) \psi_3(\sim x_1) - \psi_1(\sim x_2) \psi_2(\sim x_3) \psi_3(\sim x_1) \right] \quad (4) \end{aligned}$$

where $\sim x_i$ is now a generalized coordinate that includes spatial as well as spin degrees of freedom.

The Hartree-Fock method is a variational, wavefunction-based approach. Although it is a many-body technique, the

approach followed is that of a single-particle picture, i.e. the electrons are considered as occupying single-particle orbitals making up the wavefunction. Each electron feels the presence of the other electrons indirectly through an effective potential.

Each orbital, thus, is affected by the presence of electrons in other orbitals.

The starting point of the Hartree-Fock method is to write a variational wavefunction, which is built from these single-particle orbitals. Once we make a suitable ansatz to the wavefunction, all that is left is the application of the variational principle as described in Lecture 1. The simplest wavefunction that can be formed from these orbitals is their direct product

$$(\sim x_1, \dots, \sim x_N) = \psi_1(\sim x_1) \psi_2(\sim x_2) \dots \psi_N(\sim x_N).$$

(4) This is the Hartree approximation and it is a straightforward task to calculate the variational lowest energy from Eq. 4.

However, the Hartree wavefunction has a very important shortcoming, which is that it fails to satisfy antisymmetry, which states that a fermion wavefunction changes sign under odd permutations of the electronic variables. The permutation

operator is defined by its action on the wavefunction

$$P^{ij} (\psi_1, \dots, \psi_i, \dots, \psi_j, \dots, \psi_N) = (\psi_1, \dots, \psi_j, \dots, \psi_i, \dots, \psi_N) = - (\psi_1, \dots, \psi_i, \dots, \psi_j, \dots, \psi_N) \quad (5)$$

If an odd number of such permutation operators are applied to the wavefunction, it picks up a minus sign while no change

in sign occurs under an even number of permutations. In order to satisfy the antisymmetry condition, a more sophisticated form than that of the Hartree wavefunction is needed.

THE HARTREE-FOCK EQUATIONS

The variational principle that we will apply here is rather different from the linear variation. There the form of our approximate wavefunction was written as an expansion over a collection of predetermined functions and we minimized the expectation value (at the same time obeying the normalization constraint) with respect to the coefficients of the basis functions. Here however we employ a much more general treatment where we minimize with respect to the basis functions themselves! Needless to say, this requires functional differentiation where any change affected in the expectation value in Eq. 1 due to an infinitesimal change in any of the orbitals ψ_k should be zero

$$\delta \langle \psi_k | \hat{H}_e | \psi_k \rangle = 0$$

In addition, we demand through Lagrange multipliers that the set of orbitals ψ_k remain orthogonal throughout the minimization process.

where the first and the second term are straightforward, single-body operators and the third term is an integral operator. This is now a set of interdependent single-particle eigenvalue equations. The operator \hat{J} corresponds to the classical interaction of an electron distributions given by $|\psi_i|^2$ and $|\psi_k|^2$ and is called the direct term while \hat{K} , called the exchange term, has no classical analogue and is a direct result of the antisymmetry property of the wavefunction.

For each k there is an equivalent equation defining a system of Schrödinger-like, one-particle equations. Although it's tempting to interpret the eigen values k as the energy levels of an interacting system, this is in fact not justified because the single-electron picture is not correct. However, if interpreted correctly the Hartree-Fock eigen values do correspond to certain physical entities.

MOLECULAR ORBITAL THEORY

Electrons have certain properties of particles and certain properties of waves. Electrons have mass and charge like particles. Because they are so small and are moving so fast, electrons have no defined position. Their location is best described by wave mechanics (i.e. a three-dimensional wave) and a wave equation called the Schrödinger equation. Solutions of the Schrödinger equation are called wave functions and are represented by ψ .

The sign of the wave function can change from positive (+) to negative (-) in different parts of the same orbital. This is analogous to the way that waves can have positive or negative amplitudes. The sign of the wave function does not indicate anything about charge.

The value of the square of the wave function is proportional to the probability of finding electron density at a given point in an orbital. Note that the sign of square of the wave function is always positive, because the square of even a negative value is still positive.

In a $2p$ orbital, it is just as probable to find electron density in the negative lobe as it is to find electron density in the positive lobe. A node is any place in an orbital at which the value of the wave function is zero.

A nodal surface or nodal plane are surfaces or planes where the value of the wave function is zero. There is absolutely no electron density at a node, a nodal surface, or a nodal plane. The Schrödinger equation can in principle describe covalent bonding, but, even with powerful computers the equation is too complicated to be solved exactly for large molecules.

Valence bond Theory

The two-electron system with orbitals ψ_1 ($\sim x_1$) and ψ_2 ($\sim x_2$), the following variational wavefunction satisfies the antisymmetry condition, at the same time preserving the single-particle picture

$$(\psi_1, \psi_2) = c [\psi_1(\psi_1) \psi_2(\psi_2) - \psi_1(\psi_2) \psi_2(\psi_1)] \quad (1)$$

where c is the normalization constant. For three electrons, the equivalent antisymmetrized wavefunction would be

$$\begin{aligned} (\psi_1, \psi_2, \psi_3) = c h & \psi_1(\psi_1) \psi_2(\psi_2) \psi_3(\psi_3) - \psi_1(\psi_1) \psi_2(\psi_3) \psi_3(\psi_2) + \psi_1(\psi_3) \psi_2(\psi_1) \psi_3(\psi_2) \\ & - \psi_1(\psi_2) \psi_2(\psi_1) \psi_3(\psi_3) + \psi_1(\psi_3) \psi_2(\psi_2) \psi_3(\psi_1) - \\ & \psi_1(\psi_2) \psi_2(\psi_3) \psi_3(\psi_1) \end{aligned} \quad (2)$$

Upon closer inspection, we notice that the same permutations of orbitals with matching signs are obtained by the following determinant

$$\begin{vmatrix} \psi_1(\psi_1) & \psi_2(\psi_1) & \psi_3(\psi_1) \\ \psi_1(\psi_2) & \psi_2(\psi_2) & \psi_3(\psi_2) \\ \psi_1(\psi_3) & \psi_2(\psi_3) & \psi_3(\psi_3) \end{vmatrix} \quad (3)$$

where the factor in front ensures normalization. For an arbitrary number of electrons the wavefunction can be shown to satisfy the desired antisymmetry condition. The determinant, referred to as a Slater determinant in literature, has $N!$ terms each multiplied by -1 or 1 depending on the parity of the permutation. Each term has each orbital ψ_i only once and each of the arguments ψ_{x_i} only once. Thus, each term may be written as follows where the indices i_1, i_2, \dots take values between 1 and N and the exponent of -1 in front refers to the order of appearance of the orbital indices in the term. The term picks up a -1 in front if the corresponding permutation is odd and $+1$ if it is even. For ease of notation, we replace $P(i_1, i_2, \dots, i_N)$ by the shorthand notation $P(i)$, where i now refers to a particular arrangement (or sequence) of the N indices. The Slater determinant may then be written as

where the sum i runs over the $N!$ terms. Nothing has been said so far about the form of the orbitals $\psi_i(\psi_j)$ and they are left to be found as a result of the minimization procedure associated by the variation. In order to achieve that we now calculate the expectation value of the Hamiltonian for this variational wavefunction

$$E_H = \langle \psi | \hat{H} | \psi \rangle \quad (4)$$

Possible Questions

Part B (4 Marks each)

1. What is particle exchange operator? What are its eigen values? Show that it is a constant of motion.
2. Illustrate exchange degeneracy with examples.
3. What is Slater determinant? How does it incorporate Pauli principle?
4. Explain Fermi hole and Fermi heap.
5. What are orthohelium and parahelium?
6. Explain why the ground state of helium exists in the para form whereas the excited states come in both forms.
7. Explain central field approximation.
8. How did Hartree obtain the central field in his theory of many electron atom?
9. Explain self consistent potential.

Part C (10 marks each)

1. a. Explain what is meant by indistinguishable particles. **(5 marks)**
b. Explain symmetric and antisymmetric wave functions **(5 marks)**
2. a. Using symmetric and antisymmetric wave functions explain Pauli's exclusion principle. **(5 marks)**
b. Discuss the inclusion of spin of electrons. **(5 marks)**
3. Using the theory of indistinguishable particles, explain the ground state and first excited state of Helium atom. Distinguish between parahelium and orthohelium.
4. a. Explain central field approximation. **(5 marks)**
b. Discuss Thomas-Fermi model of the atom. **(5 marks)**
5. a. Derive Hartree equation and obtain expression for total energy of the system.
b. Derive Hartree Fock equation. **(5 marks)**

S.No	Questions	Option 1	Option 1	Option 1	Option 1	Answer
1	The central field approximation is applicable on all atoms except the _____ atom.	. heavier	alkali	lighter	none of the above	lighter
2	Every atomic electron moves in a _____ potential energy $V(r)$ that is produced by the nucleus and all other electrons	Spherically symmetric	Assymmetric	. Radially symmetric	. None of the above	Spherically symmetric
3	The fluctuating potential due to each nearby electron varies slowly with the _____ distance.	equal	infinite	separation	finite	separation
4	The potential energy $v(r)$ for a neutral atom has the coulomb form _____ at a great	$-e^2/r$	e^2/r	$-2e^2/r$	$2e^2/r$	$-e^2/r$

	distance r from the nucleus.					
5	The state of an electron in a central field is specified by the quantum numbers _____.	n and l	m_l and m_s	n, l and m_s	n, l, m_l and m_s	n, l, m_l and m_s
6	According to Thomas-Fermi statistical model $v(r)$ varies slowly enough in an _____ wavelength.	proton	neutron	electron	none of the above	electron
7	At normal temperature, the thermal energy KT is very small in comparison with _____ everywhere except at the edge of the atom.	kinetic energy	potential $V(r)$	a and b	none of the above	potential $V(r)$
8	The number of electron states in a cube of edge length L at the walls of which the wave functions	$(L/2\pi)^3 dk_x dk_y dk_z$	$-(L/2\pi)^3 dk_x dk_y dk_z$	$(L/2\pi)^3 dk_x dk_y$	$(L/2\pi)^3 dk_x dk_z$	$(L/2\pi)^3 dk_x dk_y dk_z$

	obey periodic boundary condition is _____.					
9	The relation between volume density of electron $n(r)$ and the potential energy is _____.	$n(r) = \frac{(2mV(r)/3p^2)^{3/2}}{3^{1/2}}$	$n(r) = \frac{(2mV(r)/3p^2)^{3/2}}{2}$	$n(r) = \frac{(2mV(r))^{3/2}}{3p^2}$	$n(r) = \frac{(2mV(r)/3p^2)^{3/2}}{2}$	$n(r) = \frac{(2mV(r))^{3/2}}{3p^2}$
10	As $r \rightarrow \infty$, there is no net charge inside the sphere of radius r , so that V falls off more rapidly than _____.	a. $1/r$	a. $1/r^2$	a. $-1/r$	r^2	a. $1/r$
11	If m becomes infinite and e becomes zero in such a way that $m^3 e^4$ remains constant, then the electron wavelength becomes _____.	. Infinite	. zero	. finite	. none of the above	. zero

12	According to Hartree's method, the charge density associated with an electron is _____ times its position probability density.	e	$1/e$	$-1/e$	$-e$	$-e$
13	According to Hartree's method, the entire wave function for all the electrons is a simple product of _____ functions.	one-electron	all electron	each individual electron wave	none of the above	one-electron
14	The theory of complex spectra consists in determining the linear combination of _____ suitably wave function.	symmetrical	normalised	a and b	antisymmetrical	antisymmetrical

15	When the electrostatic perturbation is included and spin-orbit energy neglected, then the total orbital- angular momentum L and the total spin angular momentum S are separately _____ of the motion.	equations	symmetrical	constants	antisymmetrical	constants
16	When the spin-orbit energy is neglected, the electrostatic energy separates states of different _____.	S	L	J	a and b	L
17	energy state can be specified by the quantum numbers _____.	J, L, S, M	J, L, M_L, M_S	J, L, S	J, L, S, M, M_L, M_S	J, L, S, M, M_L, M_S

18	For given L and S, the states specified by J and M are linear combinations of those specified by _____ and _____.	M_L and M_S	J and S	J and L	J, L and S	M_L and M_S
19	If spin-orbit energy is included, then L and S are not of _____ motion.	equations	symmetrical	constants	antisymmetrical	symmetrical
20	In JJ coupling, the spin-orbit energy is _____ in comparison with the electrostatic energy.	Small	Large	Finite	Infinite	Infinite
21	JJ coupling takes place in _____ atoms where the large $V(r)$ makes the spin-orbit energy	heavy	light	alkali	none of the above	heavy

22	In alkali atom, a single electron moves in a spherically symmetric _____ potential energy $V(r)$.	excitation	coloumb	noncoloumb	none of the above	noncoloumb
23	The configuration of an alkali atom can be specified by a single pair of quantum numbers _____.	n, l	n, l, m_l	n, l, m_l, m_s	n, l, m_s	n, l
24	The configuration of an alkali atom can be specified by a single pair of quantum numbers _____.	infinity	1	1 and 2	0	0
25	The doublet structure characterizes all the moderately excited levels of the alkali atom except those for which $l =$ _____.	negative	zero	positive	infinite	positive

26	The pair of states having j either $l+1/2$ or $l-1/2$ has attractive potential energy $V(r)$ which is _____.	$L + S$	LS	$(L+1)(S+1)$	$(L+1)(S+1/2)$	$L + S$
27	The total angular momentum $J =$ _____.	s	n and l	j and s	l	l
28	The absolute value of doublet separation depends on _____	different	proportional	same	inversely proportional	same
29	The doublet intensity of two lines can be found by assuming the radial wave functions are _____ for two excited 2P states.	diagonal	dipole	square	unity	dipole

30	The observed intensities if the two P states are equally likely to be occupied are proportional to the squares of the _____ matrix elements.	LS	JJ	LS and JJ	None of the above	LS
31	The equality of total intensities from each state formed from a given L and S is a general property of _____ coupling.	03:01	02:04	01:02	02:01	02:01
32	The two lines of the doublet have intensities in the ratio _____.	02:04	02:01	01:02	03:01	02:01
33	The lowest doublets of the alkalis are in the ratio _____.			6	12	6

34	The sum of the intensities of all the lines that originates on each of the four $^2P_{3/2}$ states is equal to _____.	8	4	4	12	8
35	The total intensity from each of the two $^2P_{1/2}$ states is equal to _____.	6	8	2	1	2
36	For higher doublets the intensity ratio exceeds _____.	4	6	function	radial function	radial function
37	In higher doublets the intensity ratio exceeds 2 due to the difference to _____.	energy state	electron wave function	a and b	$(j+1)^2$	energy state
38	$J^2 =$ _____.	$j(j+1)^2$	$-j(j+1)^2$	J.J	$j(j+1)^2$	J.J

39	The states of different j have _____ fold degeneracy.	Proportional	Same	Different	$(2j+1)$	Different
40	The states of different j with $(2j+1)$ fold degeneracy is due to _____.	$-(j+1)$	$-(2j+1)$	$(j+1)$	j and s	j and s
41	The state of different j with $(2j+1)$ fold degeneracy is due to _____.	m	l	l and s	0	m
42	The method of partial wave is an elegant procedure for the analysis of _____ scattering	elastic	inelastic	compton	differential	elastic
43	The s -particle wave will be _____ of the angle	dependent	independent	perpendicular	parallel	independent
44	The s -particle wave will be _____ symmetric	spherically	circularly	elastically	a	spherically
45	The phenomenon with out scattering is called _____	Ramsaur - Townsend effect	tuindall effect	raman effect	bohr model	Ramsaur - Townsend effect

46	The small scattering cross section for electrons of rare gas atoms at a bombarding energy of _____	0.7 eV	15 eV	35 eV	1.2 eV	0.7 eV
47	$l = \frac{h}{mv}$	k_B	0	b		k_B
48	The interaction between two particles is usually screened by the atomic electrons surrounding the _____		electrons	neutrons	protons	nucleus
49	The quantum mechanics does not satisfy the requirement of special theory of _____	resistivity	permittivity	permeability	conductivity	relativity
50	Klein-gordon equation does not say anything about _____	particle	wave	energy	space	particle
51	is the _____ operator	de alembertian	schrodinger	wave	dirac	de alembertian

52	Klein and Gordon were not able to give a explanation of _____ energy	positive	negative	zero	neutral	negative
53	_____ was resolved by Pauli and Weisskopf in 1934	dilemma	charge density	lambda	surface energy	dilemma
54	Coulomb field is described by a potential of the type _____	$V(r) = 0$	$V(r) = KB$	$v(r) = -Ze^2/r$	$v(r) = ih$	$v(r) = -Ze^2/r$

UNIT- IV

SYLLABUS

Relativistic quantum mechanics: Klein-Gordan equation – Interpretation of the Klein-Gordan equation – Particle in a coulomb field – Dirac's equation for a free particle – Dirac matrices – Covariant form of Dirac equation – Probability density – Negative energy states – Spin of the Dirac particle – Magnetic moment of the electron – Spin-orbit interaction – Radial equation for an electron in a central potential – Hydrogen atom – Lamb shift.

Klein-Gordan Equation

The Klein-Gordon equation fulfills the laws of special relativity, but contains two fundamental problems, which have to be taken care of for the equation to be physically meaningful. The problem becomes obvious when considering the solutions of the different equations.

$$\begin{aligned}\psi(x) &= a e^{i(\vec{k} \cdot \vec{x} - \omega t)} \\ &= a e^{-i k_\mu x^\mu}\end{aligned}$$

$$k_\mu = \begin{pmatrix} \frac{\omega}{c} \\ -\vec{k} \end{pmatrix}.$$

$$a \left[-k_\mu k^\mu + \left(\frac{mc}{\hbar} \right)^2 \right] = 0$$

$$k^2 = k_\mu k^\mu = \left(\frac{mc}{\hbar} \right)^2$$

from which follows

$$(k^0)^2 = \vec{k}^2 + \left(\frac{mc}{\hbar}\right)^2$$

$$k^0 = \pm \sqrt{\vec{k}^2 + \left(\frac{mc}{\hbar}\right)^2}$$

This means that the Klein-Gordon equation allows negative energies as solution. Formally, one can see that from the square of the information about the sign is lost. However, when starting all solutions have to be considered, and there is the problem of the physical interpretation of negative energies. The second problem with the Klein-Gordon equation is less obvious. It occurs when interpreting the function $\psi(x)$ as probability amplitude.

Interpretation of $\psi(x)$ as probability amplitude is only possible if there exists a probability density $\rho(x)$ and a current $\vec{j}(x)$ that ful a continuity equation

$$\frac{\partial}{\partial t} \rho + \vec{\nabla} \cdot \vec{j} = 0$$

which guarantees that no "probability" is lost. Since we deal with a covariant equation,

$$j^0(x) := c\rho(x)$$

$$j^\mu(x) := \begin{pmatrix} j^0(x) \\ \vec{j}(x) \end{pmatrix}$$

and obtain the covariant form

$$\frac{\partial}{\partial x^\mu} j^\mu = \partial_\mu j^\mu = 0$$

Non-relativistically one has

$$\rho_{NR} = \psi^* \psi$$

$$\vec{j}_{NR} = \frac{\hbar}{(2mi)} [\psi^* \vec{\nabla} \psi - \psi \vec{\nabla}^* \psi]$$

and thus one expects in the relativistic case also bilinear expressions in for ψ , ψ^* and \vec{j} . It is easy to show that this density does not fulfill a continuity equation.

$$j^\mu := \frac{i\hbar}{2m} \psi^* \overleftrightarrow{\partial}^\mu \psi$$

$$A^* \overleftrightarrow{\partial}^\mu B := A^* (\partial^\mu B) - (\partial^\mu A^*) B.$$

Consider

$$\begin{aligned} \partial_\mu j^\mu &= \frac{i\hbar}{2m} \partial_\mu (\psi^* \overleftrightarrow{\partial}^\mu \psi) \\ &= \frac{i\hbar}{2m} [\psi^* (\square \psi) - (\square \psi^*) \psi] \end{aligned}$$

the Klein-Gordon equation, the right-hand side of vanishes, and the continuity equal

$$\begin{aligned} \rho &= \frac{1}{c} j^0 \\ &= \frac{i\hbar}{2mc} \psi^* \overleftrightarrow{\partial}^0 \psi \\ &= \frac{i\hbar}{2mc^2} \left[\psi^* \frac{\partial}{\partial t} \psi - \frac{\partial \psi^*}{\partial t} \psi \right] \end{aligned}$$

Since the Klein-Gordon equation denotes a partial differential equation of hyperbolic type, one has the option to arbitrarily choose the functions

$$\psi(\vec{x}, t = 0) \quad \text{and} \quad \frac{\partial}{\partial t} \psi(\vec{x}, t = 0)$$

at the starting time ($t = 0$), and thus obtain, e.g., negative values for $\rho(\vec{x}; t = 0)$. An interpretation of ρ as probability density would mean that the theory allows negative probabilities. This is the problem of the indefinite probability density.

Interpretation of the Klein- Gordon equation

The electromagnetic interactions into the KG equation

$$\begin{aligned} p^\mu &\rightarrow p^\mu - eA^\mu \\ \left[- \left(i \frac{\partial}{\partial x^\mu} - eA_\mu \right) \left(i \frac{\partial}{\partial x_\mu} - eA^\mu \right) + m^2 \right] \Psi(x) &= 0 \\ \left[\partial_\mu \partial^\mu + m^2 + U(x) \right] \Psi(x) &= 0, \end{aligned}$$

where the generalized potential $U(x)$ consists of a scalar and vector

$$\begin{aligned} U(x) &= ie \frac{\partial}{\partial x^\mu} A^\mu + ie A^\mu \frac{\partial}{\partial x^\mu} - e^2 A^\mu A_\mu \\ &= i \frac{\partial}{\partial x^\mu} V^\mu + i V^\mu \frac{\partial}{\partial x^\mu} + S \end{aligned}$$

that the symmetrized form of the vector terms is required in order to maintain the hermicity of the interaction. For the electromagnetic case they are related

$$\begin{aligned} S &= e^2 A^\mu A_\mu \\ V^\mu &= e A^\mu \end{aligned}$$

Using the standard form, the KG equation can be written as

$$\left(i \frac{\partial}{\partial t} - e\Phi \right)^2 \Psi(\mathbf{x}, t) = \left[(-i\nabla - e\mathbf{A})^2 + m^2 \right] \Psi(\mathbf{x}, t)$$

Substituting the positive and negative energy

$$(E_p \mp e\Phi)^2 \Psi^{(\pm)}(\mathbf{x}, t) = \left[(\hat{p} \mp e\mathbf{A})^2 + m^2 \right] \Psi^{(\pm)}(\mathbf{x}, t)$$

as starting point and use it with more general potentials V

$$(E^2 + V^2 - 2EV) \Psi = (\hat{p}^2 + m^2) \Psi$$

$$(\nabla^2 + k^2) \Psi = (2EV - V^2) \Psi$$

which looks like a Schrodinger equation with the equivalent energy dependent potential

$$V^{SE} = \frac{2EV - V^2}{2m}$$

The other potential is considered as the Lorentz scalar. The KG equation with coupling to the scalar potential

$$E^2 \Psi = [\hat{p}^2 + (m + S)^2] \Psi$$

Particle in a coulomb field

Coulomb's law is a law of physics for quantifying the amount of force with which stationary electrically charged particles repel or attract each other.

$$F = k_e \frac{q_1 q_2}{r^2}$$

where k_e is Coulomb's constant ($k_e = 9.0 \times 10^9 \text{ N m}^2 \text{ C}^{-2}$), q_1 and q_2 are the signed magnitudes of the charges, and the scalar r is the distance between the charges.

Coulomb's law and Coulomb's constant can also be interpreted in various terms:

- Atomic units. In atomic units the force is expressed in hartrees per Bohr radius, the charge in terms of the elementary charge, and the distances in terms of the *Bohr radius*.
- Electrostatic units or Gaussian units. In electrostatic units and Gaussian units, the unit charge (*esu* or statcoulomb) is defined in such a way that the Coulomb constant k disappears because it has the value of one and becomes dimensionless.
- Lorentz–Heaviside units (also called *rationalized*). In Lorentz–Heaviside units the Coulomb constant is $k_e = 1/4$ and becomes dimensionless.

An electric field is a vector field that associates to each point in space the Coulomb force experienced by a test charge. In the simplest case, the field is considered to be generated solely by a single source point charge. The strength and direction of the Coulomb force F on a test charge q_t depends on the electric field E that it finds itself in, such that $F = q_t E$. If the field is generated by a positive source point charge q , the direction of the electric field points along lines directed radially outwards from it, i.e. in the direction that a positive point test charge q_t would move if placed in the field. For a negative point source charge, the direction is radially inwards.

The magnitude of the electric field E can be derived from Coulomb's law. By choosing one of the point charges to be the source, and the other to be the test charge, it follows from

Coulomb's law that the magnitude of the electric field E created by a single source point charge q at a certain distance from it r in vacuum is given by

$$|E| = \frac{1}{4\pi\epsilon_0} \frac{|q|}{r^2}$$

Dirac's equation for a free particle.

Dirac attempted to overcome some of the problems of relativistic quantum mechanics by introducing a first-order wave equation.¹

$$i \mu - m = 0. \quad (1)$$

Here, the μ are some suitably chosen operators acting locally on the wave function. This wave equation can be viewed as a factorisation of the second-order Klein-Gordon equation as follows:

$$(i + m)(i - m) = (-\mu - m^2) = 0. \quad (2)$$

The latter form becomes the Klein-Gordon equation provided that the μ 's satisfy the Clifford algebra^{2,3}

$$\{\mu, \mu\} = \mu^2 + \mu^2 = -2\mu^2. \quad (3)$$

This means that every solution of the Dirac equation also satisfies the Klein-Gordon equation and thus describes a particle of mass m .

The Dirac equation is a relativistic wave equation. Translational invariance is evident, but we have not yet shown its Lorentz covariance (although the resulting Klein-Gordon equation certainly is covariant).

Dirac Matrices

Consider a Lorentz transformation

$x_0 = \gamma - 1 x$ with $(\gamma) = \exp(\gamma)$. Suppose ψ is a solution of the Dirac equation. It is not

sufficient to use the transformation rule for scalar fields $\psi(x) = \psi(x')$. In analogy to vectors we should also transform spinors. We make the ansatz

$$\psi(x) = S(\Lambda) \psi(x'), \quad (1)$$

where $S(\Lambda)$ is a matrix that acts on Dirac spinors. We then substitute $\psi(x) = S(\Lambda) \psi(x')$ into the Dirac equation

$$\begin{aligned} (i \gamma^\mu \partial_\mu - m) \psi(x) &= (i \gamma^\mu \partial_\mu - m) S(\Lambda) \psi(x') \\ &= i S(\Lambda) \gamma^\mu \partial_\mu \psi(x') - m S(\Lambda) \psi(x') \\ &= S(\Lambda) i \gamma^\mu \partial_\mu \psi(x') - m S(\Lambda) \psi(x') \\ &= i S(\Lambda) \gamma^\mu S^{-1}(\Lambda) \partial'_\mu \psi(x') - m S(\Lambda) \psi(x'). \end{aligned} \quad (2)$$

So the term in the bracket must vanish for invariance of the Dirac equation. Indeed, the canonical Lorentz transformation of gamma-matrices

$$\gamma'_\mu = (\Lambda^{-1})^\nu{}_\mu \gamma_\nu S^{-1}(\Lambda), \quad (3)$$

where not only the vector index is transformed by Λ^{-1} , but also the spinor matrix is conjugated by the corresponding spinor transformation S . In analogy to the invariance of the Minkowski metric, $\eta_{\mu\nu} = \eta'_{\mu'\nu'}$, the Dirac equation is invariant if the gamma-matrices are invariant

$$\gamma'_\mu = \gamma_\mu. \quad (4)$$

to gamma-matrices, and we make the ansatz $S = 1 + \frac{1}{2} \omega_{\mu\nu} \Sigma^{\mu\nu}$. Substituting this into the invariance condition and using

$$[\Sigma^{\mu\nu}, \gamma^\rho] = \{\gamma^\rho, \Sigma^{\mu\nu}\} = \gamma^\rho \gamma^\mu \gamma^\nu - \gamma^\rho \gamma^\nu \gamma^\mu, \quad (5)$$

arrive at $(\Lambda^\mu{}_\nu - \delta^\mu{}_\nu) \gamma^\nu = 0$. We conclude that a Lorentz transformation for spinors is

given by the matrix

the Dirac spinor $\psi = \begin{pmatrix} L \\ R \end{pmatrix}$ transforms in the direct sum of two (irreducible) representations of the Lorentz group. The 2-spinors L and R are called left-chiral and right-chiral spinors. The massive Dirac equation, however, mixes these two representations

$$i \not{\partial} \psi - m \psi = 0. \quad (7)$$

It is therefore convenient to use Dirac spinors for massive spinor particles whereas massless spinor particles can also be formulated using 2-spinors;

The decomposition into chiral parts is not just valid in the Weyl representation of the Clifford algebra.

In the Weyl representation it reads $\gamma_5 = \text{diag}(-1, +1)$, it therefore measures the chirality of spinors. In general, it anti-commutes with all the other gamma-matrices,

$$\{\gamma_5, \gamma_\mu\} = 0. \quad (9)$$

This property implies that a single gamma-matrix maps between opposite chiralities, i.e. it inverts chirality. The property is also sufficient to prove commutation with $M_{\mu\nu}$. Alternatively, it follows by construction of γ_5 as a (pseudo)-scalar combination of gamma-matrices.

Covariant form of Dirac equation

The matrices

$$\gamma^0 = \beta, \quad \vec{\gamma} = \beta \vec{\alpha}$$

the Dirac equation in the covariant form can be written as,

$$\left(i \gamma^\mu \partial_\mu - \frac{mc}{\hbar} \right) \psi(x) = 0$$

in the Klein-Fock-Gordon equation, in the form of the inverse Compton wave length.

$\hbar c = 197.326 \text{ MeV} \cdot \text{fm}$, and using the Feynman slash, the dirac equation can be rewritten as

$$(i \not{\partial} - m)\psi(x) = 0$$

Probability density

Probability density function or density of a continuous random variable, is a function, whose value at any given sample in the sample space, the PDF is used to specify the probability of the random variable falling within a particular range of values, as opposed to taking on any one value. This probability is given by the integral of this variable's PDF over that range—that is, it is given by the area under the density function but above the horizontal axis and between the lowest and greatest values of the range. The probability density function is nonnegative everywhere, and its integral over the entire space is equal to one. The terms "probability distribution function" and "probability function" have also sometimes been used to denote the probability density function.

Negative energy states

If $E < 0$, the coefficient $-2mE/\hbar^2$ be written as

Dirac's goal had been to find a relativistic equation for electrons which was free of the negative probabilities and the "negative energy" states of the Klein-Gordon equation. By developing an equation that was first order in the time derivative, he hoped to have an equation that behaved like the Schrödinger equation, an equation for a single particle. The Dirac equation also has "negative energy" solutions. While the probability is positive, the flux that we have derived is in the opposite direction of the momentum vector for the "negative energy" solutions.

Dirac applies the Pauli-principle, where every quantum state can only be occupied with one electron. For each momentum $p = \hbar k$, there exist only four electrons, namely two with the same sign for the energy, one with spin $+1/2$ and one with spin $-1/2$. According to Dirac the states with the negative energies is completely. Thus, one has an "underworld," the Dirac sea with the following properties:

total energy : 1

total charge : 1

total momentum : 0

total angular momentum

Then there would be a hole in the Dirac sea. If the original electron in the sea had the properties

$$\begin{aligned} \text{momentum} &: \vec{p} \\ \text{energy} &: E = -\sqrt{\vec{p}^2 + m^2} \\ \text{charge} &: \ell = -|e| \end{aligned}$$

then one obtains the hole rotation. Thus the "hole" represents the antiparticle to the electron e^- with the mass m_e and a positive charge $+|e|$, namely the positron e^+ . According to the preceding consideration, it should be created with a high energy -particle. To full momentum conservation one needs, e.g., the nucleus of an atom, the, namely the positron e^+ .

Magnetic moment of the electron

The electron is a charged particle of charge $-1e$, where e is the unit of elementary charge. Its angular momentum comes from two types of rotation: spin and orbital motion. From classical electrodynamics, a rotating electrically charged body creates a magnetic dipole with magnetic poles of equal magnitude but opposite polarity. This analogy holds as an electron indeed behaves like a tiny bar magnet. One consequence is that an external magnetic field exerts a torque on the electron magnetic moment depending on its orientation with respect to the field.

Spin-orbit interaction

The spin-orbit interaction for an electron bound to an atom, up to first order in perturbation theory, using some semiclassical electrodynamics and non-relativistic quantum mechanics. This gives results that agree reasonably well with observations. A more rigorous derivation of the same result would start with the Dirac equation, and achieving a more precise result would involve calculating small corrections from quantum electrodynamics.

Radial equation for an electron in a central potential

The kinetic energy operator in spherical polar coordinates is

$$\frac{\hat{p}^2}{2m_0} = -\frac{\hbar^2}{2m_0} \nabla^2 = -\frac{\hbar^2}{2m_0 r^2} \left[\frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \hat{l}^2 \right]$$

The spherical harmonics satisfy

$$\hat{l}^2 Y_{lm}(\theta, \phi) \equiv \left\{ -\frac{1}{\sin^2 \theta} \left[\sin \theta \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{\partial^2}{\partial \phi^2} \right] \right\} Y_{lm}(\theta, \phi) = l(l+1) Y_{lm}(\theta, \phi).$$

Substituting this into the Schrödinger equation

$$\left\{ -\frac{\hbar^2}{2m_0 r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{\hbar^2 l(l+1)}{2m_0 r^2} + V(r) \right\} R(r) = ER(r)$$

the radial equation becomes

$$-\frac{\hbar^2}{2m_0} \frac{d^2 u}{dr^2} + V_{\text{eff}}(r)u(r) = Eu(r)$$

which is precisely a Schrödinger equation for the function $u(r)$ with an effective potential given by

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2m_0 r^2}$$

where the radial coordinate r ranges from 0 to ∞ . The correction to the potential $V(r)$ is called the centrifugal barrier term.

Hydrogen atom

Spectral lines of H found to be composed of closely spaced *doublets*. Splitting is due to interactions between electron spin s and the orbital angular momentum l . Spin-orbit coupling produces fine-structure splitting of ~ 0.016 nm corresponds to an internal magnetic field on the electron of about 0.4 Tesla.

Orbital and spin angular momenta couple together via the spin-orbit interaction. Internal magnetic field produces torque which results in precession of l and s about their sum, the *total angular momentum*:

This kind of coupling is called *L-S coupling* or *Russell-Saunders coupling*

The Hydrogen Atom

A hydrogenic (hydrogen-like) atom is a two-particle system consisting of a nucleus and an electron. The two particles interact through the potential given by Coulomb's law:

$$V(r) = -\frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r}$$

where

- ϵ_0 is the permittivity of the vacuum,
- Z is the atomic number (eZ is the charge of the nucleus),
- e is the elementary charge (charge of the electron),
- r is the distance between the electron and the nucleus.

The mass m_0 , introduced above, is the reduced mass of the system. Because the electron mass is about 1836 smaller than the mass of the lightest nucleus (the proton), the value of m_0 is very close to the mass of the electron m_e for all hydrogenic atoms.

A hydrogen atom is an atom of the chemical element hydrogen. The electrically neutral atom contains a single positively charged proton and a single negatively charged electron bound to the nucleus by the Coulomb force. Atomic hydrogen constitutes about 75% of the baryonic mass of the universe.

In everyday life on Earth, isolated hydrogen atoms (called "atomic hydrogen") are extremely rare. Instead, hydrogen tends to combine with other atoms in compounds, or with itself to form ordinary (diatomic) hydrogen gas, H_2 .

Lamb Shift in Atomic Hydrogen

To measure the Lamb shift in the Balmer transition of atomic hydrogen. The Lamb shift cannot be explained by the Schrödinger or Dirac formulations of quantum mechanics. It can be explained by a theory known as quantum electrodynamics—a theory whose development was intimately linked to experimental observation of the Lamb shift.

The spectrum of the hydrogen atom was the first to be described quantitatively and modeled from first principles. In 1885 Balmer discovered that the wavelengths of the then known lines in the hydrogen spectrum.

In 1890 Rydberg discovered a more general form of Balmer's formula which, when applied to the hydrogen spectrum. In 1887 Michelson, using his interferometer to investigate the shape of spectral lines, discovered that the Balmer line consisted of not a single line but of two lines separated by a fraction of an angstrom. Bohr's simple model of the atom had no means of accounting for this feature.

In 1916 Arnold Sommerfeld presented a model of the hydrogen atom allowing for the possibility of elliptical in addition to strictly circular electron orbits. Applying relativistic corrections to these elliptical orbits, Sommerfeld's model predicted the Balmer line to consist of more than one component, just as Michelson had observed. But, being an ad hoc combination of classical and quantum physics, the Sommerfeld model was restricted in scope and left much to be desired. Quantitatively it was unable to account for features such as magnetic effects or the different intensities of the components of the Balmer line.

POSSIBLE QUESTIONS

PART B (4 Marks each)

1. Derive Klein-Gordon equation for a relativistic particle
2. Explain how Klein-Gordon equation leads to positive and negative probability density values.
3. Derive Dirac's relativistic equation for a free particle.
4. Explain the concept of negative energy states and Dirac's explanation for it.
5. Write a short note on Lamb shift.
6. Prove that the operator c , where c is the Dirac's matrix, can be interpreted as the velocity operator.
7. Give the energy spectrum of a free Dirac particle and explain pair production and pair annihilation
8. Give the physical interpretation of Dirac's α -matrix.
9. Starting from Klein-Gordon equation, obtain the equation of continuity.
10. Derive expressions for probability density and probability current density in the Dirac theory.

PART C (10 Marks each)

1. Discuss the relativistic motion of a particle in a Coulomb field and derive expression for energy.
2. a. Obtain Dirac's equation for a free particle, and deduce the co-variant form of the Dirac equation. **(5 Mark)**

- b. Explain Dirac matrices for α and β . **(5 Mark)**
3. a. Discuss the magnetic moment of an electron. **(5 Mark)**
- b. Explain spin-orbit interaction. **(5 Mark)**
4. Derive the radial equation for a relativistic electron in a central potential.
5. Using the radial equations in a central potential, derive the energy eigen values of a hydrogen atom.

S.No	Questions	Option 1	Option 1	Option 1	Option 1	Answer
1	The basis of all molecular approximation is the large ratio of _____.	electron mass to nuclear mass	electron mass to neutron mass	electron mass to atomic mass	nuclear mass to electron mass	nuclear mass to electron mass
2	The energy associated with the motion of then nuclei is much _____ than the energy associated with the motion of electron about the nuclei.	larger	smaller	varied	none of the above	smaller
3	The period of nuclear motion is of the order of _____ divided by its energy.		e	–	–e	
4	The nuclear periods are _____ than the electronic periods.	smaller	stable	longer	a and b	longer
5	The nuclear motion are classified into translation and rotational motion of the _____ equilibrium arrangement and internal vibrations of the nuclei about the equilibrium.	quasi-rigid	stable	unstable	neutral	quasi-rigid

6	Molecular energy levels are classified into _____ vibrational and rotational energy levels	static	rigid	translational	electronic	electronic
7	The energy E_e associated with the motion of a valence is of order of _____, where m is the electronic mass	$-\frac{2}{ma^2}$	$-\frac{2}{ma^2}$	$-\frac{2}{ma^2} + 1$	$\frac{2}{ma^2} + 1$	$-\frac{2}{ma^2}$
8	The only nuclear coordinates R_j of the hydrogen molecule is the magnitude, _____ of the distance between the two hydrogen nuclei.	R	r	$-R$	R^2	R
9	The linear combination of unperturbed degenerate wave function which gives lower energy than the separate wave function is the basis of _____ binding molecules	heteropolar	nuclei	homopolar	atomic	homopolar
10	The property of degeneracy is known as _____.	resonance	doublet separation	doublet intensity	none of the above	resonance

11	An interaction between two resonant (degenerate) states in quantum mechanics give rise to a lower energy _____.	eigen function	eigen value	wave	wave function	eigen value
12	The wave function based on a simple product of two ground state _____ functions gives good result.	alkali atom	helium atom	hydrogen molecule	hydrogen atom.	hydrogen atom.
13	In case of hydrogen molecule, the equilibrium value for r_{AB} is theoretically calculated as _____.	0.74 Å	0.8 Å	1.06 Å	1.32 Å	0.8 Å
14	The ground state of a hydrogen molecule is _____	a triplet state	a mixture of single and triplet state	neither a singlet nor a triplet state	a singlet state	a singlet state
15	The interaction between valence electrons give rise to _____ forces between atom which hold the atoms together in molecule	bonding	electrostatic	coloumbic	repulsive	bonding
16	Heitler and London theory of hydrogen molecule helps us to develop the picture of _____ bond.	covalent	chemical	ionic	none of the above	chemical

17	The spin functions of two electrons are $\alpha(1)$ and $\alpha(2)$, then the total spin wave function is the product of _____ such spin functions.	either one	wavelength with	a and b	two	two
18	The complete wavefunction of an electron is the product of _____ wave function multiplied by one of the spin function.	unperturbed orbital	perturbed orbital	orbital	none of the above.	orbital
19	The symmetric orbital functions of an electron will be associated with _____ spin function.	skew symmetric	symmetric	a and b	antisymmetric	antisymmetric
20	The antisymmetric orbital function will be associated with _____ spin function.	symmetric	skew symmetric	antisymmetric	b and c	symmetric
21	If r_{12} is the distance between two electrons, then the interaction between these electrons 1 and 2 is given	$-e^2/r_{12}^2$	$-e^2/r_{12}$	$-2e^2/r_{12}^2$	$-3e^2/r_{12}^2$	$-e^2/r_{12}$
22	If the system consists of two hydrogen nuclei 'a' and 'b' and two electrons 1 and 2 separated by distance r_{12} ,	$e^2/r_{ab} + e^2/r_{12} + e^2/r_{a1} + e^2/r_{b1} + e^2/r_{a2} + e^2/r_{b2}$	$e^2/r_{ab} + e^2/r_{12} + e^2/r_{a1} + e^2/r_{b1} + e^2/r_{a2} - e^2/r_{b2}$	$e^2/r_{ab} + e^2/r_{12} - e^2/r_{a1} + e^2/r_{b1} + e^2/r_{a2} + e^2/r_{b2}$	$e^2/r_{ab} + e^2/r_{12} - e^2/r_{a1} - e^2/r_{b1} - e^2/r_{a2} - e^2/r_{b2}$	$e^2/r_{ab} + e^2/r_{12} - e^2/r_{a1} - e^2/r_{b1} - e^2/r_{a2} - e^2/r_{b2}$

	then the potential energy or two nuclei is $V = \underline{\hspace{2cm}}$.					
23	_____ theory is also an approximation method for explaining bonding between H-atom in H_2 molecule.	vander walls	valence bond	scattering theory	partial wave.	valence bond
24	The attraction of two hydrogen atom give rise to the formation of _____ molecule.	stable	unstable	colloidal	suspension	stable
25	If we assume both the hydrogen atom are in ground state, then both the wave function are _____.	imaginary	integer	real	none of the above	real
26	The schroedinger equation for hydrogen molecule is given by _____.	$\tilde{N}_1^2 y + \tilde{N}_2^2 y + (2m/\hbar^2)(E-V)y = 0$	$\tilde{N}_1^2 y + \tilde{N}_2^2 y + (2m/\hbar^2)(E-V)y = 1$	$\tilde{N}_1^2 y + \tilde{N}_2^2 y + (2m/\hbar^2)(E-V)y = H y$	$\tilde{N}_1^2 y + \tilde{N}_2^2 y - (2m/\hbar^2)(E-V)y = H y$	$\tilde{N}_1^2 y + \tilde{N}_2^2 y + (2m/\hbar^2)(E-V)y = 0$
27	If the co-ordinates of 1 st electron is (x_1, y_1, z_1) and of 2 nd electron is (x_2, y_2, z_2) , then $r_{12} = \underline{\hspace{2cm}}$.	$(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2$	$(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2$	$(x_2 - x_1)^2 - (y_2 - y_1)^2 - (z_2 - z_1)^2$	$(x_2 - x_1)^2 + (y_2 - y_1)^2 - (z_2 - z_1)^2$	$(x_2 - x_1)^2 - (y_2 - y_1)^2 - (z_2 - z_1)^2$

28	The SP^3 hybridisation leads to _____ equivalent bonds.	3	4	6	2	3
29	The ground state of a hydrogen atom is _____.	a triplet	a mixture of singlet and triplet	neither singlet nor a triplet	singlet	singlet
30	If the spins of electron in two atoms are parallel then the atoms _____ each other	singlet	attract	coagulate	none of the above	singlet
31	If the spins of the electrons in two atoms are antiparallel, then two atoms _____ each other	repel	attract	coagulate	none of the above	attract
32	If two spins S_1 and S_2 of the electron combine to give a resultant spin $S=0$, then it will give rise to _____ state	doublet	triplet	multiplet	singlet	singlet
33	If two spins S_1 and S_2 of the electron combine to give a resultant spin $S=1$, then it will give rise to _____ state.	triplet	doublet	singlet	multiplet	triplet

34	Hartree-Fock method incorporates the effect of _____ symmetry.	skew	anti	exchange	none of the above	exchange
35	The molecular wave function as a linear combination of atomic orbitals is called _____ method.	LCAO	Exchange	MO	none of the above	LCAO
36	The effect of exchange symmetry has been incorporated in _____.	Hartree-Fock method	Hartree's self consistent method	Thomas – Fermi model	None of the above	Hartree's self consistent method
37	The effect of exchange symmetry has been incorporated in _____.	109°28'	180°	0°	120°	109°28'
38	In case of hydrogen molecule ion, the minimum potential energy equivalent to dissociation energy is theoretically calculated as _____.	2.78 eV	4.72 eV	3.14 eV	1.76 eV	1.76 eV
39	Resonance is the property of _____	degeneracy	doublet	singlet	triplet	degeneracy
40	The symmetric spin function will be associated with	skew symmetric	hermitian	antisymmetric	triplet	antisymmetric

	_____ orbital function.					
41	Dirac require the equation must be of _____ order in time and space	first	second	zero	none	first
42	Diracs equation is relativistically _____	invariant	variant	covariant	all the above	invariant
43	Lorentz is covariant from _____	μ	δ			
44	The spin of an electron carries no _____	energy	particle	time	wave function	energy
45	The empty space is called _____	hole	spintron	neutron	positron	hole

Field theory: Introduction – Classical approach to field theory – Relativistic Lagrangian and Hamiltonian of a charged particle in an electromagnetic field – Field: Lagrangian and Hamiltonian formulations – Quantum equation for the field – Second quantisation – Quantisation of non-relativistic Schrodinger equation – Creation, annihilation and number operators.

CLASSICAL THEORY OF ELECTROMAGNETIC FIELDS

The classical electrodynamics is based on Maxwell's equations for the electric and magnetic fields E and B . In rationalised units, also called Heaviside Lorentz units, these equations can be written as:

$$\nabla \cdot E = \rho \quad \text{.....(1)}$$

$$\nabla \times E = -\frac{\partial B}{\partial t} \quad \text{.....(2)}$$

$$\nabla \cdot B = 0 \quad \text{.....(3)}$$

$$\nabla \times B = \frac{\partial E}{\partial t} + j \quad \text{.....(4)}$$

Here $\rho(x, t)$ is the charge density and $j(x, t)$ is the current density. Instead of E and B , the field equations can also be expressed in terms of a vector potential A and a scalar potential ϕ . Equation (3) implies

$$B = \nabla \times A \quad \text{.....(5)}$$

With this definition of B , Equation (2) takes the form :

$$\nabla \times \left(E + \frac{\partial A}{\partial t} \right) = 0 \quad \text{.....(6)}$$

Since the curl of the gradient of a scalar function is zero, from Equation (6) We have

$$E + \frac{\partial A}{\partial t} = -\nabla \phi \quad (\phi \text{ is scalar potential})$$

$$E = -\frac{\partial A}{\partial t} - \nabla \phi \quad \text{....(7)}$$

Which gives the electric field in terms of the potential A and ϕ .

The other two equations, Eqs (1) and (4) can also be expressed in terms A and ϕ .

Substituting the value of E in Eq(1)

$$\nabla^2 \phi + \frac{\partial}{\partial t} (\nabla \cdot A) = -\rho \quad \text{.....(8)}$$

Substituting Eqs (5) and (7) in Eq (4), we have

$$\begin{aligned} \nabla \times (\nabla \times A) + \frac{\partial}{\partial t} \left(\frac{\partial A}{\partial t} + \nabla \phi \right) &= j \\ \nabla (\nabla \cdot A) - \nabla^2 A + \frac{\partial^2 A}{\partial t^2} + \nabla \frac{\partial \phi}{\partial t} &= j \\ \nabla^2 A - \frac{\partial^2 A}{\partial t^2} - \nabla \left(\nabla \cdot A + \frac{\partial \phi}{\partial t} \right) &= -j \quad \text{.....(9)} \end{aligned}$$

The solution of Maxwell's equations is thus reduced to solving the coupled equation (8) and (9) for A and ϕ .

$$A \rightarrow A' = A + \nabla \Lambda \quad \text{.....(10)}$$

$$\phi \rightarrow \phi' = \phi - \frac{\partial \Lambda}{\partial t} \quad \text{.....(11)}$$

Where Λ an arbitrary scalar function leaves B and E unchanged. The fact that $\nabla \times \nabla \Lambda = 0$

leaves B unchanged by the transformation. The electric field E , Eq (7)

$$\begin{aligned} E &= \frac{\partial}{\partial t} (A + \nabla \Lambda) - \nabla \left(\phi - \frac{\partial \Lambda}{\partial t} \right) \\ &= -\frac{\partial A}{\partial t} - \nabla \phi \\ \nabla \cdot A + \frac{\partial \phi}{\partial t} &= 0 \quad (12) \end{aligned}$$

The freedom available in the definition of Eqs (10) and (11) together is called gauge transformation and the condition in Eq (12) is known as Lorentz gauge condition.

Eqn(12) can be written as:

$$\frac{\partial A_1}{\partial x_1} + \frac{\partial A_2}{\partial x_2} + \frac{\partial A_3}{\partial x_3} + \frac{\partial(i\varphi)}{\partial(it)} = 0$$

$$\frac{\partial A_1}{\partial x_1} + \frac{\partial A_2}{\partial x_2} + \frac{\partial A_3}{\partial x_3} + \frac{\partial A_4}{\partial x_4} = 0$$

$$\frac{\partial A_\mu}{\partial x_\mu} = 0 \quad \text{or} \quad \partial_\mu A_\mu = 0 \quad \dots\dots(13)$$

It can easily be shown that the three components of vector \mathbf{j} and charge density ρ form the four vector

$$\mathbf{j} = (\mathbf{j}, ic\rho) \quad \dots\dots(14)$$

The components of the vector potential \mathbf{A} and the scalar potential φ form the four-vector potential:

$$\mathbf{A} = (\mathbf{A}, i\varphi) \quad \dots\dots(15)$$

From eq we have

$$B_1 = \frac{\partial A_3}{\partial x_2} - \frac{\partial A_2}{\partial x_3} \quad \dots\dots(16)$$

$$B_2 = \frac{\partial A_1}{\partial x_3} - \frac{\partial A_3}{\partial x_1} \quad \dots\dots(17)$$

$$B_3 = \frac{\partial A_2}{\partial x_1} - \frac{\partial A_1}{\partial x_2} \quad \dots\dots(18)$$

From eq

$$E_1 = -\frac{\partial A_1}{\partial t} - \frac{\partial \varphi}{\partial x_1} \quad \text{or} \quad iE_1 = \frac{\partial A_4}{\partial(it)} - \frac{\partial(i\varphi)}{\partial x_1}$$

$$\frac{\partial A_1}{\partial x_4} - \frac{\partial A_4}{\partial x_1} iE_1 = - = F_{41}$$

$$\frac{\partial A_2}{\partial x_4} - \frac{\partial A_4}{\partial x_2} iE_2 = - = F_{42}$$

$$\frac{\partial A_3}{\partial x_4} - \frac{\partial A_4}{\partial x_3}$$

$$\dots iE_3 = - = F_{43}$$

In general

$$F_{k4} = -iE_k, \quad F_{ij} = \epsilon_{ijk} B_k$$

$$\epsilon_{ijk} = 0 \text{ if two indices are equal}$$

$$\epsilon_{ijk} = 1 \text{ if } i, j, k \text{ are distinct and in cyclic order}$$

$$\epsilon_{ijk} = -1 \text{ if } i, j, k \text{ are distinct and not in cyclic order.}$$

These are component of the anti symmetric tensor $F_{\mu\nu}$ defined by

$$F_{\mu\nu} = \begin{bmatrix} 0 & B_z & B_y & -iE_x/c \\ -B_z & 0 & B_x & -iE_y/c \\ B_y & -B_x & 0 & -iE_z/c \\ iE_x/c & iE_y/c & iE_z/c & 0 \end{bmatrix}$$

Which is the electromagnetic field four tensor.

Relativistic Lagrangian and Hamiltonian of a charged particle in an electromagnetic field

The action is the Lagrangian integrated over time, so the units of action are just the units of the Lagrangian multiplied by the units of time. The Lagrangian has units of energy, so the units of action are

$$[S] = M \frac{L^2}{T^2} T = \frac{ML^2}{T}$$

the action S_{nr} for a free non-relativistic particle is given by the time integral of the kinetic energy

$$S_{nr} = \int \frac{1}{2} m v^2(t) dt, \quad v^2 \equiv \vec{v} \cdot \vec{v}, \quad \vec{v} = \frac{d\vec{x}}{dt}$$

The equation of motion following by Hamilton's principle is

$$\frac{d\vec{v}}{dt} = 0$$

The free particle moves with constant velocity. Since even a free relativistic particle must move with constant velocity. The velocity of light does not even appear in this action. S_{nr} cannot be the action for a relativistic point particle. The path traced out in spacetime by the motion of a particle is called its world-line. It would be inconsistent for one observer to state that a certain motion is allowed and for another to state that the same motion is forbidden. If the equations of motion hold in a fixed Lorentz frame, they must hold in all Lorentz frames. If the action is a Lorentz scalar, the equations of motion will be Lorentz invariant.

Lagrangian and Hamiltonian formulations

Lagrange function or Lagrangian to be $L=T-V$

where

$$T = \sum_{i=1}^N \frac{1}{2} m_i |\mathbf{v}_i|^2$$

is the total kinetic energy for the system, and V is its potential energy.

The correct path of motion of a mechanical system with holonomic constraints and conservative external forces, from time t_1 to t_2 , is a stationary solution of the action. Indeed, the correct path of motion $q = q(t)$, with $q = (q_1, \dots, q_n)^T$, necessarily and sufficiently satisfies Lagrange's

equations of motion for $j = 1, \dots, n$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0$$

it is Hamilton's form of the principle of least action, because in many cases the action of $q = q(t)$ is not only an extremal but also a minimum value of the action functional. Hamilton's principle the equations of motion are given by Lagrange's equations, which here, taking the generalized coordinates to be $q_1 = r$ and $q_2 = \theta$, are the pair of ordinary differential equation

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{r}} \right) - \frac{\partial L}{\partial r} = 0$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\theta}} \right) - \frac{\partial L}{\partial \theta} = 0$$

Using the form for the Lagrangian,

$$\frac{\partial L}{\partial \dot{r}} = m\dot{r}, \quad \frac{\partial L}{\partial r} = mr\dot{\theta}^2 - \frac{\mu m}{r^2}, \quad \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta} \quad \text{and} \quad \frac{\partial L}{\partial \theta} = 0.$$

Substituting these expressions into Lagrange's equations

$$m\ddot{r} - mr\dot{\theta}^2 + \frac{\mu m}{r^2} = 0,$$

$$\frac{d}{dt} (mr^2\dot{\theta}) = 0.$$

Hamiltonian mechanics

Consider mechanical systems that are holonomic and conservative (or for which the applied forces have a generalized potential). For such a system we can construct a Lagrangian $L(q, \dot{q}, t)$, where $q = (q_1, \dots, q_n)^T$, which is the difference of the total kinetic T and potential V energies. These mechanical systems evolve according to the n Lagrange equations

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0$$

for $j = 1, \dots, n$. These are each second order ordinary differential equations and so the system is determined for all time once $2n$ initial conditions $q(t_0), \dot{q}(t_0)$ are specified (or n conditions at two different times). The state of the system is represented by a point $q = (q_1, \dots, q_n)$ T in configuration space.

Lagrange's equations of motion imply Hamilton's canonical equations, for $i = 1, \dots, n$

$$\dot{q}_i = \frac{\partial H}{\partial p_i},$$

$$\dot{p}_i = - \frac{\partial H}{\partial q_i}$$

Constraint

Mechanical systems with some types of non-holonomic constraints can also be treated, in particular constraints of the form

$$\sum_{j=1}^n A(\mathbf{q}, t)_{kj} \dot{q}_j + b_k(\mathbf{q}, t) = 0,$$

For $k = 1, \dots, m$, where $q = (q_1, \dots, q_n)$ T . Note the assumption is that these equations are not integrable, in particular not exact, otherwise the constraints would be holonomic.

Quantum equation for the field

Field equation is a partial differential equation which determines the dynamics of a physical field, specifically the time evolution and spatial distribution of the field. The solutions to the equation are mathematical functions which correspond directly to the field, as functions of time and space. Since the field equation is a partial differential equation, there are

families of solutions which represent a variety of physical possibilities. Usually, there is not just a single equation, but a set of coupled equations which must be solved simultaneously. Field equations are not ordinary differential equations since a field depends on space and time, which requires at least two variables.

Whereas the "wave equation", the "diffusion equation", and the "continuity equation" all have standard forms (and various special cases or generalizations), there is no single, special equation referred to as "the field equation".

The topic broadly splits into equations of classical field theory and quantum field theory. Classical field equations describe many physical properties like temperature of a substance, velocity of a fluid, stresses in an elastic material, electric and magnetic fields from a current, etc.

They also describe the fundamental forces of nature, like electromagnetism and gravity. In quantum field theory, particles or systems of "particles" like electrons and photons are associated with fields, allowing for infinite degrees of freedom (unlike finite degrees of freedom in particle mechanics) and variable particle numbers which can be created or annihilated.

Non-Relativistic Field Theory and Second Quantization

The problem of an N-particle system as a nonrelativistic field theory. The procedure described in the previous section is commonly known as Second Quantization. If the (identical) particles are bosons, the operators $\hat{a}(\mathbf{x})$ obey canonical commutation relations. If the (identical) particles are Fermions, the operators $\hat{a}(\mathbf{x})$ obey canonical anticommutation relations. In position space, it is customary to represent $\hat{a}^\dagger(\mathbf{x})$ by the operator $\hat{\psi}^\dagger(\mathbf{x})$ which obeys the equal-time algebra

$$\begin{aligned} [\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})]_{-\xi} &= \delta^d(\mathbf{x} - \mathbf{y}) \\ [\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{y})]_{-\xi} &= [\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})]_{-\xi} = 0 \end{aligned}$$

the one-particle Schrodinger equation becomes classical field equation

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - V(\mathbf{x}) \right] \hat{\psi} = 0$$

The Hamiltonian \hat{H} for this system is

$$\hat{H} = \int d^d x \left[\frac{\hbar^2}{2m} \nabla \hat{\psi}^\dagger \cdot \nabla \hat{\psi} + V(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \right] + \frac{1}{2} \int d^d x \int d^d x' \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}') U(\mathbf{x} - \mathbf{x}') \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x})$$

For Fermions the fields $\hat{\psi}$ and $\hat{\psi}^\dagger$ satisfy equal-time canonical anticommutation relations

$$\{\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\} = \delta(\mathbf{x} - \mathbf{x}')$$

while for Bosons they satisfy

$$[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}')$$

The Fock space picture of the many-body problem is equivalent to the Grand Canonical Ensemble of Statistical Mechanics. Thus, instead of fixing the number of particles we can introduce a Lagrange multiplier μ , the chemical potential, to weigh contributions from different parts of the Fock space.

Second Quantization: Creation and Annihilation Operators

A basis state can be completely specified in terms of the occupation number n_i for each member of a complete set of orthonormal single-particle states, $\{|i\rangle, i = 1, 2, 3, \dots\}$. The set of occupation numbers contains all the information necessary to construct an appropriately symmetrized or antisymmetrized basis vector, denoted

$$|i\rangle = |n_1, n_2, \dots, n_i, \dots\rangle$$

For bosons, n must be a non-negative integer; for fermions, the Pauli exclusion principle restricts n to be either 0 or 1.

The vector space spanned by the set of all such basis states is called the *Fock space*. A feature of the Fock space is that the total number of particles is not a fixed parameter, but rather is a dynamical variable associated with a total number operator

$$N = \sum n .$$

There is a unique *vacuum* or no-particle state:

$$|0\rangle = |0, 0, 0, 0, \dots\rangle .$$

The single-particle states can be represented

$$|i\rangle = |0, 0, \dots, 0, n_i = 1, 0, \dots\rangle \quad |0_1, 0_2, \dots, 0_{-1}, 1, 0_{+1}, \dots\rangle .$$

Bosonic operators. Let us define the bosonic *creation operator* and the corresponding *annihilation operator* a

Equations (1) and (2) allow us to define the number operator $N = a^\dagger a$, such that

$$N |n_1, n_2, \dots, n, \dots\rangle = n |n_1, n_2, \dots, n, \dots\rangle$$

The simplest application of the creation and annihilation operators involves the single-particle states:

$$a^\dagger |0\rangle = |i\rangle, \quad a |i\rangle = 0 .$$

When applied to multi-particle states, the properties of the creation and annihilation operators must be consistent with the symmetry of bosonic states under pairwise interchange of particles. It is clear from Eqs. (1) and (2) that for any pair of single particle state,

The properties described in the preceding paragraph can be summarized in the commutation relations

One consequence of these commutation relations is that any multi-particle basis state can be written or equally well, as any permutation of the above product of operators acting on the vacuum.

Equations (1)–(3) define the key properties of bosonic creation and annihilation operators. Note the close formal similarity to the properties of the harmonic oscillator raising and lowering operators.

Fermionic operators. The fermionic case is a little trickier than the bosonic one because we have to enforce antisymmetry under all possible pairwise interchanges. We define the fermionic creation operator c^\dagger by

$$\begin{aligned} c^\dagger |n_1, n_2, \dots, n_{-1}, 0, n_{+1}, \dots, i\rangle &= (-1)^{n_{+1} + \dots + n_i} |n_1, n_2, \dots, n_{-1}, 1, n_{+1}, \dots, i\rangle, \\ c^\dagger |n_1, n_2, \dots, n_{-1}, 1, n_{+1}, \dots, i\rangle &= 0, \end{aligned} \quad (4)$$

and the annihilation operator c by

$$\begin{aligned} c |n_1, n_2, \dots, n_{-1}, 1, n_{+1}, \dots, i\rangle &= (-1)^{n_{+1} + \dots + n_i} |n_1, n_2, \dots, n_{-1}, 0, n_{+1}, \dots, i\rangle, \\ c |n_1, n_2, \dots, n_{-1}, 0, n_{+1}, \dots, i\rangle &= 0. \end{aligned} \quad (5)$$

In both Eqs. (4) and (5),

$$= \sum_{i=1}^N N_i, \quad \text{where } N_i = c_i^\dagger c_i, \quad (6)$$

measures the total number of particles in single-particle states having an index i . It is straightforward to check that Eqs. (4)–(6) are self-consistent, in the sense that with the phase factor $(-1)^{N_i}$ as defined above,

$$N_i |n_1, n_2, \dots, n_i, \dots\rangle = n_i |n_1, n_2, \dots, n_i, \dots\rangle \quad \text{for } n_i = 0 \text{ or } 1. \quad (7)$$

$$c_i |i=0\rangle = -c_i |i=1\rangle. \text{ Similarly, } c_i |i=1\rangle = -c_i |i=0\rangle \text{ for } i \neq j, \text{ and } c_i c_i |i=0\rangle = 0.$$

ny $c_i^\dagger c_i |i\rangle = |i\rangle$ basis state $|i\rangle$, whereas $c_i c_i^\dagger |i\rangle = (1 - n_i) |i\rangle$.

Thus, for any $|i\rangle$ in the Fock space.

The properties above can be summarized in the anticommutation relations where

$\{A, B\} = AB + BA$ is the anticommutator of A and B . These anticommutation properties fundamentally distinguish the fermionic operators from their commuting bosonic counterparts. The $(-1)^{N_i}$ phase factors entering Eqs. (4) and (5) were chosen specifically to ensure that Eqs. (7) are satisfied. Alternative phase conventions can be adopted, so long as the anticommutation relations are preserved.

Given the anticommutation relations, any multi-particle basis state can be or equally well, as any permutation of the above product of creation operators with a sign change for each pairwise interchange of adjacent operators.

For example,

Equations (4)–(7) define the key properties of fermionic creation and annihilation operators.

Basis transformations.

Creation and annihilation operators defined above were constructed for a particular basis of single-particle states $\{|i\rangle\}$. We will use the notation b_i^\dagger and b_i to represent these operators in situations where it is unnecessary to distinguish between the bosonic and fermionic cases.

Consider an alternative single-particle basis $\{|\tilde{i}\rangle\}$, which—like $\{|i\rangle\}$ —is complete and Prepared by Dr. A.SARANYA, Asst. Prof, Dept. of PHYSICS, KAHE

orthonormal. The Fock space can be spanned by many-particle basis states of the form

$$|\tilde{i}\rangle = |n_1, n_2, \dots, n_i, \dots\rangle,$$

It is important to note that the vacuum state $|0\rangle$ can (and will) be chosen to be the same in both the original and new bases.

all consistent with the unitary transformation

An important special case of a basis transformation involves single-particle basis states of well-defined position \mathbf{r} and spin z component : $\{|\tilde{i}\rangle\} = \{|\mathbf{r}, i\rangle\}$, where $\langle \mathbf{r}, i | \mathbf{r}', j \rangle = \delta(\mathbf{r} - \mathbf{r}') \delta_{ij}$.

The corresponding operators are called the field creation and annihilation operators, and are given the special notation $\hat{\psi}^\dagger(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$. For bosons or fermions, where $\psi(\mathbf{r})$ is the wave function of the single-particle state $|i\rangle$. The field operators create/annihilate a particle of spin- z at position \mathbf{r} :

Dynamical variables.

Now we consider how to represent dynamical variables in terms of the creation and annihilation operators introduced above

The simplest dynamical variables are additive *one-particle operators* of the form $\hat{O} = \sum_j \hat{O}_j$, where \hat{O}_j acts just on the j 'th particle. Examples of one-particle operators include the momentum $\hat{P} = \sum_j \hat{P}_j$, the kinetic energy $K = \sum_j \hat{K}_j$, where

$$\hat{K}_j = \hat{P}_j^2 / 2m, \text{ and the external potential } V = \sum_j V_j, \text{ where } V_j = v(\mathbf{r}_j).$$

If we choose a single-particle basis $\{|\tilde{i}\rangle\}$ in which \hat{P}_j is diagonal (e.g., momentum eigenstates in the cases of \hat{P}_j and \hat{K}_j , position eigenstates for V_j), then the total operator can be represented as $\hat{O} = \sum_{i,j} \tilde{O}_{ij} \tilde{a}_i^\dagger \tilde{a}_j$.

In any other basis $\{|i\rangle\}$, related to $\{|\tilde{i}\rangle\}$ by Eq. (8), the most general form of an additive one-particle operator is

$$\hat{O} = \sum_{i,j} \langle i | \hat{O} | j \rangle a_i^\dagger a_j.$$

We will also consider *additive two-particle operators*, most commonly encountered as a pairwise interaction potential $U = \sum_{i < j} u(\mathbf{r}_i, \mathbf{r}_j)$.

Note the reversal of the order of the operators a and b in Eq. (9), which allows the same expression to be used for bosons and fermions.

We are now in a position to consider applications of the formalism outlined above to many-boson and many-fermion systems.

QUANTIZATION OF THE FIELD

To quantize the field, we regard the field variables Ψ and π as operator functions. Just as the quantum conditions.

$$[q_i, q_j] = [P_i, P_j] = 0; \quad [q_i, P_j] = i\hbar \delta_{ij} \quad \dots\dots\dots (1)$$

Were used for the transition from classical to quantum particle mechanics , we achieve the transition from classical to quantum field theory by requiring that

$$[P_i, P_j] = 0 \text{ and } [\Psi_i, P_j] = i\hbar \delta_{ij} \quad \dots\dots\dots (2)$$

Assuming the cell volumes are very small, Eq. (2) can be rewritten in terms of Ψ and π in the following forms:

$$[\Psi(r, t), \Psi(r', t)] = [\pi(r, t), \pi(r', t)] = 0 \quad \dots\dots\dots (3)$$

$$[\Psi(r, t), \pi(r', t)] = i \delta(r, r') \quad \dots\dots\dots (4)$$

Where $\delta(r, r') = \frac{1}{V} \delta_{ii}$ if r and r' are in the same cell and zero otherwise in the limit, the cell volume approach zero , $\delta(r, r')$ can be replaced by the three dimensional Dirac δ – function $\delta(r-r')$. The quantum conditions for the canonical field variables Ψ and π the become

$$[\Psi(r, t), \Psi(r', t)] = [\pi(r, t), \pi(r', t)] = 0 \quad \dots\dots\dots (5)$$

$$[\Psi(r, t), \pi(r', t)] = i \delta(r, r') \quad \dots\dots\dots (6)$$

By making Ψ and π non –commuting operators, we convert H, L etc., also into operators which have eigenvalues , eigenstates , etc.

The equation of motion for any quantum dynamical variable F is obtained from by replacing the Poisson bracket by the commutator bracket divided by i or from Eq.

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{1}{i\hbar} [F, H] \quad \dots\dots\dots (7)$$

Equations (5) and (7) completely describe the behaviour of the quantized field specified by the Hamiltonian.

Quantization Of Schrodinger Equation

As an example of the field quantization technique, we shall consider the quantization of the non-relativistic Schrodinger equation in this section. The name Schrodinger field is used for a field $\Psi(r, t)$ satisfying the Schrodinger equation.

$$i \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi \quad \text{.....(1)}$$

Equation (1) is the quantized equation of motion of a particle of mass m moving in a potential V . Here $\Psi(r, t)$ is thought of as a classical field, which can be quantized by converting it into an operator using the procedure described earlier. Since it is the second time the equation is being quantised, it is referred to as the second quantization.

To start with, we note that the Lagrangian density \mathcal{L} taken in the form:

$$\mathcal{L} = i \Psi^* \frac{\partial \Psi}{\partial t} - \frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi - V(r, t) \Psi^* \Psi \quad \text{.....(2)}$$

Reduce the classical field equation to the familiar Schrodinger equation, Eq (1). Ψ and Ψ^* in Eq. (2) can be considered as independent fields giving the Lagrange's equations of motion. The variation with respect to Ψ^* in Eq directly gives Eq(1) while variation with respect in Ψ gives the complex conjugate of Eq(1).

$$-i \frac{\partial \Psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V \Psi^* \quad \text{.....(3)}$$

The momentum canonically conjugate to Ψ is :

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\Psi}} = i \Psi^* \quad \text{.....(4)}$$

Where we have used the expression for \mathcal{L} given in Eq 2. Using Equation (2)

Hamiltonian density \mathcal{H} now becomes
and(4),the

$$\mathcal{H} = \pi \dot{\Psi} - \mathcal{L} = \frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi + V(r, t) \Psi^* \Psi \quad \text{.....(5)}$$

$$= -\frac{i\hbar}{2m} \nabla(i\hbar \Psi^*) \cdot \nabla \Psi - \frac{i}{\hbar} V(i\hbar \Psi^*) \Psi$$

Using Eq (5), the Hamiltonian H is given by

$$H = \int_V \mathcal{H} d^3r = \int_V \left(\frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi + V \Psi^* \Psi \right) d^3r$$

The classical field equation in the Hamiltonian form are given by eq it follow from the discussed on function derivation eq

$$\frac{\partial H}{\partial \pi} = \frac{\partial \mathcal{H}}{\partial \pi} - \nabla \cdot \frac{\partial \mathcal{H}}{\partial (\nabla \pi)} \quad \dots\dots(7)$$

$$\pi = \frac{\partial H}{\partial \Psi} = \left(\frac{\partial \mathcal{H}}{\partial \Psi} - \nabla \cdot \frac{\partial \mathcal{H}}{\partial \nabla \Psi} \right) \quad \dots\dots(8)$$

These equations can be expressed in the familiar form by substituting the value of \mathcal{H} from eq now

$$= -\frac{i}{\hbar} V + \frac{i\hbar}{2m} \nabla^2 \Psi \quad \dots\dots(9)$$

Multiplying by i ,

$$i \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi$$

Replacement of \mathcal{H} in eq this equation

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

Since $\pi = i \Psi^*$ this equation becomes

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

Equation (9) and (10) are the familiar classical equation and its complex conjugate for the Schrodinger field. This validates the expressed for Lagrangian density

Since $\hat{\Psi}$ is now an operator, $\hat{\Psi}^*$ is to be interpreted as the Hamiltonian adjoint of $\hat{\Psi}$ rather than its complex conjugate and its usually denoted by $\hat{\Psi}^\dagger$.

$$[\hat{\Psi}(\mathbf{r},t), \hat{\Psi}^\dagger(\mathbf{r}',t)] = \delta(\mathbf{r}-\mathbf{r}').$$

QUANTIZATION OF THE FIELD

To quantize the field, we regard the field variables $\hat{\Psi}$ and $\hat{\pi}$ as operator functions. Just as the quantum conditions.

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$$[\hat{\Psi}(\mathbf{r},t), \hat{\Psi}(\mathbf{r}',t)] = [\hat{\pi}(\mathbf{r},t), \hat{\pi}(\mathbf{r}',t)] = 0 \quad \dots\dots\dots (3)$$

$$[\hat{\Psi}(\mathbf{r},t), \hat{\pi}(\mathbf{r}',t)] = i\delta(\mathbf{r}-\mathbf{r}') \quad \dots\dots\dots (4)$$

Where $\delta(\mathbf{r}, \mathbf{r}') = \frac{1}{\Delta V} \delta_{ij}$ if \mathbf{r} and \mathbf{r}' are in the same cell and zero otherwise in the limit, the cell volume approach zero, $\delta(\mathbf{r}, \mathbf{r}')$ can be replaced by the three dimensional Dirac δ -function $\delta(\mathbf{r}-\mathbf{r}')$. The quantum conditions for the canonical field variables $\hat{\Psi}$ and $\hat{\pi}$ the become

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Equations (5) and (7) completely describe the behaviour of the quantized field specified by the Hamiltonian.

QUANTIZATION OF THE SCHRODINGER EQUATION

As an example of the field quantization technique ,we shall consider the quantization of the non-relativistic Schrodinger equation in this section. The name Schrodinger field is used for a field $\Psi(r, t)$ satisfying the Schrodinger equation.

$$I \frac{\partial \Psi}{\partial t} = - \frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi \quad \dots\dots\dots(1)$$

Equation (1) is the quantized equation of motion of a particle of mass m moving in a potential V. Here $\Psi(r,t)$ is thought of as a classical field , which can be quantized by converting it into an operator using the procedure described earlier. Since it is the second time the equation is being quantised , it is referred to as the second quantization.

To start with, we note that the Lagrangian density \mathcal{L} taken in the form:

$$\mathcal{L} = i \Psi^* \Psi - \frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi - V(r,t) \Psi^* \Psi \quad \dots\dots\dots(2)$$

Reduce the classical field equation to the familiar Schrodinger equation , Eq (1). Ψ and Ψ^* in Eq. (2) can be considered as independent fields giving the Lagrange's equations of

motion. The variation with respect to Ψ^* in Eq directly gives Eq(1) while variation with respect in Ψ gives the complex conjugate of Eq(1).

$$-i \frac{\partial \Psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V \Psi^* \quad \dots\dots\dots(3)$$

The momentum canonically conjugate to Ψ is :

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\Psi}} = i \Psi^* \quad \dots\dots\dots(4)$$

Where we have used the expression for \mathcal{L} given in Eq 2. Using Equation (2) and (4), the Hamiltonian density \mathcal{H} now becomes

$$\mathcal{H} = \pi \dot{\Psi} - \mathcal{L} = \frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi + V(r,t) \Psi^* \Psi \quad \dots\dots\dots(5)$$

$$= -\frac{i\hbar}{2m} \nabla (i\hbar \Psi^*) \cdot \nabla \Psi - \frac{i}{\hbar} V (i\hbar \Psi^*) \Psi$$

$$= -\frac{i\hbar}{2m} \nabla \pi \cdot \nabla \Psi - \frac{i}{\hbar} V \pi \Psi \quad \dots\dots\dots(6)$$

Using Eq (5), the Hamiltonian H is given by

$$H = \int_V \mathcal{H} d^3 r = \int_V \left(\frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi + V \Psi^* \Psi \right) d^3 r$$

The classical field equation in the Hamiltonian form are given by eq it follow from the discussed on function derivation eq

$$\frac{\partial H}{\partial \pi} = \frac{\partial \mathcal{H}}{\partial \pi} = \nabla \cdot \frac{\partial \mathcal{H}}{\partial (\nabla \pi)} \quad \dots\dots\dots(7)$$

$$\pi = \frac{\partial H}{\partial \dot{\Psi}} = -\left(\frac{\partial \mathcal{H}}{\partial \dot{\Psi}} - \nabla \cdot \frac{\partial \mathcal{H}}{\partial \nabla \Psi} \right) \quad \dots\dots\dots(8)$$

These equations can be expressed in the familiar form by substituting the value of \mathcal{H} from eq now

$$= -\frac{i}{\hbar} V + \frac{i\hbar}{2m} \nabla^2 \Psi \quad \text{.....(9)}$$

Multiplying by i ,

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Since $\pi = i \Psi^*$ this equation becomes

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Equation (9) and (10) are the familiar classical equation and its complex conjugate for the Schrodinger field. This validates the expressed for Lagrangian density .

Since π is now an operator , Ψ^* is to be interpreted as the Hamiltonian adjoint of Ψ rather than its complex conjugate and its usually denoted by Ψ^* .

$$[\Psi(r,t), \Psi^*(r',t)] = \delta(r-r').$$

POSSIBLE QUESTIONS

PART B (4 Marks each)

1. State and explain the classical field equation in Hamiltonian form.
2. State the classical field equation and explain the quantities involved therein.
3. What is meant by a conjugate field? Explain.
4. What are creation, annihilation and number operators? Why are they called so? Explain.
5. What is meant by second quantization? Why is it called so? Explain
6. Explain quantization of non-relativistic Schrodinger equation.
7. Write a short note on Lagrangian density
8. Explain what is meant by functional derivative.
9. Explain the need of quantization of fields. What is the necessity of quantizing fields? In what context is it important?
10. For a system of fermions, define the number operator N_k and show that its eigen values are zero and one.

PART C (10 Marks each)

1. Derive the classical field equation in the Hamiltonian form, and explain quantization of fields. Explain the terms Hamiltonian density, functional density and conjugate field.
2. Explain quantization of Schrodinger equation. Explain creation and annihilation operators and their significance.
3. Explain in detail Dirac field.
4. Explain classical theory of electromagnetic fields.
5. Explain quantization of electromagnetic fields.

S.No	Questions	Option 1	Option 2	Option 3	Option 4	Answer
1	A system of particles is specified by the _____ co-ordinates and their dependence on the time.	momentum	space	positional	phase-space	positional
2	The field lagrangian is expressed as the integral over all space of a _____ density.	Lagrangian	Hamiltonian	Volume	Surface	Lagrangian
3	The Hamiltonian equation for the time rate of change of a functional F of y and p is given by _____.	$\frac{dF}{dt} = \frac{F}{t} - \{F, H\}$	$\frac{dF}{dt} = \frac{F}{t} + \{F, H\}$	$\frac{dF}{dt} = \frac{F}{x} - \{F, H\}$	$\frac{dF}{dt} = \frac{F}{x} + \{F, H\}$	$\frac{dF}{dt} = \frac{F}{t} + \{F, H\}$
4	In the equation $\frac{dF}{dt} = \frac{F}{t} + \{F, H\}$, H represents the _____ energy of the field.	total	partial	kinetic	none of the above	total
5	The Lagrangian $L(q_i, \dot{q}_i, t)$ is a function of time and a functional of the possible paths of _____ of the system.	y(t)	dy/dt	$q_i(t)$	none of the above	$q_i(t)$
6	The field lagrangian is a function of the field amplitude _____.	\tilde{N}_y	dy/dt	q(r,t)	y(r,t)	y(r,t)
7	The appearance of \tilde{N}_y is a continuous dependence of y on r i.e., continuously _____ number of degrees of freedom.	finite	infinite	constant	a and c	infinite
8	The variational principle for the lagrangian is given by _____.	$\frac{dL}{dt} = 0$	$\frac{dL}{dt} = 1$	$\frac{dL}{dt} = -1$	$\frac{dL}{dt} = y(r,t)$	$\frac{dL}{dt} = 0$

9	The momentum canonically conjugate to y can be defined to be the ratio of dL to the infinitesimal change dy when all the other d and all the _____ are zero.	y	L	\tilde{N}_y	dy	dy
10	The functional density $F(y, p, t)$ is assumed not to depend explicitly on _____	time	momentum	space co-ordinate	none of the above	none of the above
11	The $dF/dt =$ _____.	$-F/t + \{F, H\}$	$-F/t - \{F, H\}$	$F/t + \{F, H\}$	$F/t - \{F, H\}$	$F/t + \{F, H\}$
12	If H does not depend on explicitly on the time, then H is a _____ of motion.	equation	constant	lagrangian equation	Hamiltonian equation	constant
13	According to quantum equation for the field, the wave field from a real numerical function can be converted to a hermitian operator in the _____ picture.	quantum	classical	skew hermitian	Heisenberg	Heisenberg
14	According to quantum equation for the field, $[y_i, y_j] = [P_i, P_j] =$ _____	1	-1	0	2	0
15	The function $d(r, r')$ has the property that _____ is equal to the average value of f for the cell in which r' is situated.	$f(r) d(r, r') / d^3r$	$-f(r) d(r, r') / d^3r$	$-f(r) d(r, r') / d^2r$	$f(r) d(r, r') / d^2r$	$f(r) d(r, r') / d^3r$
16	The equation of motion for any quantum dynamical variable F is given by _____	$dF/dt = -F/t + 1/i [F, H]$	$dF/dt = F/t - 1/i [F, H]$	$dF/dt = F/t + 1/i [F, H]$	$dF/dt = -F/t - 1/i [F, H]$	$dF/dt = F/t + 1/i [F, H]$

17	The field quantization is often called as _____.	wave quantisation	second quantisation	wave function quantisation	none of the above	second quantisation
18	If the commutation relations for the operators a_k and a_k^* are solved, then _____ is diagonal, consists of matrices.	$a_k^* a_k$	$a_k^* a_k^2$	$a_k^* a_k$	$a_k^* a_k$	$a_k^* a_k$
19	The states of the quantized field in the representation in which each N_k is diagonal, are the kets given by _____.	$ n_1, n_2, n_3, \dots, n_k, \dots\rangle$	$ n_1, n_2, n_3, \dots, n_k, \dots\rangle$	$ n_1, n_2, n_3, \dots, n_k, \dots\rangle$	$ N_1, N_2, N_3, \dots, N_k, \dots\rangle$	$ n_1, n_2, n_3, \dots, n_k, \dots\rangle$
20	The a_k^* is called _____ operator for the state k of the field.	none of the above	creation	number	destruction	number
21	The spin of the electron carries no _____	charge	particles	energy	density	energy
22	The N_k is called _____ operator for the state k of the field.	number	creation	destruction	none of the above	number
23	The number operator need not be a _____.	equation of motion	constant of motion	lagrangian motion	Hamiltonian motion	constant of motion

24	The rate of change of N_k is given by _____.	$\frac{dN_k}{dt} = i [a_k^*, a, H]$	$\frac{dN_k}{dt} = -i [a_k^*, a, H]$	$\frac{dN_k}{dt} = [a_k^*, a, H]$	$i \frac{dN_k}{dt} = [a_k^*, a, H]$	$i \frac{dN_k}{dt} = [a_k^*, a, H]$
25	The necessary and sufficient condition that N_k to be a constant of the motion is that all off-diagonal elements that involve the state U_k be _____.	0	-1	1	none of the above	0
26	If U_k and E_k are the eigen function and eigen value, then the field hamiltonian becomes _____.	$H = N_k E_k^2$	$H = N_k E_k^3$	$H = N_k E_k$	$H = N_k E_k^4$	$H = N_k E_k$
27	According to anticommutation relation, $[a_k, a_l] =$ _____.	$a_k a_l + a_l a_k = 1$	$a_k a_l + a_l a_k = 0$	$a_k a_l + a_l a_k = -1$	$a_k a_l - a_l a_k = 0$	$a_k a_l + a_l a_k = 0$
28	If the eigenvalues of each N_k are 0 and 1, then the particles obey the _____ principle.	variational	lagrangian	Hamiltonian	Exclusion	Exclusion
29	The eigen values of H can be found by the linear combination of the _____ wave amplitudes	spherical	polarized	plane	circular	plane
30	H is formally equivalent to the sum of the energies of a number of _____ oscillators.	harmonic	simple harmonic	sinusoidal	none of the above	harmonic
31	The momentum density of an electromagnetic field is the pointing vector _____ divided by c^2 .	$-(c/4\pi) \mathbf{E}(\mathbf{r}, t) \times \mathbf{H}(\mathbf{r}, t)$	$(c/\pi) \mathbf{E}(\mathbf{r}, t) \times \mathbf{H}(\mathbf{r}, t)$	$-(c/\pi) \mathbf{E}(\mathbf{r}, t) \times \mathbf{H}(\mathbf{r}, t)$	$(c/4\pi) \mathbf{E}(\mathbf{r}, t) \times \mathbf{H}(\mathbf{r}, t)$	$(c/4\pi) \mathbf{E}(\mathbf{r}, t) \times \mathbf{H}(\mathbf{r}, t)$
32	According to quantized field, the energy and momentum of each plane wave are quantized in	$\hbar \omega$ and $\hbar \mathbf{k}$	$\hbar \omega$ and $\hbar \mathbf{k}$	$\hbar \omega$ and $-\hbar \mathbf{k}$	$\hbar \omega$ and $-\hbar \mathbf{k}$	$\hbar \omega$ and $\hbar \mathbf{k}$

33	According to Planck's quantum hypothesis, the energy associated with each plane electromagnetic wave is an integer multiple of the fundamental quantum _____.	K	- K	hn	h	hn
34	The quantized electromagnetic field propagates with the _____ speed of light.	classical	quantum	a and b	none of the above	classical
35	The Hamiltonian density is given by H= _____.	-p	p	0	p	p
36	A physical system with _____ degrees of freedom is referred as a field.	finite	infinite	constant	none of the above	infinite
37	A transition from classical particle mechanics to quantum mechanics is _____ degeneracy.	doubly	triply	singly	none of the above	doubly
38	The electromagnetic wave travels in free space with the velocity of _____.	sound	ultrasonic wave	ultrasonic wave	infrasonic wave	ultrasonic wave