

	SEMESTER III	L T P C
16PHP301	QUANTUM MECHANICS – II	4 - - 4

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 – Clebsch-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-Gordon equation – Interpretation of the Klein-Gordon 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.

6. Chatwal R.G. and Sk. Anand, 4th editin 2004, Quantum Mechanics, Himalaya Publishing House, New Delhi
7. Thangappan. V. K., 2nd edition 2007, Quantum Mechanics, Tata McGraw Hill, New Delhi

UNIT-I

S No	Lecture Duration (Hr)	Topics to be covered	Support materials
1.	1Hr	Angular momentum: Angular momentum operators - Angular momentum commutation relations	T1-170-171
2.	1Hr	Eigen values and Eigen functions of L^2 and L_z General angular momentum	T1-172-173
3.	1Hr	Eigen values of J^2 and J_z - Ladder operators (J_+ and J_-)	T1-173-176
4.	1Hr	Angular momentum matrices - Matrices for J^2 , J_z , J_+ , J_- , J_x and J_y	T1-176-179
5.	1Hr	Spin angular momentum, Spin $\frac{1}{2}$ systems	T1-179
6.	1Hr	Spin vectors for spin $\frac{1}{2}$ systems - Addition of angular momentum	T1-179-180
7.	1Hr	Clebsch-Gordan coefficients.	T1-180-182
8.	1Hr	Revision	
9.	1Hr	Discussion of possible 2 mark question	
10.	1Hr	Discussion of possible 8 mark question	
11.	1Hr	Test in 2 mark question	
12.	1Hr	Test in 8 mark question	
Total no of hours			

Text Book

T1: Aruldas. G, 2008, Quantum Mechanics, 2nd Edition, Prentice-Hall of India, New Delhi.

Reference Book

R1: Gupta, Kumar and sharma, 2002, Quantum Mechanics, 22nd edition, Jaiprakash nath & Co, Meerut

UNIT-II

S No	Lecture Duration (Hr)	Topics to be covered	Support materials
1.	1Hr	Scattering: Scattering cross-section- Scattering amplitude , Partial waves - Scattering by a central potential:	T1 - 283-290
2.	1Hr	partial wave analysis - Significant number of partial waves	T1 - 290-291
3.	1Hr	Scattering by an attractive square-well potential	T1 – 291
4.	1Hr	Briet-Wigner formula, Scattering length	T1 - 292-294
5.	1Hr	Expression for phase shift - Integral equation	T1 - 295-298
6.	1Hr	The Born approximation - Scattering by screened coulomb potential	T1 – 298-300
7.	1Hr	Validity of Born approximation - Laboratory and center of mass co-ordinate systems	T1- 300-303
8.	1Hr	Revision	
9.	1Hr	Discussion of possible 2 mark question	
10.	1Hr	Discussion of possible 8 mark question	
11.	1Hr	Test in 2 mark question	
12.	1Hr	Test in 8 mark question	
Total no of hours			12

Text Book

T1:Aruldas. G, 2008, Quantum Mechanics, 2nd Edition, Prentice-Hall of India, NewDelhi.

Reference Book

R1:Gupta, Kumar and sharma ,2002, Quantum Mechanics, 22nd edition, Jaiprakash nath & Co, Meerut

UNIT-III

S No	Lecture Duration (Hr)	Topics to be covered	Support materials
1.	1Hr	Many Electron Problem: Indistinguishable particles, Pauli principle, Inclusion of spin - Spin functions for three electrons	T1-260-265
2.	1Hr	Spin functions for three electrons - The Helium atom	T1-266-269
3.	1Hr	Central field approximation	T1-269- 270
4.	1Hr	Thomas-Fermi model of the atom - Hartree equation , Hartree-Fock equation	T1-270- 276
5.	1Hr	Molecular orbital theory: Hydrogen molecule ion H_2^+ -	R2-433- 444
6.	1Hr	Valence bond theory , Heitler-London theory of hydrogen molecule.	R2-457
7.	1Hr	Revision	
8.	1Hr	Discussion of possible 2 mark question	
9.	1Hr	Discussion of possible 8 mark question	
10.	1Hr	Test in marks 2	
11.	1Hr	Test in 8 mark question	
		Total no of hours	11

Text Book

T1:Aruldas. G, 2008, Quantum Mechanics, 2nd Edition, Prentice-Hall of India, NewDelhi.

R2:Satya Prakash, 2003, Quantum Mechanics, New Edition Kedar Nath & Ram Nath & Co, Meerut.

Reference Book

R1:Gupta, Kumar and sharma ,2002,Quantum Mechanics, 22nd edition, Jaiprakash nath & Co, Meerut

UNIT-IV

S No	Lecture Duration (Hr)	Topics to be covered	Support materials
1.	1Hr	Relativistic quantum mechanics: Klein-Gordan equation - Interpretation of the Klein-Gordan equation	T1 -310-312
2.	1Hr	Particle in a coulomb field - Dirac's equation for a free particle - Dirac matrices , Covariant form of Dirac equation	T1-312-318
3.	1Hr	Probability density ,Negative energy states	T1-318-322
4.	1Hr	Spin of the Dirac particle, Magnetic moment of the electron - Spin-orbit interaction - Radial equation for an electron in a central potential	T1 322-331
5.	1Hr	Hydrogen atom , Lamb shift	T1-331-333
6.	1Hr	Revision	
7.	1Hr	Discussion of possible 2 mark question	
8.	1Hr	Discussion of possible 8 mark question	
9.	1Hr	Test in 2 mark question	
10.	1Hr	Test in 8 mark question	
		Total no of hours	10

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T1:Aruldas. G, 2008, Quantum Mechanics, 2nd Edition, Prentice-Hall of India, NewDelhi.

Reference Book

R1:Gupta, Kumar and sharma ,2002,Quantum Mechanics, 22nd edition, Jaiprakash nath & Co, Meerut

UNIT-V

S No	Lecture Duration (Hr)	Topics to be covered	Support materials
1.	1Hr	Field theory: Introduction , Classical approach to field theory	R2-410
2.	1Hr	Relativistic Lagrangian and Hamiltonian of a charged particle in an electromagnetic field	R2-412
3.	1Hr	Lagrangian - Hamiltonian formulations	R2-413-414
4.	1Hr	Quantum equation for the field - Second quantisation	R2-414-418
5.	1Hr	Quantisation of non-relativistic Schroedinger equation	R2-419-420
6.	1Hr	Creation, annihilation and number operators.	R2-420-422
7.	1Hr	Revision	
8.	1Hr	Old question paper discussion	
9.	1Hr	Old question paper discussion	
10.	1Hr	Old question paper discussion	
11.	1Hr	Test in Unit 1 & 2	
12.	1Hr	Test in Unit 3 & 4	
13.	1Hr	Test in Unit 5	
14.	2Hr	Full portion test	
	Total no of hours		15

Text Book

R2:..Satya Prakash, 2003, Quantum Mechanics, New Edition Kedar Nath & Ram Nath & Co, Meerut.

Reference Book

R1:Gupta, Kumar and Sharma, 2002, Quantum Mechanics, 22nd Edition, Jai Prakash Nath & Co, Meerut.

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

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

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

in these commutations p_z stands for $-i \frac{d}{dz}$. 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

$$[(y p_z - z p_y), p_x] = y p_x [p_z, z] = -i y p_x$$

based on similar arguments, we get

$$[z p_x - x p_z] = p_y x [z, p_z] = -i x p_y$$

Hence

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

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

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

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 commutation relations hold for the components of total angular momentum $L = L_i$ of a system of particle also. The commutation relation can be written in a compact form as

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

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

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

$$= 0 + L_y [L_y, L_x] + [L_y, L_x] L_y + L_z [L_z, L_x] + [L_z, L_x] L_z$$

$$=L_y(-iL_z)+(-iL_z)L_y+iL_zL_y+iL_yL_z$$

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 by 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 representations in which all the four are diagonal.

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

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

the reason for the names would be clear in section.

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

and

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

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

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

we also have

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

and

$$L_+L_- = L^2 - L_z^2 + L_z, L_-L_+ = L^2 - L_z^2 - L_z$$

EIGENVALUES AND EIGENFUNCTIONS OF L^2 AND L_z :

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

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

where $l(l+1)$ is the eigen value of L^2 and Y is the corresponding eigen function rearranging we get

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

which is the same as the angular part of the schrodinger equation of a system moving in a potential $V(r)$. The solution gives $l(l+1)$ 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

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

and $Y_{lm} = (-1)^m$ for $m > 0$ and $Y_{l0} = 1$ for $m = 0$. The form of L_z , immediately gives

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

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

$$J^2 |l, m\rangle = \lambda |l, m\rangle$$

and

$$J_z |l, m\rangle = m |l, m\rangle$$

equation 1 can be written as

$$J_x^2 + J_z^2 |l, m\rangle + m^2 |l, m\rangle = \lambda |l, m\rangle$$

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

$$\langle l, m| J^2 |l, m\rangle + \langle l, m| J_z^2 |l, m\rangle = \lambda \langle l, m| |l, m\rangle$$

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

$$-\lambda \leq 0 \text{ or } \lambda \geq 0$$

operating eq 1 from left by J_+ , we get

$$J_+ J^2 |l, m\rangle = J_+ \lambda |l, m\rangle$$

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

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

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

we get

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

or

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

thus $J_+ |l, m\rangle$ is an eigenket 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 \hbar , 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

$$J_z |l, \mu\rangle = \mu |l, \mu\rangle$$

operation by J_+ from left gives

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

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

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

premultiplying by J_- and using the result

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

we get

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

therefore

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

as

$$(\mu^2 - \mu) = 0 \text{ so}$$

$$\mu(\mu + 1) = 0$$

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

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

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

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

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

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

since $(\mu - n) \neq 0$

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

or

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

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

$$[-(\mu-n)^2 + (\mu-n)]J^{n+1}\mu = 0$$

As $J^{n+1}\mu > 0$, $-(\mu-n)^2 + (\mu-n) = 0$, substituting the value of μ from we find

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

since $(n+1) \neq 0$

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

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 the possible value of j are $0, 1/2, 1, 3/2, \dots$ thus half integral quantum number 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 $j(j+1)$ and m by $|j, m\rangle$ we get

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

and

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

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 $\langle j', m' | J | j, m \rangle$. 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 commute 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 $J^2 |j, m\rangle = j(j+1) |j, m\rangle$ and $J_z |j, m\rangle = m |j, m\rangle$ from left by $\langle j', m' |$ gives

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

and

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

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

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

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

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

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

similar we get

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

where

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

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

compare the two equations gives

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

operating of eq from left by J_- , we have

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

replacing $J_- J_+$ we get

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

or

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

or

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

with the value of a_m

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

or

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

similarly

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

last two give equation give the matrix element for J_+ and J_- they are infinite dimensional matrices like the J^2 and J_z matrices. The nature of the Kronecker deltas in last two equations indicates that all nonvanishing elements occur in blocks 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 $j=1/2$

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

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

for $j=1$

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

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

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

$$\mu_s = -e/m \mathbf{S}$$

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

\mathbf{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

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

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

$$x^2 = y^2 = z^2 = 1$$

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

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

Pauli was the first to recognize the necessity of two component state vectors 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 $\psi(r, m_s)$ 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

$$\psi(r, m_s) = \psi(r) \psi(m_s)$$

where $\psi(r)$ represented that depends on the space coordinates and $\psi(m_s)$ 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

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

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

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

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

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

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

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

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”

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

and all results will be equally. 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.

Clebsh – Gordon Coefficient

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.

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

Substituting this value of the coefficient in equation (3)

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

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

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

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

And

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

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

$$m = m_1 + m_2$$

we shall next find out how 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 , m_1 can have values from j_1 to $-j_1$ and j_2 to $-j_2$, m_2 in integral step.

The smallest value 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?

DEPARTMENT OF PHYSICS
CLASS:II M.Sc PHYSICS
QUANTUM MECHANICS-II (16PHP301)

Equation of Linear momentum	$P = mv$	$P = dv$	$P = md$	$P = m^2v$	$P = mv$
Torque τ	$r \times F$	$r^2 \times F$	$r^2 \times$	$r \times F^2$	$r \times F$
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
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
Angular momentum =	$\hbar(r \times \Delta)$	$\hbar/I r \times \Delta$	$\hbar(r^2 \times \Delta)$	$\hbar/i r \times \Delta$	$\hbar/i r \times \Delta$
$L \times L =$	$i\hbar L$	$i\hbar L$	$i\hbar L^2$	$i\hbar^2 L$	$i\hbar L$
Total angular momentum is defined by	$J^2 = J_x^2 + J_y^2 + J_z^2$	$J^3 = J_x^3 + J_y^3 + J_z^3$	$J^2 = J_x + J_y + J_z$	$J = J_x^2 + J_y^2 + J_z^2$	$J^2 = J_x^2 + J_y^2 + J_z^2$
Commutative law $[J_x, J_y]$ is equal to	$i\hbar J_z$	$i\hbar J_z$	$i\hbar J_y$	$i\hbar J_{z+x+y}$	$i\hbar J_z$
$[J^2, J_y] =$	1	2	0	3	0
$J_+ =$	$J_x + iJ_y$	$J_x - iJ_y$	$J_x^2 + iJ_y^2$	$J_x^2 - iJ_y^2$	$J_x + iJ_y$
$J_- =$	$J_x + iJ_y$	$J_x - iJ_y$	$J_x^2 + iJ_y^2$	$J_x^2 - iJ_y^2$	$J_x - iJ_y$
$[J_x^2, J_x] =$	$J_x [J_x J_x] + J_x$	J_x	$J_x [J_x J_x] + [J_x J_x] J_x$	J_x^2	$J_x [J_x J_x] + [J_x J_x] J_x$
$[J_z, J_+] =$	$\hbar J_+$	$\hbar J_x$	$\hbar J_z$	$\hbar J_x J_y$	$\hbar J_+$
$[J^2, J_+] =$ is equal to	1	2	4	0	0
$[J_+, J_-] =$ is equal to	$\hbar J$	$\hbar J_z$	$\hbar J^2$	$\hbar J$	$\hbar J$
Torque is defined as	moment of force	moment of inertia	rate of change of force	rate of change of distance	moment of force
Momentum is a	vector	scalar	dimensionless	product of vector and scalar	vector
In quantum mechanics operator associated with linear momentum is	$\hbar/i r \times \Delta$	$\hbar/i \Delta$	$\hbar/i r$	$\hbar/i (r \times \Delta)^2$	$\hbar/i r \times \Delta$
The operator that increases or decreases eigen value another operator is called	. Hamilton operator	Ladder operator	Hermitian operator	angular momentum operator	Ladder operator
$[J_x^2, J_x] =$	1	2	4	0	0
The operator for energy is	$i\hbar \partial/\partial t$	$-i\hbar \partial/\partial t$	$i\hbar \partial/\partial x$	$-i\hbar v$	$i\hbar \partial/\partial t$
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
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
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
The orbital corresponding to $l = 0$ is called	s orbital	p orbital	d orbital	f orbital	s orbital
The orbital corresponding to $l = 1$ is called	s orbital	p orbital	d orbital	f orbital	p orbital
The orbital corresponding to $l = 2$ is called	s orbital	p orbital	d orbital	f orbital	d orbital
The orbital corresponding to $l = 3$ is called	s orbital	p orbital	d orbital	f orbital	f orbital
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
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, $\pm 1, \pm 2, \pm 3, \pm 4 \dots$
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.
The correct form of the angular momentum for quantum number l is	$\hbar h$	$\hbar h$	$[l(l+1)\hbar]$	$[l(l+1)]^{1/2} \hbar$	$[l(l+1)]^{1/2} \hbar$

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
An energy level with orbital angular momentum quantum number l, is _____ fold degenerate.	2-fold	3-fold	(2l+1) fold	l-fold	(2l+1) fold
The potential involved outside the nucleus is _____	gravitational	electromagnetic	nuclear	Coulombic	Coulombic
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
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	$dP_{10}/dr = 0$	$dP_{10}/dr = \text{a constant}$	none of the above	$dP_{10}/dr = 0$
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
The binding energy of deuteron is _____	2.226 MeV	2.226 eV	2.226 keV	Zero	2.226 MeV
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
The energy value of two electrons relative to axes with the nucleus at the origin, in ground state of helium atom is _____	$2Z^2 E_H$	$2ZE_H$	$- 2ZE_H$	$- 2Z^2 E_H$	$- 2Z^2 E_H$
For $n = 1, l = 0, m = 0$, the wave function for He atom becomes _____	$(Z/\pi a_0)^{1/2} e^{-\rho/2}$	$(Z^3/\pi a_0^3)^{1/2} e^{-\rho/2}$	$(Z/\pi a_0)^{3/2} e^{-\rho/2}$	$(Z/\pi a_0^3)^{1/2} e^{-\rho/2}$	$(Z^3/\pi a_0^3)^{1/2} e^{-\rho/2}$
The secular equation in which all the elements are zero, except _____	principal diagonal	lower diagonal	upper diagonal	lower and upper diagonal	principal diagonal
The perturbation $H^{(1)}$ which is the extra energy of nucleus and electron due to external field in H atom is _____	$eEr \cos\theta$	$er \cos\theta$	$- eEr \cos\theta$	$- er \cos\theta$	$- eEr \cos\theta$
The ground state for H atom is non-degenerate state, the wave function ψ_{100} is given by _____	$(1/\pi a_0^3)^{1/2} \exp(-r/a_0)$	$(1/\pi a_0^3)^{1/2} \exp(r/a_0)$	$(1/\pi a_0^3)^{3/2} \exp(-r/a_0)$	$(1/\pi a_0^3)^{3/2} \exp(r/a_0)$	$(1/\pi a_0^3)^{1/2} \exp(-r/a_0)$
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
The Bohr radius of the first orbit is _____	5.267 Å	0.05267 Å	0.5267 Å	52.67 Å	0.5267 Å
By expansion theorem ψ may be expanded in terms of a complete set of ortho-normal functions $\phi_0, \phi_1, \phi_2, \dots$ if _____	$\psi = 1$	$\psi = 0$	$\psi = \psi_0$	$\psi \neq \psi_0$	$\psi \neq \psi_0$
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 by an attractive square well potential

The Schrodinger equation for the perturbed system can be written as

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

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, $|\psi\rangle$ and E are both

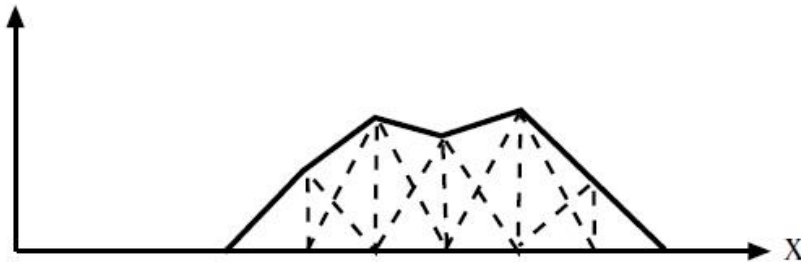


Figure 1: The triangle functions for a piecewise linear approximation of a function. This is a basis that is not orthogonal but yet can be used to seek approximate solutions .

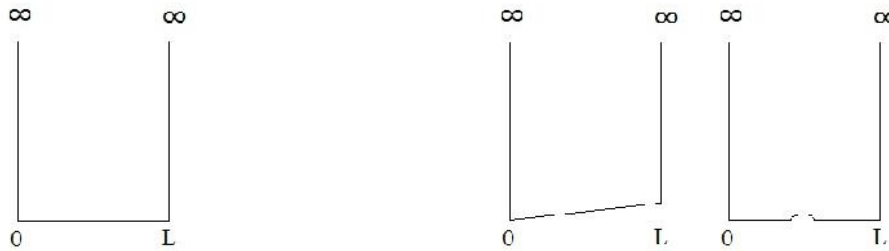


Figure 2: The infinite potential well on the left represents the unperturbed problem. The middle figure represents a perturbation due to a tiny electric field. The right figure represents a perturbation due to imperfection in fabrication or impurities.

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

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

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

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

$$a_0 + a_1 \epsilon + a_2 \epsilon^2 + \dots \quad (5)$$

while the right-hand side is similarly written as

$$b_0 + b_1 \epsilon + b_2 \epsilon^2 + \dots \quad (6)$$

These two power series in ϵ 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:

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

We assume that the zeroth order equation is known in terms of an eigenstate $|^{(0)}m\rangle$ with energy E_m .

In other words

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

We will use this knowledge to solve the first order equation (7) above.

Before we proceed further, a 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) as we shall see later. To achieve uniqueness, it is best to pin down the length of the total eigenvector given by (2). We fix the length of the eigenvector $|\mathbf{i}\rangle$ by requiring that

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

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

because

$|\langle \mathbf{0} \rangle \mathbf{i}\rangle = |\mathbf{m} \mathbf{i}\rangle$, it is easy to show that $\langle \mathbf{m} | \langle \mathbf{i} \rangle \mathbf{i} \rangle = 0$, $i > 0$. As a consequence, $|\langle \mathbf{i} \rangle \mathbf{i}\rangle$ is orthogonal to $|\mathbf{m} \mathbf{i}\rangle$. 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 $|\langle \mathbf{1} \rangle \mathbf{i}\rangle$ to the left of (8). We then have

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

where we have made use of (6.3.10). Notice that the above equation is non-unique since the operator $\hat{H}_0 - E_m$ has a null space with a null space vector $|\mathbf{m} \mathbf{i}\rangle$.

Testing the above equation with $\langle \mathbf{m} |$, we

have

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

$$|m\rangle \quad (10)$$

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

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

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

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

We choose $a^{(1)} = 0$ for a number of reasons: It makes the correction term unique since $|^{(1)}\rangle$ is orthogonal to $|^{(0)}\rangle$. It makes the normalization of the eigenvector $|m\rangle$ 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 $|^{(2)}\rangle$ on the left hand side. Then (9) becomes

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

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

Consequently,

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

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

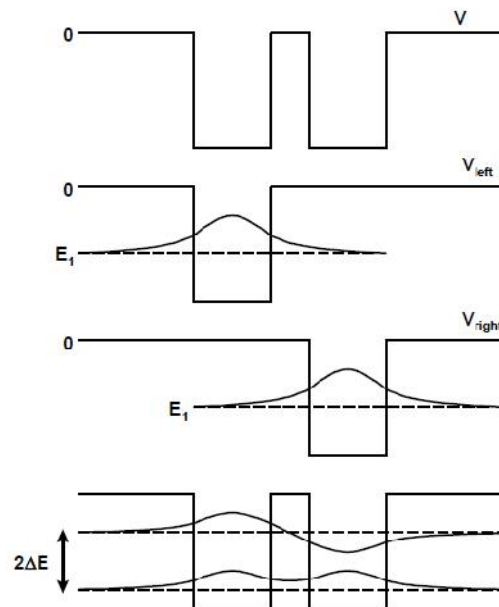
The above procedure can be generalized to arbitrary order. By induction, we notice that the equivalence of to p-th order is

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

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

There is a significant exception to the independence of the cross-section on energy mentioned

$$\sqrt{2m|V_0|a^2/\hbar^2} \quad \pi/2$$

above. Suppose that the quantity is slightly less than $\pi/2$. As the

incident energy increases, $k'a$, which, can reach the value $\frac{\pi}{2}$. In this case, $\tan(k'a)$ becomes infinite, so we can no longer assume that the right-hand side is small. In fact, it

follows from $k'a = \frac{\pi}{2}$ that at the value of the incident energy when $k'a = \frac{\pi}{2}$ then we also have $k'a + \delta_0 = \frac{\pi}{2}$, or $\delta_0 \simeq \frac{\pi}{2}$ (since we are assuming that $k'a \ll 1$). This implies that

$$\sigma_{\text{total}} = \frac{4\pi}{k^2} \sin^2 \delta_0 = 4\pi a^2 \left(\frac{1}{k^2 a^2} \right). \quad (1)$$

Note that the cross-section now depends on the energy. Furthermore, the magnitude of the cross-section is much larger than that given in Eq. (1) for $k'a \neq \frac{\pi}{2}$ (since $k'a \ll 1$).

The origin of this rather strange behaviour is quite simple. The condition

$$\sqrt{\frac{2m|V_0|a^2}{\hbar^2}} = \frac{\pi}{2} \quad (2)$$

is equivalent to the condition that a spherical well of depth V_0 possesses a *bound state* at zero energy. Thus, for a potential well which satisfies the above equation, 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.

We have seen that there is a resonant effect when the phase-shift of the *S*-wave takes the value $\frac{\pi}{2}$. There is nothing special about the $l = 0$ partial wave, so it is reasonable to

assume that there is a similar resonance when the phase-shift of the l th partial wave is $\pi/2$.

Suppose that δ_l attains the value $\pi/2$ at the incident energy E_0 , so that

$$\delta_l(E_0) = \frac{\pi}{2}. \quad (3)$$

Let us expand $\cot \delta_l$ in the vicinity of the resonant energy:

$$\begin{aligned} \cot \delta_l(E) &= \cot \delta_l(E_0) + \left(\frac{d \cot \delta_l}{dE} \right)_{E=E_0} (E - E_0) + \dots \\ &= - \left(\frac{1}{\sin^2 \delta_l} \frac{d\delta_l}{dE} \right)_{E=E_0} (E - E_0) + \dots \end{aligned} \quad (4)$$

Defining

$$\left(\frac{d\delta_l(E)}{dE} \right)_{E=E_0} = \frac{2}{\Gamma}, \quad (5)$$

we obtain

$$\cot \delta_l(E) = -\frac{2}{\Gamma} (E - E_0) + \dots \quad (6)$$

that the contribution of the l th partial wave to the scattering cross-section is

$$\sigma_l = \frac{4\pi}{k^2} (2l+1) \sin^2 \delta_l = \frac{4\pi}{k^2} (2l+1) \frac{1}{1 + \cot^2 \delta_l}. \quad (7)$$

Thus,

$$\sigma_l \simeq \frac{4\pi}{k^2} (2l+1) \frac{\Gamma^2/4}{(E - E_0)^2 + \Gamma^2/4}. \quad (8)$$

This is the famous *Breit-Wigner formula*. The variation of the partial cross-section σ_l with the incident energy has the form of a classical *resonance curve*. The quantity Γ is the width of the resonance (in energy). We can interpret the Breit-Wigner formula as describing the absorption of an incident particle to form a metastable state, of energy E_0 , and lifetime $\tau = \hbar/\Gamma$.

THE BORN APPROXIMATION:

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

replacing $\psi(r')$ in the integral equation by $\exp(iK \cdot r')$, we get

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

where k and k' are the wave vector in the incident and scattered direction 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

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

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 θ'

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

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

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

we get

$$\int_0^\pi \exp(iqr' \cos \theta) \sin \theta d\theta = \int_{-1}^1 \exp(iqr'x) dx \\ = \exp(iqr') - \exp(-iqr') \quad (5)$$

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

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

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 $q = 2k \sin(\theta/2)$

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 N , the number of relative separations is always larger than the number of particles (six versus four for $N = 4$, for example). In conclusion, from $N = 3$ 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 as

$$\mathbf{R} = \frac{1}{M} \sum_{i=1}^N m_i \mathbf{r}_i \quad (1)$$

where N is the total number of particles, m_i and \mathbf{r}_i are the mass and the position of

$$M = \sum_{i=1}^N m_i$$

particle i , and M is the total mass of the system. We can interpret the right hand side as a type of lever arm equation. 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. See any textbook on classical dynamics for a derivation of this property. In the case of an isolated N -body system, there are no external forces, and therefore the center of mass will move in a straight line.

Starting with a given coordinate system, and subtracting the center of mass position vector \mathbf{R} from all particle positions allows us to construct a representation of the N -body system in its c.o.m. system (a short hand for 'center of mass'). Subtracting the c.o.m. position is not enough, however. While this causes a momentary centering, it is still quite possible that the N -body will start drifting off soon thereafter. To keep the system in place, at least on average, we also have to subtract the velocity of the c.o.m. \mathbf{V} from all particle velocities. Differentiation of Eq. 1 gives:

$$\mathbf{V} = \frac{1}{M} \sum_{i=1}^N m_i \mathbf{v}_i \quad (2)$$

This shows, incidentally, that the total momentum of all particles is zero in the c.o.m. coordinate system. Since the c.o.m. moves in a straight line.

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.
8. Derive integral equation for wave function.

9. Derive Born approximation.
10. Discuss the validity of Born Approximation.
11. Explain the difference between laboratory coordinate system and centre of mass coordinate system.

DEPARTMENT OF PHYSICS
CLASS:II M.Sc PHYSICS
QUANTUM MECHANICS-II (16PHP301)

In _____ a beam of particle is allowed to pass close to a scattering material	scattering	target	energy	wave	scattering
Scattering material is called _____	discrete	particles	frequency	energy	target
In bound states the energy of eigen values are _____	positive	negative	infinity	zero	negative
The angular distribution of the scattered particles are related to _____	light	energy	particle	wave function	wave function
The study of scattering is important in studying the properties of _____ atom		energy	spectral line	material	atom
The angle between the initial and final straight line paths is called _____ scattering angle		polarization	spectral line	scattering	scattering angle
Cross-sections are usually measured in _____	barn	cm	mm	ampere	barn
The probability that a particle will be scattered as it traverses a given thickness of matter can be expressed in terms of a quantity called the _____.	Total scattering cross-section	Differential scattering cross-section	Scattering cross-section	scattering	Scattering cross-section
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
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
In wave mechanics, an incident beam of particles is represented by a _____ wave.		Longitudinal	Stationary wave	ordinary	Longitudinal
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
The complete time dependent solution of the schrodinger equation for central potential $V(r)$ is _____.	$y(r,t) = y(r) e^{iEt/\hbar}$	$y(r,t) = -y(r) e^{-iEt/\hbar}$	$y(r,t) = -y(r) e^{iEt/\hbar}$	$y(r,t) = y(r) e^{-iEt/\hbar}$	$y(r,t) = y(r) e^{iEt/\hbar}$
The Schrodinger equation for central potential $V(r)$ is written as _____.	$[-(\hbar^2/2m)\nabla^2 + V(r)]y = Ey$	$[-(\hbar^2/2m)\nabla^2 + V(r)]y = Ey$	$[-(\hbar^2/2m)\nabla^2 - V(r)]y = Ey$	$[-(\hbar^2/2m)\nabla^2 - V(r)]y = Ey$	$[-(\hbar^2/2m)\nabla^2 - V(r)]y = Ey$
_____ 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	$[-(\hbar^2/2m)\nabla^2 + V(r)]y = Ey$

The delta function of Green's function is _____ everywhere except at $r=0$.	zero	finite	infinite	constant	Bessel's function
Green's function has proper _____ form.	differential	integral	asymptotic	none of the above	asymptotic
The scattering amplitude $f(q, f)$ for the scattering problem of stationary wave is given by _____.	$(m/2p \hbar^2) \int_0^\infty V(r) Y(r) dr$	$(m/2p \hbar^2) \int_0^\infty e^{ik \cdot r} V(r) Y(r) dr$	$(m/4p \hbar^2) \int_0^\infty e^{-ik \cdot r} V(r) Y(r) dr$	$-(m/2p \hbar^2) \int_0^\infty e^{-ik \cdot r} V(r) Y(r) dr$	$-(m/2p \hbar^2) \int_0^\infty e^{-ik \cdot r} V(r) Y(r) dr$
Born approximation is applicable for the scattering centres which are _____.	strong	Weak	moderate	none of the above	Weak
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
The first Born approximation is given by	$Y = e^{ikr} - (m/2p \hbar^2) \int_0^\infty G(r, r') V(r') e^{ik \cdot r'} dr'$	$Y = -e^{ikr} - (m/2p \hbar^2) \int_0^\infty G(r, r') V(r') e^{ik \cdot r'} dr'$	$Y = e^{ikr} + (m/2p \hbar^2) \int_0^\infty G(r, r') V(r') e^{ik \cdot r'} dr'$	$Y = -e^{ikr} + (m/2p \hbar^2) \int_0^\infty G(r, r') V(r') e^{ik \cdot r'} dr'$	$Y = -e^{ikr} - (m/2p \hbar^2) \int_0^\infty G(r, r') V(r') e^{ik \cdot r'} dr'$
The first Born approximation scattering amplitude is _____.	$f(q, f) = (m/2p \hbar^2) \int_0^\infty e^{i(k-k') \cdot r'} V(r') dr'$	$f(q, f) = (m/2p \hbar^2) \int_0^\infty -e^{i(k-k') \cdot r'} V(r') dr'$	$f(q, f) = -(m/2p \hbar^2) \int_0^\infty e^{i(k-k') \cdot r'} V(r') dr'$	$f(q, f) = -(m/2p \hbar^2) \int_0^\infty e^{i(k-k') \cdot r'} V(r') dr'$	$f(q, f) = -(m/2p \hbar^2) \int_0^\infty e^{i(k-k') \cdot r'} V(r') dr'$
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 _____.	$\sqrt{(m/2p \hbar^2 E)} V_0 a \gg 1$	$\sqrt{(m/2p \hbar^2 E)} V_0 a = 0$	$\sqrt{(m/2p \hbar^2 E)} V_0 a \ll 1$	$\sqrt{(m/2p \hbar^2 E)} V_0 a = a$	$\sqrt{(m/2p \hbar^2 E)} V_0 a \ll 1$
The ordinary coulomb potential is $V(r) =$ _____.	$(1/4\pi\epsilon_0) (Ze^2/r)$	$-(1/4\pi\epsilon_0) (Ze^2/r)$	$(1/4\pi\epsilon_0) (Z^2 e^2/r)$	$(1/4\pi\epsilon_0) (Z^2 e^2/r)$	$-(1/4\pi\epsilon_0) (Ze^2/r)$
The screened coulomb potential is _____.	$(-Ze^2/4\pi\epsilon_0) e^{-r/r_0}$	$Ze^2/4\pi\epsilon_0 e^{-r/r_0}$	$(-Ze^2/4\pi\epsilon_0) e^{r/r_0}$	$(Ze^2/4\pi\epsilon_0) e^{r/r_0}$	$Ze^2/4\pi\epsilon_0 e^{-r/r_0}$
The method of partial waves is mainly applicable to _____.	Coulomb potential	Screened coulomb potential	Weak potential	Spherically symmetric potential	Spherically symmetric potential
In higher perturbation theory, a plane wave is equivalent to _____.	transverse waves	longitudinal waves	number of spherical waves	radial waves	number of spherical waves
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}	$R(r) \ddot{A}(q) j(f)$
If the incident wave travels along Z-axis, the value of $j(f) =$ _____.	differentiable	infinite	finite	constant	constant
In the method of partial wave, the Legendre polynomial is _____.	$P_l(\cos q)$	$P_l(\cos q)$	$P_l(\sin q)$	$P_l(\sin q)$	$P_l(\cos q)$
A plane wave is equivalent to the superposition of a number of _____.	Stationary	Transverse	Spherical	Longitudinal	Spherical

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
The Green's function has a singularity at $r =$ _____	finite	infinity	0	none of the above	0
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
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
Born approximation is poor for the _____.	alkali	c and d	lighter	heavier	heavier
Green's function is _____ in nature.	asymptotic	differentiable	symmetrical	antisymmetrical	asymptotic
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
The plane wave term e^{ikr} represents a wave unit density and of current density _____.	$\hbar k/m$	$-\hbar k/m$	$\hbar k/m^2$	$-\hbar k^2/m$	$\hbar k/m$
$d(r)$ satisfies the first requirement of a delta function i. e. , it is zero everywhere except at $r =$ _____.	1	-1	infinity	0	0
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
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
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
_____ has proper asymptotic form.	Legendre's function	Green's function	Hermite's function	Bessel's function	Green's function
The method of _____ waves is mainly applicable to spherically symmetric potential.	polarized	unpolarised	circular	partial	partial
In _____ perturbation theory, a plane wave is equivalent to number of spherical waves.	Higher	Lower	Linear	Spherical	Higher
_____ approximation is poor for heavier atoms.	Maclaurin's	Rolle's	Born's	Lagrangian's	Born's

An angular momentum is also called _____	spin	half spin	eigen value	momentum	spin
In study of angular momentum the commutation relations obeyed by the _____	operator	spin	momentum	spin	operator
The classical particle do not get scattered if _____	$l > kr_0$	$l = 0$	$l > k$	$l < k$	$l > kr_0$
If the cross-section of the scattering reaches the value is called _____	absorbance	phase shift	function	resonance	resonance
The concept of scattering length is extensively used in the investigations relating to the scattering of thermal _____	positrons	electrons	neutrons	protons	neutrons
The scattering cross-section depends on the momentum of the incident _____	particle	wave	light	energy	particle

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

$$| \text{identical-bosons } i \propto \sum \hat{P} |1, a_i |2, b_i |3, c_i \dots |N, n_i \quad (3)$$

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, \dots, n . The above

wavefunction remains unchanged when we permute the positions of two particles, because for every $|1, a_i \dots i, l_i \dots j, p_i \dots N, n_i\rangle$, there is a $|1, a_i \dots j, l_i \dots i, p_i \dots N, n_i\rangle$ in the 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

$$|a_1 \dots a_N\rangle \propto \sum_P \hat{P} |1, a_i |2, b_i |3, c_i \dots |N, n_i\rangle \quad (4)$$

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 $|1, a_i \dots i, l_i \dots j, p_i \dots N, n_i\rangle$, there always exists another term:

$-|1, a_i \dots j, l_i \dots i, p_i \dots N, n_i\rangle$ in the above summation since they differ by one per-

mutation. 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 term 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).
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Suppose their wavefunction is $\psi(x_1, x_2)$, where x_i is the coordinate of the i th particle, e.g., $x = (r, \sigma)$ with r the spatial position and $\sigma = \uparrow, \downarrow$ the spin of the particle, etc.

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

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

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

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

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

$$\hat{P}_{12}^2 \psi(x_1, x_2) = \psi(x_1, x_2), \quad \text{or } p^2 = 1$$

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

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

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

Now let us consider its consequence. A general Hamiltonian of N -particle system is

$$\hat{H} = \sum_{i=1}^N \hat{H}_i + \hat{V}$$

$$i=1$$

where v is the interaction potential.

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_x, J_y, J_z 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,

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

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 (later, we will include some corrections due to Coulomb repulsion by empirical Hund's rule). Assume that we have solved the single-particle Schrödinger eq.

$$\hat{H}_{1k}(\mathbf{x}_1) = E_{k-1}(\mathbf{x}_1)$$

the total wavefunction may be written as

$$(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) \propto \psi_1(\mathbf{x}_1) \psi_2(\mathbf{x}_2) \dots \psi_N(\mathbf{x}_N)$$

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

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}} [\psi_1(\mathbf{x}_1) \psi_2(\mathbf{x}_2) + \psi_1(\mathbf{x}_2) \psi_2(\mathbf{x}_1)] \quad \text{for Boson}$$

[or $\psi_1(x_1) \psi_1(x_2)$ etc.] and 1

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_1(x_1) \psi_2(x_2) - \psi_1(x_2) \psi_2(x_1)] \quad \text{for Fermions}$$

so that $\psi(x_1, x_2) = \psi(x_2, x_1)$ for Bosons and $\psi(x_1, x_2) = -\psi(x_2, x_1)$ for Fermions. One can also construct a symmetric wavefunction for two Bosons by a single wavefunction as $\psi(x_1, x_2) = \psi_1(x_1) \psi_1(x_2)$, or $\psi_2(x_1) \psi_2(x_2)$.

Notice that if $k_1 = k_2$, $\psi(x_1, x_2) = 0$, but not $\psi(x_1, x_2)$. This indicates that two Fermions cannot occupy the same state, but two bosons are allowed to occupy the same state. It can be extended to a more general statement:

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 -electron system is given by the Slater determinant constructed from the lowest N single particle states. For atoms, these single particle 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 states at different nuclear configurations. We will discuss QM of molecules in the last chapter. Sometimes it is convenient to separate total wavefunction as discussed above into product of spatial and spin parts of wavefunctions, namely

$$\psi(x_1, \dots, x_N) = \psi(r_1, \dots, r_N) \chi(s_1, \dots, s_N).$$

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 Schrodinger 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

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

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,

orbitals (shells) :	1s	2s	2p	3s	3p	4s	3d	4p	5s	...
electron no. :	2	4	10	12	18	20	30	36	38	...

In the above table, we also list 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. As we are mainly interested 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

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

We notice that a given electron configuration will not uniquely determine some basic

properties (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 ($Z = 7$): $\text{He}(2s)^2(2p)^3$. 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 ($Z = 8$): $\text{He}(2s)^2(2p)^4$. 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.

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. To facilitate the upcoming math, let's make the following definition

$$\hat{H}_e = \sum \hat{h}_i(\mathbf{x}_i)$$

where \mathbf{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.

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

$$\begin{aligned} \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \frac{1}{\sqrt{6}} & [\psi_1(\mathbf{r}_1) \psi_2(\mathbf{r}_2) \psi_3(\mathbf{r}_3) - \psi_1(\mathbf{r}_1) \psi_2(\mathbf{r}_3) \psi_3(\mathbf{r}_2) + \psi_1(\mathbf{r}_3) \psi_2(\mathbf{r}_2) \psi_3(\mathbf{r}_1) \\ & - \psi_1(\mathbf{r}_2) \psi_2(\mathbf{r}_1) \psi_3(\mathbf{r}_3) + \psi_1(\mathbf{r}_3) \psi_2(\mathbf{r}_1) \psi_3(\mathbf{r}_2) - \psi_1(\mathbf{r}_2) \psi_2(\mathbf{r}_3) \psi_3(\mathbf{r}_1)] \quad (4) \end{aligned}$$

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

$$(\sim x_1, \dots, \sim x_N) = \frac{1}{\sqrt{N!}} (\sim x_1)^2 (\sim x_2) \dots (\sim x_N).$$

(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

$$P^{ij} (\sim x_1, \dots, \sim x_i, \dots, \sim x_j, \dots, \sim x_N) = (\sim x_1, \dots, \sim x_j, \dots, \sim x_i, \dots, \sim x_N) = - (\sim x_1, \dots, \sim x_i, \dots, \sim x_j, \dots, \sim x_N) \quad (5)$$

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

$$\delta \langle \psi_k | \hat{H} | \psi_k \rangle = 0 \quad (1)$$

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}_i 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}_i , called the exchange term, has no classical analogue and is a direct result of the antisymmetry property of the wavefunction. The Fock operator

$$\hat{F}_i = \hat{h}_i + \sum_k (\hat{J}_k - \hat{K}_k) \quad (2)$$

and using this definition Eq. 2 takes the simple form

$$\hat{F}_k = \sum_{i=1}^N (\hat{J}_i - \hat{K}_i) \quad (3)$$

There are several different solutions to the equations in Eq. 3 each corresponding to a different set of ψ_k . We have the freedom to concentrate upon those ψ_k which satisfies

$$\psi_k = \psi_{k_i} \quad (4)$$

where ϵ_k is essentially a new name for the Lagrange multipliers[1]. With this, Eq.4 may be written as

$$\hat{F}_k = \epsilon_k \phi_k. \quad (5)$$

In this form, Eq. 5 is a traditional eigen value equation. 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 ϵ_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.

Valence bond Theory

The two-electron system with orbitals $\phi_1(\mathbf{r}_1)$ and $\phi_2(\mathbf{r}_2)$, the following variational wavefunction satisfies the antisymmetry condition, at the same time preserving the single-particle picture

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = c [\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) - \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_1)] \quad (1)$$

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

$$\begin{aligned} \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \frac{1}{\sqrt{6}} & [\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\phi_3(\mathbf{r}_3) - \phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_3)\phi_3(\mathbf{r}_2) + \phi_1(\mathbf{r}_3)\phi_2(\mathbf{r}_1)\phi_3(\mathbf{r}_2) \\ & - \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_1)\phi_3(\mathbf{r}_3) + \phi_1(\mathbf{r}_3)\phi_2(\mathbf{r}_2)\phi_3(\mathbf{r}_1) - \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_3)\phi_3(\mathbf{r}_1)] \end{aligned} \quad (2)$$

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

$$\frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_2(\mathbf{r}_1) & \dots & \phi_N(\mathbf{r}_1) \\ \phi_1(\mathbf{r}_2) & \phi_2(\mathbf{r}_2) & \dots & \phi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r}_N) & \phi_2(\mathbf{r}_N) & \dots & \phi_N(\mathbf{r}_N) \end{vmatrix} \quad (3)$$

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 i only once and each of the arguments ψ_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 ψ_i ($\sim \psi_j$) 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. **(5 marks)**
b. Derive Hartree Fock equation. **(5 marks)**

DEPARTMENT OF PHYSICS
CLASS:II M.Sc PHYSICS

QUANTUM MECHANICS-II (16PHP301)

The central field approximation is applicable on all atoms except the _____ atom.	. heavier	alkali	lighter	none of the above	lighter
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
The fluctuating potential due to each nearby electron varies slowly with the _____ distance.	equal	infinite	separation	finite	separation
The potential energy $v(r)$ for a neutral atom has the coulomb form _____ at a great distance r from the nucleus.	$-e^2/r$	e^2/r	$-2e^2/r$	$2e^2/r$	$-e^2/r$
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	n , l , l and m_s	n , l , l and m_s
According to Thomas-Fermi statistical model $v(r)$ varies slowly enough in an _____ wavelength.	proton	neutron	electron	none of the above	electron
At normal temperture, 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 $V(r)$
The number of electron states in a cube of edge length L at the walls of which the wave functions obey periodic boundary condition is _____.	$(L/2\pi)^3 dk_x dk_y dk_z$	$-(L/2\pi)^3 dk_x dk_y dk_z$	$(L/2\pi)^3 dk_x dk_y$	$(L/2\pi)^3 dk_x dk_z$	$(L/2\pi)^3 dk_x dk_y dk_z$
The relation between volume density of electron $n(r)$ and the potential energy is _____.	$n(r) = (2mV(r)/3\pi^2 \hbar^3)^{1/2}$	$n(r) = (2mV(r)/3\pi^2 \hbar^3)^{3/2}$	$n(r) = (-2mV(r))^{3/2}/3\pi^2 \hbar^3$	$n(r) = -(2mV(r)/3\pi^2 \hbar^3)^{3/2}$	$n(r) = (-2mV(r))^{3/2}/3\pi^2 \hbar^3$
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	$a. 1/r$

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
According to Hartree's method, the charge density associated with an electron is _____ times its position probability density.	e	$1/e$	$-1/e$	$-e$	$-e$
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
The theory of complex spectra consists in determining the linear combination of suitably _____ wave function.	symmetrical	normalised	a and b	antisymmetrical	antisymmetrical
When the electrostatic perturbation is included and spin-orbit energy neglected, the total orbital- angular momentum L and the total spin angular momentum S are separately _____ of the motion.	equations	symmetrical	constants	antisymmetrical	constants
When the spin-orbit energy is neglected, the electrostatic energy separates states of different _____.	S	L	J	a and b	L
energy state can be specified by the quantum numbers _____.	J, L, S, M	$J, L, M-M$	J, L, S	J, L, S, M, M	J, L, S, M, M
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
If spin-orbit energy is included, then L and S are not _____ of motion.	equations	symmetrical	constants	antisymmetrical	symmetrical
In JJ coupling, the spin-orbit energy is _____ in comparison with the electrostatic energy.	Small	Large	Finite	Infinite	Infinite
JJ coupling takes place in _____ atoms where the large $V(r)$ makes the spin-orbit energy	heavy	light	alkali	none of the above	heavy

In alkali atom, a single electron moves in a spherically symmetric _____ potential energy $V(r)$.	excitation	coloumb	noncoloumb	none of the above	noncoloumb
The configuration of an alkali atom can be specified by a single pair of quantum numbers _____.	n, l	n, l, m	n, l, m, m_s	n, l, s, m	n, l
The configuration of an alkali atom can be specified by a single pair of quantum numbers _____.	infinity	1	1 and 2	0	0
The doublet structure characterizes all the moderately excited levels of the alkali atom except those for which $l =$ _____.	negative	zero	positive	infinite	positive
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	$(L+1)(S+1)$	$(L+1)(S+1/2)$	$L + S$
The total angular momentum $J =$ _____.	s	n and l	j and s	l	l
The absolute value of doublet separation depends on _____.	different	proportional	same	inversely proportional	same
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
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
The equality of total intensities from each state formed from a given L and S is a general property of _____ coupling.	3:01	2:04	1:02	2:01	2:01
The two lines of the doublet have intensities in the ratio _____.	2:04	2:01	1:02	3:01	2:01
The lowest doublets of the alkalis are in the ratio _____.			6	12	6
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

The total intensity from each of the two $^2P_{1/2}$ states is equal to _____.	6	8	2	1	2
For higher doublets the intensity ratio exceeds _____.	4	6		radial function	radial function
In higher doublets the intensity ratio exceeds 2 due to the difference to _____.	energy state	electron wave function	a and b	$(j+1) \hbar^2$	energy state
$J^2 =$ _____.	$j(j+1) \hbar^2$	$-j(j+1) \hbar^2$	J.J	$j(j+1) \hbar^2$	J.J
The states of different j have _____ fold degeneracy.	Proportional	Same	Different	$(2j+1)$	Different
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
The state of different j with $(2j+1)$ fold degeneracy is due to _____.	m	l	l and s	0	m
The method of partial wave is an elegant procedure for the analysis of _____ scattering	elastic	inelastic	compton	differential	elastic
The s-particle wave will be _____ of the angle θ	dependent	independent	perpendicular	parallel	independent
The s-particle wave will be _____ symmetric	spherically	circularly	elastically	a	spherically
The phenomenon with out scattering is called _____	Ramsaur - Townsend effect	tuindall effect	raman effect	bohr model	Ramsaur - Townsend effect
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
$l\hbar =$ _____	$k\hbar b$	0	αb	$\rho\lambda$	$k\hbar b$
The interaction between two particles is uasually screened by the atomic electrons surrounding the _____		electrons	neutrons	protons	nucleus
The quantum mechanics does not satisfy the requirement of special theory of _____	resistivity	permitivity	permiability	conductivity	relativity
Klein-gordan equation does not say anything about _____	particle	wave	energy	space	particle
\square is the _____ operator	de alembertian	schrodinger	wave	dirac	de alembertian
Klein and gordan were not able to give a explanation of _____ energy	positive	negative	zero	neutral	negative

_____ was resolved by pauli and weisskopf in 1934	dilemma	charge density	lamda	surface energy	dilemma
coulomb field is described by a potential of the type _____	$V(r) = 0$	$V(r) = KB$	$v(r) = -Ze^2/r$	$v(r) = ih$	$v(r) = -Ze^2/r$

Relativistic quantum mechanics: Klein-Gordon equation – Interpretation of the Klein-Gordon 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 – GORDON EQUATION

The non relativistic Schrodinger equation was obtained by replacing P by $-i\hbar\nabla$ and E by $i\hbar\frac{\partial}{\partial t}$ in the classical energy expression of a free particle $E = \frac{P^2}{2m}$ and allowing the resulting operator equation to operate on the wave function. The corresponding relativistic energy relation is:

$$E^2 = c^2 p^2 + m^2 c^4 \quad \text{.....(1)}$$

Where m is the rest mass of the particle. For convenience, rest mass will be denoted by m in this chapter. Replacing E and P by the respective operators, we get the operator equation

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

Allowing this operator equation to operate on the wave function $\psi(r,t)$

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

Which is Klein – Gordon equation or Schrodinger's relativistic equation

Rearranging, we get

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

$$\psi(r,t) = \frac{m^2 c^2}{2} \psi(r,t)$$

$$\square = \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \quad \text{.....(5)}$$

Where \square is the de Alembertian operator which is relativistically invariant. Therefore eq(5) is relativistically invariant if ψ transforms like a scalar

Plane Wave Solution

The plane wave represented by

$$\Psi(r, t) = \exp[i(k \cdot r - \omega t)] \quad \text{.....(6)}$$

Is an eigenfunction of both energy and momentum operator with eigenvalues ω and k respectively. Substitution of Eq (6) in Eq (4) gives

$$\begin{aligned} (\omega^2) &= (c^2 \hbar^2 k^2 + m^2 c^4) \\ (\omega) &= \pm (c^2 \hbar^2 k^2 + m^2 c^4)^{1/2} \end{aligned}$$

This means that the energy eigenvalue can have both positive and negative values. Klein – Gordon were not able to give a consistent explanation for the negative energy.

Dirac Equation.

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

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

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:

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

The latter form becomes the Klein–Gordon equation provided that the μ 's satisfy the Clifford algebra

$$\{\mu_i, \mu_j\} = \mu_i \mu_j + \mu_j \mu_i = -2 \delta_{ij}. \quad (3)$$

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 $\gamma = \exp(\dots)$. Suppose ψ is a solution of the Dirac equation. It is

not sufficient to use the transformation rule for scalar fields $\psi(x_0) = \psi(x)$. In

analogy to vectors we should also transform spinors. We make the ansatz

$$\psi(x_0) = S(\gamma) \psi(x), \quad (1)$$

where $S(\gamma)$ is a matrix that acts on Dirac spinors. We then substitute

$\psi(x) = S^{-1}(\gamma) \psi(x_0)$ into the Dirac equation

$$0 = i \gamma^\mu \partial_\mu \psi - m \psi \quad 0(x) = i \gamma^\mu \partial_\mu \psi - m \psi \quad S^{-1}(\gamma) \psi(x)$$

$$= i S^{-1} \gamma^\mu \partial_\mu \psi - S^{-1} m \psi \quad (\gamma) \psi(x)$$

$$= S^{-1} i \gamma^\mu \partial_\mu \psi - S^{-1} m \psi \quad (\gamma) \psi(x)$$

$$= i S^{-1} \gamma^\mu S \partial_\mu \psi - S^{-1} m \psi \quad (\gamma) \psi(x). \quad (2)$$

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

$$0_\mu = (\gamma^{-1})_\mu \quad S \quad S^{-1}, \quad (3)$$

where not only the vector index is transformed by γ^{-1} , but also the spinor matrix is conjugated by the corresponding spinor transformation S . In analogy to the

invariance of the Minkowski metric, $0 = \dots$, the Dirac equation is invariant if the

gamma-matrices are invariant

$$0_\mu = \gamma_\mu. \quad (4)$$

This condition relates S to the Lorentz transformation. The infinitesimal form of the invariance condition reads

$$[S, \mu] - \mu = 0. \quad (5)$$

This implies that S must be proportional to μ . The latter carries two vector indices, while S carries none. The only possibility is to contract the vector indices by S from the left, co-spinors by the S^{-1} from the right.

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

$$[\mu, \mu] = \{\mu, \mu\} - \{\mu, \mu\}, \quad (6)$$

we arrive at $(2 - 1) \mu = 0$. We conclude that a Lorentz transformation for spinors is given by the matrix

the Dirac spinor $\psi = (L, R)$ 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

$$i \mu \mu R - m L = 0,$$

$$i \mu \mu L - m R = 0. \quad (7)$$

It is therefore convenient to use Dirac spinors for massive spinor particles whereas massless spinor particles can also be formulated using 2-spinors; we shall discuss the massless case later on.

The decomposition into chiral parts is not just valid in the Weyl representation of the Clifford algebra. More abstractly, it is due to the existence of the matrix

$$\gamma_5 = i \mu \mu = i \gamma_0 \gamma_1 \gamma_2 \gamma_3. \quad (8)$$

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.

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.

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

H α line is single line according to the Bohr or Schrödinger theory. occurs at 656.47 nm for Hydrogen and 656.29 nm for Deuterium (isotope shift, ~ 0.2 nm).

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

The energy eigenvalues of hydrogen atom . For hydrogen atom, $V(r) = -Ze^2/4\pi\epsilon_0 r$

.

It is convenient to introduce numerical substitutions defined by

$$\alpha = \frac{(m^2 c^4 - E^2)^{1/2}}{c\hbar} = \left(\frac{mc^2 + E}{c\hbar} \right)^{1/2} \left(\frac{mc^2 - E}{c\hbar} \right)^{1/2} = \alpha_1^{1/2} \alpha_2^{1/2}$$

$$\alpha_1 = \frac{mc^2 + E}{c\hbar}, \quad \alpha_2 = \frac{mc^2 - E}{c\hbar}$$

Introducing a new variable ρ defined by

$$\rho = \alpha\gamma$$

We can be reduced to

$$\frac{dF}{d\rho} - \frac{kF}{\rho} - \left(\frac{\alpha_1}{\alpha} + \frac{\gamma}{\rho} \right) G = 0, \quad \gamma = \frac{Ze^2}{4\pi\epsilon_0 c\hbar}$$

$$\frac{dG}{d\rho} + \frac{kF}{\rho} - \left(\frac{\alpha_2}{\alpha} - \frac{\gamma}{\rho} \right) F = 0$$

As in the nonrelativistic case let us look for solution of the form

$$F(\rho) = \sum_{n=0}^{\infty} a_n \rho^{s+n} e^{-\rho}, \quad a_0 \neq 0$$

And

$$G(\rho) = \sum_{n=0}^{\infty} b_n \rho^{s+n} e^{-\rho}, \quad b_0 \neq 0$$

Substituting these equation in Eqs(4) and (5) and equating the coefficients of ρ^{s+n-1} to zero, we get

$$(s + n - k) a_n - a_{n-1} - \gamma b_n - \frac{\alpha_1}{\alpha} b_{n-1} = 0$$

$$(s + n - k) b_n - b_{n-1} + \gamma a_n - \frac{\alpha_1}{\alpha} a_{n-1} = 0$$

When $n = 0$

$$(s - k) a_0 - \gamma b_0 = 0 \quad (s + k) b_0 - \gamma a_0 = 0$$

For eqn to have nonvanishing solution, the determinant

$$\begin{vmatrix} s - k & -\gamma \\ \gamma & s + k \end{vmatrix} = 0 \quad \text{or} \quad s = \pm (k^2 - \gamma^2)^{1/2}$$

The negative solution is not acceptable as it would make F and G diverge at the origin. Hence the positive sign is the only acceptable solution. When $n > 0$, a relation between a_n and b_n can be obtained by multiplying by α and by α_2 and substituting

$$b_n [(s + n + k)\alpha + \alpha_2 \gamma] = a_n [\alpha_2 (s + n - k) - \alpha \gamma]$$

Where we have used the relation $\alpha^2 = \alpha_1 \alpha_2$. As in the nonrelativistic case regular solution are possible only if both the series terminate. Let this occurs at $n=n'$ so that $a_{n'+1} = b_{n'+1} = 0$. Replacing n by $(n'+1)$ in eq we have

$$(s + n' + 1 - k) a_{n'+1} - a_{n'} - \gamma b_{n'+1} - \frac{\alpha_1}{\alpha} b_n = 0$$

In view of the condition $a_{n'+1} = b_{n'+1} = 0$ reduce to

$$b_n = -\frac{\alpha}{\alpha_1} a_{n'} \quad n' = 0, 1, 2, \dots$$

Equation also gives the same condition between b_n and a_n . The energy levels can be

Obtained by setting $n=n'$ in eq and

$$-\frac{\alpha}{\alpha_1} a_n' [(s + n' + k)\alpha + \alpha_2 \gamma] = a_n' [\frac{1}{2} (s + n - k) - \alpha \gamma]$$

$$2\alpha (s + n') = \gamma (\alpha_1 \alpha_2)$$

Substituting the values of $\alpha_1, \alpha_2, \alpha$ and squaring, we get

$$(m^2 c^4 - E^2) (s+n')^2 = E^2 \gamma^2$$

$$E = mc^2 \left[1 + \frac{\gamma^2}{s+n} \right]^{1/2}$$

Expanding in power of γ^2 and retaining terms of order γ^4

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

Where $n=n' + |k| = n' + j + \frac{1}{2}$ is the total quantum number of hydrogen atom and $|k|$ takes the

value 1,2,.....,n. To label the energy levels by l the orbital angular momentum quantum

number we have to extend the discussion to nonrelativistic limit. When this is done, the

values of l in terms of k are

$$l = |k| = j + \frac{1}{2} \quad \text{for } k < 0$$

$$l = k - 1 = j - \frac{1}{2} \quad \text{for } k > 0$$

the complete degeneracy of the energy level for a given n in the nonrelativistic one is partly lifted by relativistic effect. The energy level given below

$$n=3, k=3 \quad 3D_{5/2}$$

$$n=3, k=2 \quad 3P_{\frac{3}{2}}$$

$$n=3, k=2 \quad 3D_{\frac{3}{2}}$$

$$n=3, k=1 \quad 3S_{\frac{1}{2}}$$

$$n=3, k=1 \quad 3P_{\frac{1}{2}}$$

$$n=2, k=2 \quad 2P_{\frac{3}{2}}$$

$$n=2, k=1 \quad 2S_{\frac{1}{2}}$$

$$n=2, k=1 \quad 2P_{\frac{1}{2}}$$

$$n=1, k=0 \quad 1S_{\frac{1}{2}}$$

this is the scheme of hydrogen atom $n=1,2,3$

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 α 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 β -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.

DEPARTMENT OF PHYSICS
CLASS:II M.Sc PHYSICS
QUANTUM MECHANICS-II (16PHP301)

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
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
The period of nuclear motion is of the order of _____ divided by its energy.	\hbar	e	$-\hbar$	$-e$	\hbar
The nuclear periods are _____ than the electronic periods.	smaller	stable	longer	a and b	longer
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
Molecular energy levels are classified into _____ vibrational and rotational energy levels	static	rigid	translational	electronic	electronic
The energy E_e associated with the motion of a valence is of order of _____, where m is the electronic mass	$-\hbar^2/ma^2$	$-\hbar^2/ma^2$	$-\hbar^2/ma^2 + 1$	$\hbar^2/ma^2 + 1$	$-\hbar^2/ma^2$
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
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
The property of degeneracy is known as _____.	resonance	doublet separation	doublet intensity	none of the above	resonance
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
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.
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°
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
The interaction between valence electrons give rise to _____ forces between atom which hold the atoms together in molecule	bonding	electrostatic	coloumbic	repulsive	bonding
Heitler and London theory of hydrogen molecule helps us to develop the picture of _____ bond.	covalent	chemical	ionic	none of the above	chemical
The spin functions of two electrons are $a(1)$ and $a(2)$, then the total spin wave function is the product of _____ such spin functions.	either one	wavelength with	a and b	two	two

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
The symmetric orbital functions of an electron will be associated with _____ spin function.	skew symmetric	symmetric	a and b	antisymmetric	antisymmetric
The antisymmetric orbital function will be associated with _____ spin function.	symmetric	skew symmetric	antisymmetric	b and c	symmetric
If r_{12} is the distance between two electrons, then the interaction between these electrons 1 and 2 is given	$-e^2/r_{12}^2$	$-e^2/r_{12}$	$-2e^2/r_{12}^2$	$-3e^2/r_{12}^2$	$-e^2/r_{12}$
If the system consists of two hydrogen nuclei 'a' and 'b' and two electrons 1 and 2 separated by distance r_{12} , then the potential energy or two nuclei is $V =$ _____.	$e^2/r_{ab} + e^2/r_{12} + e^2/r_{a1} + e^2/r_{b1} + e^2/r_{a2} + e^2/r_{b2}$	$e^2/r_{ab} + e^2/r_{12} + e^2/r_{a1} + e^2/r_{b1} + e^2/r_{a2} - e^2/r_{b2}$	$e^2/r_{ab} + e^2/r_{12} - e^2/r_{a1} + e^2/r_{b1} + e^2/r_{a2} + e^2/r_{b2}$	$e^2/r_{ab} + e^2/r_{12} - e^2/r_{a1} - e^2/r_{b1} - e^2/r_{a2} - e^2/r_{b2}$	$e^2/r_{ab} + e^2/r_{12} - e^2/r_{a1} - e^2/r_{b1} - e^2/r_{a2} - e^2/r_{b2}$
_____ 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
The attraction of two hydrogen atom give rise to the formation of _____ molecule.	stable	unstable	colloidal	suspension	stable
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
The schroedinger equation for hydrogen molecule is given by _____.	$\tilde{N}_1^2 y + \tilde{N}_2^2 y + (2m/\hbar^2)(E-V)y = 0$	$\tilde{N}_1^2 y + \tilde{N}_2^2 y + (2m/\hbar^2)(E-V)y = 1$	$\tilde{N}_1^2 y + \tilde{N}_2^2 y + (2m/\hbar^2)(E-V)y = H y$	$\tilde{N}_1^2 y + \tilde{N}_2^2 y - (2m/\hbar^2)(E-V)y = H y$	$\tilde{N}_1^2 y + \tilde{N}_2^2 y + (2m/\hbar^2)(E-V)y = 0$
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 $r_{12} =$ _____.	$\sqrt{(x_2-x_1)^2 + (y_2-y_1)^2 + (z_2-z_1)^2}$	$\sqrt{(x_2-x_1)^2 + (y_2-y_1)^2 + (z_2-z_1)^2}$	$\sqrt{(x_2-x_1)^2 - (y_2-y_1)^2 - (z_2-z_1)^2}$	$\sqrt{(x_2-x_1)^2 + (y_2-y_1)^2 - (z_2-z_1)^2}$	$\sqrt{(x_2-x_1)^2 - (y_2-y_1)^2 - (z_2-z_1)^2}$
The SP^3 hybridisation leads to _____ equivalent bonds.	3	4	6	2	3
The ground state of a hydrogen atom is _____.	a triplet	a mixture of singlet and triplet	neither singlet nor a triplet	singlet	singlet
If the spins of electron in two atoms are parallel then the atoms _____ each other	singlet	attract	coagulate	none of the above	singlet
If the spins of the electrons in two atoms are antiparallel, then two atoms _____ each other	repel	attract	coagulate	none of the above	attract
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
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
Hartree-Fock method incorporates the effect of _____ symmetry.	skew	anti	exchange	none of the above	exchange
The molecular wave function as a linear combination of atomic orbitals is called _____ method.	LCAO	Exchange	MO	none of the above	LCAO
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
The effect of exchange symmetry has been incorporated in _____.	$109^\circ 28'$	180°	0°	120°	$109^\circ 28'$

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
Resonance is the property of _____	degeneracy	doublet	singlet	triplet	degeneracy
The symmetric spin function will be associated with _____ orbital function.	skew symmetric	hermitian	antisymmetric	triplet	antisymmetric
Dirac require the equation must be of _____ order in time and space	first	second	zero	none	first
Diracs equation is relativistically _____	invariant	variant	covariant	all the above	invariant
Lorentz is covariant from _____	μ	δ	Ω	ψ	ψ
The spin of an electron carries no _____	energy	particle	time	wave function	energy
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 current density $j(x, t)$ 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)

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

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

$$\nabla \times (\nabla \times \mathbf{A}) + \frac{\partial}{\partial t} \left(\frac{\partial \mathbf{A}}{\partial t} + \nabla \phi \right) = \mathbf{j}$$

$$\nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} + \frac{\partial^2 \mathbf{A}}{\partial t^2} + \nabla \frac{\partial \phi}{\partial t} = \mathbf{j}$$

$$\nabla^2 \mathbf{A} - \frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla \left(\nabla \cdot \mathbf{A} + \frac{\partial \phi}{\partial t} \right) = -\mathbf{j} \quad \dots(9)$$

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

$$\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla \chi \quad \dots(10)$$

$$\phi \rightarrow \phi' = \phi - \frac{\partial \chi}{\partial t} \quad \dots(11)$$

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

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

$$\mathbf{E} = \frac{\partial}{\partial t}(\mathbf{A} + \nabla \chi) - \nabla \left(\phi - \frac{\partial \chi}{\partial t} \right)$$

$$= - \frac{\partial \mathbf{A}}{\partial t} - \nabla \phi$$

$$\nabla \cdot \mathbf{A} + \frac{\partial \phi}{\partial t} = 0 \quad (12)$$

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:

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

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

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

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

$$\mathbf{j} = (\mathbf{j}, i c \rho) \quad \text{.....(14)}$$

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

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

From eq we have

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

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

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

From eq

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

$$iE_1 = \frac{\partial A_2}{\partial x_4} - \frac{\partial A_4}{\partial x_2} = F_{41} \quad \text{.....(19)}$$

$$iE_2 = \frac{\partial A_3}{\partial x_4} - \frac{\partial A_4}{\partial x_3} = F_{42} \quad \text{.....(20)}$$

$$iE_3 = \frac{\partial A_1}{\partial x_4} - \frac{\partial A_4}{\partial x_1} = F_{43} \quad \text{.....(21)}$$

In general

$$F_{\mu\nu} = \frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu}, \quad F_{\mu\nu} = -F_{\nu\mu} \quad \text{.....(22)}$$

$$F_{k4} = -iE_k, \quad F_{ij} = \epsilon_{ijk} B_k \quad \text{.....(23)}$$

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

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

$\epsilon_{ijk} = -1$ if i,j,k 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.

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, $\{ \phi_i \}$, $i = 1, 2, \dots$

$3, \dots\}$. 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_i must be a non-negative integer; for fermions, the Pauli exclusion principle restricts n_i 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

$$N = \sum_i n_i.$$

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

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

The single-particle states can be represented

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

Bosonic operators. Let us define the bosonic *creation operator* a^\dagger by

$$a^\dagger |n_1, n_2, \dots, n_{i-1}, n_i, n_{i+1}, \dots\rangle = \sqrt{n_i + 1} |n_1, n_2, \dots, n_{i-1}, n_i + 1, n_{i+1}, \dots\rangle, \quad (1)$$

and the corresponding *annihilation operator* a by

$$a |n_1, n_2, \dots, n_{i-1}, n_i, n_{i+1}, \dots\rangle = \sqrt{n_i} |n_1, n_2, \dots, n_{i-1}, n_i - 1, n_{i+1}, \dots\rangle. \quad (2)$$

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

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

and

$$N = \sum_i N_i.$$

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

$$|n_1, n_2, \dots, n, \dots\rangle = a_1^{\dagger n_1} a_2^{\dagger n_2} \dots a^{\dagger n} \dots |0\rangle, \quad (3)$$

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

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

and the annihilation operator c by

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

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,

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

$$c_i |n_1, n_2, \dots, n_i, \dots\rangle = 0 \quad \text{for } n_i = 0, \quad \text{and } c_i |n_1, n_2, \dots, n_i, \dots\rangle = 0 \quad \text{for } n_i = 1.$$

Similarly, $c_i^\dagger |n_1, n_2, \dots, n_i, \dots\rangle = 0$ for $n_i = 1$, and $c_i^\dagger |n_1, n_2, \dots, n_i, \dots\rangle = |n_1, n_2, \dots, n_i + 1, \dots\rangle$ for $n_i = 0$. 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 written

$$|n_1, n_2, \dots, n_i, \dots\rangle = c_1^{\dagger n_1} c_2^{\dagger n_2} \dots c_i^{\dagger n_i} \dots |0\rangle,$$

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.

The creation and annihilation operators defined above were constructed for a

particular basis of single-particle states $\{|i\rangle$. We will use the notation b^\dagger

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

$$|\tilde{i}\rangle = |\tilde{n}_1, \tilde{n}_2, \dots, \tilde{n}_i, \dots\rangle,$$

and one can define operators \tilde{b}_i^\dagger and \tilde{b}_i by analogy with those for $\{|i\rangle$. 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

$$\tilde{b}_i^\dagger = \sum_h |h\rangle \langle i| b_h^\dagger, \quad \tilde{b}_i = \sum_h \langle i| h\rangle b_h. \quad (8)$$

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 $\psi^\dagger(\mathbf{r})$ and $\psi(\mathbf{r})$. For bosons or fermions,

$$\psi(\mathbf{r}) = \sum_i \langle \mathbf{r} | i \rangle b_i = \sum_i \psi(\mathbf{r}, i) b_i,$$

where $\psi(\mathbf{r}, i)$ 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} :

The total number operator can be written $N = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})$.

$$N = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}). \quad (9)$$

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 $\hat{O} = \sum_{j=1}^N \hat{O}_j$, where \hat{O}_j acts just on the j 'th particle. Examples of one-particle

quantities include the momentum $\mathbf{P} = \sum_j \mathbf{P}_j$, the kinetic energy $K = \sum_j K_j$, where

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

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

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 b 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

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

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 $\delta(r, r') = \frac{1}{\Delta\tau\Delta i} \delta_{ij}$ 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) and (4), the Hamiltonian density \mathcal{H} now becomes

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

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

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

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

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

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

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

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

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

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

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

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

$$[\hat{H}, \hat{H}^*] = 0$$

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Assuming the cell volumes are very small, Eq. (2) can be rewritten in terms of $\hat{\psi}$ and $\hat{\pi}$ in the following forms:

$$[\hat{\psi}(\mathbf{r}, t), \hat{\psi}(\mathbf{r}', t)] = [\hat{\pi}(\mathbf{r}, t), \hat{\pi}(\mathbf{r}', t)] = 0 \quad \dots\dots\dots (3)$$

$$[\hat{\psi}(\mathbf{r}, t), \hat{\pi}(\mathbf{r}', t)] = i\hbar \delta(\mathbf{r}, \mathbf{r}') \quad \dots\dots\dots (4)$$

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 $\hat{\pi}$ become

$$[\hat{\psi}(\mathbf{r}, t), \hat{\psi}(\mathbf{r}', t)] = [\hat{\pi}(\mathbf{r}, t), \hat{\pi}(\mathbf{r}', t)] = 0 \quad \dots\dots\dots (5)$$

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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:

$$\mathcal{L} = i \left[\Psi^* \frac{\partial \Psi}{\partial t} - \frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi - V(r, t) \Psi^* \Psi \right] \quad \dots\dots\dots(2)$$

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 :

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

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

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

$$\begin{aligned} &= -\frac{i\hbar}{2m} \nabla (i\hbar \Psi^*) \cdot \nabla \Psi - \frac{i}{\hbar} \nabla (i\hbar \Psi^*) \Psi \\ &= -\frac{i\hbar}{2m} \nabla \pi \cdot \nabla \Psi - \frac{i}{\hbar} \nabla \pi \Psi \quad \dots\dots\dots(6) \end{aligned}$$

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

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

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

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

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

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

$$\pi = \frac{i}{\hbar} \nabla \cdot \mathbf{p} - \frac{i\hbar}{2m} \nabla^2 \pi$$

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

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

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 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.

DEPARTMENT OF PHYSICS
CLASS:II M.Sc PHYSICS
QUANTUM MECHANICS-II (16PHP301)

A system of particles is specified by the _____ co-ordinates and their dependence on the time.	momentum	space	positional	phase-space	positional
The field lagrangian is expressed as the integral over all space of a _____ density.	Lagrangian	Hamiltonian	Volume	Surface	Lagrangian
The Hamiltonian equation for the time rate of change of a functional F of y and p is given by _____.	$dF/dt = \partial F/\partial t - \{F, H\}$	$dF/dt = \partial F/\partial t + \{F, H\}$	$dF/dt = \partial F/\partial x - \{F, H\}$	$dF/dt = \partial F/\partial x + \{F, H\}$	$dF/dt = \partial F/\partial t + \{F, H\}$
In the equation $dF/dt = \partial F/\partial t + \{F, H\}$, H represents the _____ energy of the field.	total	partial	kinetic	none of the above	total
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	$q_i(t)$
The field lagrangian is a function of the field amplitude _____.	\tilde{N}_y	dy/dt	$q(r,t)$	$y(r,t)$	$y(r,t)$
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
The variational principle for the lagrangian is given by _____.	$d/L dt = 0$	$d/L dt = 1$	$d/L dt = -1$	$d/L dt = y(r,t)$	$d/L dt = 0$
The momentum canonically conjugate to _____ can be defined to be the ratio of dL to the infinitesimal change _____ when all the other _____ and all the _____ are zero.	y	L	\tilde{N}_y	dy	dy
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
The $dF/dt =$ _____.	$-\partial F/\partial t + \{F, H\}$	$-\partial F/\partial t - \{F, H\}$	$\partial F/\partial t + \{F, H\}$	$\partial F/\partial t - \{F, H\}$	$\partial F/\partial t + \{F, H\}$
If H does not depend on explicitly on the time, then H is a _____ of motion.	equation	constant	lagrangian equation	Hamiltonian equation	constant
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
According to quantum equation for the field, $[y_i, y_j] = [P_i, P_j] =$ _____.	1	-1	0	2	0
The function $d(r, \dot{r})$ has the property that _____ is equal to the average value of f for the cell in which r' is situated.	$\int f(r) d(r, \dot{r}) d^3r$	$-\int f(r) d(r, \dot{r}) d^3r$	$-\int f(r) d(r, \dot{r}) d^2r$	$\int f(r) d(r, \dot{r}) d^2r$	$\int f(r) d(r, \dot{r}) d^3r$
The equation of motion for any quantum dynamical variable F is given by _____.	$dF/dt = -\partial F/\partial t + 1/i\hbar [F, H]$	$dF/dt = \partial F/\partial t - 1/i\hbar [F, H]$	$dF/dt = \partial F/\partial t + 1/i\hbar [F, H]$	$dF/dt = -\partial F/\partial t - 1/i\hbar [F, H]$	$dF/dt = \partial F/\partial t + 1/i\hbar [F, H]$
The field quantization is often called as _____.	wave quantisation	second quantisation	wave function quantisation	none of the above	second quantisation
If the commutation relations for the operators a_k and a_k^* are solved, then _____ is diagonal, consists of matrices.	$a_k^* a_k$	$a_k^* a_k$	$a_k^* a_k$	$a_k^* a_k$	$a_k^* a_k$
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$
The a_k^* is called _____ operator for the state k of the field.	none of the above	creation	number	destruction	number
The spin of the electron carries no _____.	charge	particles	energy	density	energy
The N_k is called _____ operator for the state k of the field.	number	creation	destruction	none of the above	number
The number operator need not be a _____.	equation of motion	constant of motion	lagrangian motion	Hamiltonian motion	constant of motion
The rate of change of N_k is given by _____.	$dN_k/dt = i\hbar [a_k^*, a, H]$	$dN_k/dt = -i\hbar [a_k^*, a, H]$	$dN_k/dt = [a_k^*, a, H]$	$i\hbar dN_k/dt = [a_k^*, a, H]$	$i\hbar dN_k/dt = [a_k^*, a, H]$
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

If U_k and E_k are the eigen function and eigen value, then the field hamiltonian becomes _____.	$H = \sum N_k E_k^2$	$H = \sum N_k E_k^3$	$H = \sum N_k E_k$	$H = \sum N_k E_k^4$	$H = \sum N_k E_k$
According to anticommutation relation, $[a_k, a_l] =$ _____.	$a_k a_l + a_l a_k = 1$	$a_k a_l + a_l a_k = 0$	$a_k a_l + a_l a_k = -1$	$a_k a_l - a_l a_k = 0$	$a_k a_l + a_l a_k = 0$
If the eigenvalues of each N_k are 0 and 1, then the particles obey the _____ principle.	variational	lagrangian	Hamiltonian	Exclusion	Exclusion
The eigen values of H can be found by the linear combination of the _____ wave amplitudes	spherical	polarized	plane	circular	plane
H is formally equivalent to the sum of the energies of a number of _____ oscillators.	harmonic	simple harmonic	sinusoidal	none of the above	harmonic
The momentum density of an electromagnetic field is the pointing vector _____ divided by c^2 .	$-(c/4\pi) E(r,t) \times H(r,t)$	$(c/\pi) E(r,t) \times H(r,t)$	$-(c/\pi) E(r,t) \times H(r,t)$	$(c/4\pi) E(r,t) \times H(r,t)$	$(c/4\pi) E(r,t) \times H(r,t)$
According to quantized field, the energy and momentum of each plane wave are quantized in	$-\hbar c$ and $\hbar K$	$\hbar c$ and $\hbar K$	$-\hbar c$ and $-\hbar K$	$\hbar c$ and $-\hbar K$	$\hbar c$ and $\hbar K$
According to Planck's quantum hypothesis, the energy associated with each plane electromagnetic wave is an integer multiple of the fundamental quantum _____.	$\hbar K$	$-\hbar K$	$\hbar n$	\hbar	$\hbar n$
The quantized electromagnetic field propagates with the _____ speed of light.	classical	quantum	a and b	none of the above	classical
The Hamiltonian density is given by $H =$ _____.	-p	p	0	p	p
A physical system with _____ degrees of freedom is referred as a field.	finite	infinite	constant	none of the above	infinite
A transition from classical particle mechanics to quantum mechanics is _____ degenerate.	doubly	triply	singly	none of the above	doubly
The electromagnetic wave travels in free space with the velocity of _____.	sound	ultrasonic wave	ultrasonic wave	infrasonic wave	ultrasonic wave

Reg No.....
(16PHP301)

KARPAGAM ACADEMY OF HIGHER EDUCATION

COIMBATORE-21

(Under Section 3 of UGC Act 1956)

DEPARTMENT OF PHYSICS

II M.Sc PHYSICS

Third Semester

I-Internal Examination (July 2017)

Quantum Mechanics II

Time: 2 hours

Maximum: 50 marks

PART-A (20x1=20Marks)

Answer all questions

1. Equation of Linear momentum _____
a. $P = mv$ b. $P = dv$ c. $P = md$ d. $P = m^2v$
2. Total angular momentum is equal to _____
a. orbital angular momentum + spin angular momentum
b. spin angular momentum c. linear angular momentum d. torque.
3. J. _____

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a. $J_x + iJ_y$ **b. $J_x - iJ_y$** c. $J_x^2 + iJ_y^2$ d. $J_x^2 - iJ_y^2$

4. $[J_x^2, J_x] =$ _____

a. $J_x [J_x J_x] + J_x$ b. J_x **c. $J_x [J_x J_x] + [J_x J_x] J_x$** d. J_x^2

5. $[J_z, J_+] =$ _____

a. J_+ b. J_x c. J_z d. $J_x J_y$

6. The scattering amplitude $f(\theta, \phi)$ for the scattering problem of stationary wave is given by _____.

a. $(m/2\pi^2) \int e^{-ik \cdot r} V(r) \Psi(r) dt$ b. $(m/2\pi^2) \int e^{ik \cdot r} V(r) \Psi(r) dt$

c. $(m/4\pi^2) \int e^{-ik \cdot r} V(r) \Psi(r) dt$ **d. $-(m/2\pi^2) \int e^{-ik \cdot r} V(r) j(r) dz$**

7. Born approximation is applicable for the scattering centres which are _____.

a. Strong **b. weak** c. moderate d. none of the above

8. In the equation $\Psi(r) = e^{ikr} + f(\theta) e^{ikr}/r$, the first term represents the _____.

a. scattered wave function b. re-scattered wave function

c. incident wave function d. recoiled wave function

9. Every atomic electron moves in a _____ potential energy $V(r)$ that is produced by the nucleus and all other electrons.

a. Spherically symmetric b. Assymmetric c. Radially symmetric d. None of the above

10. The state of an electron in a central field is specified by the quantum numbers _____.
a. n and l b. m_l and m_s c. n , l and m_s **d. n , l , m_l and m_s**
11. The basis of all molecular approximation is the large ratio of _____.
a. electron mass to nuclear mass b. electron mass to neutron mass c. electron mass to atomic mass **d. nuclear mass to electron mass**
12. The probability that a particle will be scattered as it traverses a given thickness of matter can be expressed in terms of a quantity called the _____.
a. Total scattering cross-section **b. Differential scattering cross-section** **Scattering cross-section** c. Coulomb scattering d. Partial wave analysis
13. In wave mechanics, an incident beam of particles is represented by a _____ wave.
a. Transverse b. Plane **c. Longitudinal** d. Stationary wave
14. Born approximation is applicable for the scattering centres which are _____.
a. Strong **b. weak** c. moderate d. none of the above
15. In the equation $\Psi(r) = e^{ikr} + f(\theta) e^{ikr}/r$, the first term represents the _____.
a. scattered wave function b. re-scattered wave function **c. incident wave function** d. recoiled wave function
16. In alkali atom, a single electron moves in a spherically symmetric _____ potential energy $V(r)$.
a. Excitation b. coulomb **c. noncoulomb** d. none of the above

17. The configuration of an alkali atom can be specified by a single pair of quantum numbers _____.

a.n, l b. n, l, m_l c. n, l, m_l , m_s d. n, l, m_s

18. The doublet structure characterizes all the moderately excited levels of the alkali atom except those for which $l =$ _____.

a.Infinity **b. 1** c. 1 and 2 d. 0

19. The central field approximation is applicable on all atoms except the _____ atom.

a.heavier b.alkali **c.lighter** d.smaller

20. Every atomic electron moves in a _____ potential energy

$V(r)$ that is produced by the nucleus and all other electrons.

a.Spherically symmetric b.asymmetric c. Radially symmetric d.None of the above

PART-B (3x2=6 Marks)

Answer all the questions

21. Write a short note on angular momentum.

The angular momentum of a particle with momentum p and position r is defined by

$$L = r \times p = (yp_z - zp_y) i + (zp_x - xp_z) j + (xp_y - yp_x) k$$

22. What are ladder Operators ?

In linear algebra application to quantum mechanics, the raising and lowering operator collectively called ladder operators.

$$J^+ = J_x + iJ_y$$

$$J^- = J_x - iJ_y$$

23. Write a short note on scattering.

In scattering a beam of particles pass to scattering material called target.

Target remains original state – elastic

Target remains different state – in elastic

PART-C (3x8=24 Marks)

Answer all the questions

24. a. For a spin- $1/2$ system, obtain the matrices for S_x , S_y and S_z . What are their eigen values and eigen vectors?

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

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

the σ_x , σ_y and σ_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

$$x^2 + y^2 + z^2 = 1$$

$$x_y = i z, \quad y_z = i x, \quad x_z = i y$$

$$x_y + y_x = y_z + z_y = z_x + x_z = 0$$

pauli was the first to recognize the necessity of two component state vectors 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 (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

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

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

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

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

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

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

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

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.

b. (i) What are Clebsch-Gordon Coefficients? Explain their significance.

(ii) Obtain the matrix of Clebsh-Gordon coefficients for $j_1 = 1, j_2 = 1$.

For the total angular momentum vector $J = J_1 + J_2$,

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

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.

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

Substituting this value of the coefficient in equation (3)

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

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

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

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

And

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

Second rules

Operating eq from left by J_z , we have

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

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

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

$$m = m_1 + m_2$$

we shall next find out how 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 , m_1 can have values from j_1 to $-j_1$ and j_2 to $-j_2$, m_2 in integral step.

The smallest value 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.

25. a. Write in detail about Partial waves

b. Explain The Born approximation and Validity of Born approximation.

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

replacing $\psi(r')$ in the integral equation by $\exp(iK \cdot r')$, we get

$$f(\mathbf{k}) = -1/4 \int \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}'] U(\mathbf{r}') d\mathbf{r}' \quad (1)$$

where k and k' are the wave vector in the incident and scattered direction 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

$$f(\theta) = -1/4 \int_0^\infty \exp(iq.r') U(r') dr' \quad (3)$$

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 θ'

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

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

$$-\cos \theta' = x \quad \text{or} \quad -\sin \theta' d\theta' = dx$$

we get

$$\begin{aligned} \int_0^\pi \exp(iqr' \cos \theta') \sin \theta' d\theta' &= \int_{-1}^1 \exp(iqr'x) dx \\ &= \exp(iqr') - \exp(-iqr') \end{aligned} \quad (5)$$

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

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

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 $q = 2k \sin(\theta/2)$

26.a. Explain the principle of Central Field. Explain Hartree's theory of many electron atom using central field approximation.

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. To facilitate the upcoming math, let's make the following definition

$$\hat{H}_e = \sum_i \hat{h}(x_i)$$

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

$$(\psi_1, \dots, \psi_N) = \psi_1(x_1) \psi_2(x_2) \dots \psi_N(x_N). \quad (1)$$

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

$$P^{ij}(\psi(x_1, \dots, x_i, \dots, x_j, \dots, x_N)) = \psi(x_1, \dots, x_j, \dots, x_i, \dots, x_N) = -\psi(x_1, \dots, x_i, \dots, x_j, \dots, x_N) \quad (2)$$

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.

(OR)

b. Derive Hartree-Fock equation

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 ϕ_k should be zero

$$\delta \langle H \rangle = 0 \Rightarrow \langle \phi_k | H | \phi_k \rangle = 0 \quad (1)$$

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 J^i 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 K^i , called the exchange term, has no classical analogue and is a direct result of the antisymmetry property of the wavefunction. The Fock operator

$$F^i = h^i + \sum_k (J^i_{kk} - K^i_{kk}) \psi_k \quad (2)$$

ψ_i

and using this definition Eq. 2 takes the simple form

$\sum_{i=1}^N$

$$F^i \psi_i = \epsilon_i \psi_i \quad (3)$$

ψ_i

There are several different solutions to the equations in Eq. 3 each corresponding to a different set of ϵ_i . We have the freedom to concentrate upon those ϵ_i which satisfies

$$\epsilon_i = \epsilon_i + \epsilon_k \quad (4)$$

where ϵ_k is essentially a new name for the Lagrange multipliers[1]. With this, Eq.4 may be written as

$$\hat{F} \psi_k = \epsilon_k \psi_k. \quad (5)$$

In this form, Eq. 5 is a traditional eigen value equation. 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 ϵ_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.

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DEPARTMENT OF PHYSICS

II M.Sc PHYSICS

Third Semester

II-Internal Examination

Quantum Mechanics II

Time: 2 hours

Maximum: 50 marks

PART-A (20x1=20Marks)

Answer all questions

1. The nuclear motion are classified into translation and rotational motion of the _____ equilibrium arrangement and internal vibrations of the nuclei about the equilibrium.
a. **quasi-rigid** b. stable c. unstable d. rigid
2. A system of particles is specified by the _____ co-ordinates and their dependence on the time.
a. Momentum b. space c. **positional** d. phase-space
3. The field lagrangian is expressed as the integral over all space of a _____ density.
a. **Lagrangian** b. Hamiltonian c. Volume d. Surface
4. In the equation $dF/dt = F/t + \{F, H\}$, H represents the _____ energy of the field.

- a. **Total** b. partial c. kinetic d. none of the above
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.
a. $\psi(t)$ b. $d\psi/dt$ c. $q_i(t)$ d. none of the above
6. The field lagrangian is a function of the field amplitude _____.
a. $\nabla\psi$ b. $d\psi/dt$ c. $q(r,t)$ d. $\mathcal{E}(r,t)$
c. $(m/4\pi^2) \int e^{-ik \cdot r} V(r) \Psi(r) dt$ d. $-(m/2\pi^2) \int e^{-ik \cdot r} V(r) \Psi(r) dt$
7. As $r \rightarrow \infty$, there is no net charge inside the sphere of radius r , so that V falls off more rapidly than _____.
a. $1/r$ b. $1/r^2$ c. $-1/r$ d. r^2
8. Molecular energy levels are classified into _____ vibrational and rotational energy levels.
a. Static b. rigid c. translational d. **electronic**
9. The energy E_e associated with the motion of a valence is of order of _____, where m is the electronic mass.
a. $-2/ma^2$ b. $2/ma^2$ c. $-A^2/ma^2 + 1$ d. $2/ma^2 + 1$
10. The only nuclear coordinates R_j of the hydrogen molecule is the magnitude, _____ of the distance between the two hydrogen nuclei.
a. **R** b. r c. $-R$ d. R^2
11. The linear combination of unperturbed degenerate wave function which gives lower energy than the separate wave function is the basis of _____ binding molecules.
a. Heteropolar b. nuclei c. **homopolar** d. atomic

12. The property of degeneracy is known as _____.
a. **Resonance** b. doublet separation c. doublet intensity d. none of the above
13. A _____ oscillator emits radiation spontaneously.
a. Quantum b. **classical** c. sinusoidal d. damped
14. A _____ oscillator emits radiation spontaneously.
a. Quantum b. **classical** c. sinusoidal d. damped
15. If the spins of electron in two atoms are parallel then the atoms _____ each other.
a. **Repel** b. attract c. coagulate d. none of the above
16. If the spins of the electrons in two atoms are antiparallel, then two atoms _____ each other.
a. Repel b. **attract** c. coagulate d. none of the above
17. 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.
a. Doublet b. triplet c. multiplet d. **singlet**
18. The quantum analogue of _____ density function is known as the density operator.
a. Particle b. momentum c. **quantum** d. classical
19. A _____ state can be described by a non-negative density function.
a. classical b. statistical c. **quantum** d. none of the above

20. The doublet structure characterizes all the moderately excited levels of the alkali atom except those for which $l =$ _____.
a. Infinity b. 1 c. 1 and 2 d. 0

PART-B (3x2=6 Marks)

Answer all the questions

21. Write a short note on particle in a coulomb field.

A coulomb field is a vector field can be associated with each point in space for the coulomb force of the electric charge.

22. What are quantization?

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

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

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

23. Write a short note on creation.

The creation and annihilation should be a add (or) remove the particle for the many system of the body. This operates lies a core for each second quantization.

PART-C (3x8=24 Marks)

Answer all the questions

24. a. Describe Klein-Gordon field and Klein-Gordon field equation

The non relativistic Schrodinger equation was obtained by replacing P by $-i \nabla$ and E by $i \frac{\partial}{\partial t}$ in the classical energy

expression of a free particle $E = \frac{p^2}{2m}$ and allowing the resulting operator equation to operate on the wave function. The

corresponding relativistic energy relation is:

$$E^2 = c^2 p^2 + m^2 c^4 \quad \text{.....(1)}$$

Where m is the rest mass of the particle. For convenience, rest mass will be denoted by m in this chapter. Replacing E and P by the respective operators, we get the operator equation

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

Allowing this operator equation to operate on the wave function $\Psi(r, t)$

$$-\hbar^2 \frac{\partial^2 \Psi(r, t)}{\partial t^2} = -c^2 \hbar^2 \nabla^2 \Psi(r, t) + m^2 c^4 \Psi(r, t) \quad \text{.....(3)}$$

Which is Klein – Gordon equation or Schrodinger's relativistic equation

Rearranging, we get

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \Psi(r, t) = \frac{m^2 c^2}{\hbar^2} \Psi(r, t) \quad \text{..... (4)}$$

$$\Psi(r, t) = \frac{m^2 c^2}{2} \Psi(r, t)$$

$$\square = \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \quad \text{.....(5)}$$

Where \square is the de Alembertian operator which is relativistically invariant. Therefore eq(5) is relativistically invariant if transforms like a scalar

Plane Wave Solution

The plane wave represented by

$$\Psi(r, t) = \exp[i(k \cdot r - \omega t)] \quad \text{.....(6)}$$

Is an eigenfunction of both energy and momentum operator with eigenvalues ω and k respectively. Substitution of Eq (6) in Eq (4) gives

$$\begin{aligned} (\omega^2) &= (c^2 \hbar^2 k^2 + m^2 c^4) \\ (\omega) &= \pm (c^2 \hbar^2 k^2 + m^2 c^4)^{1/2} \end{aligned}$$

This means that the energy eigenvalue can have both positive and negative values. Klein – Gordon were not able to give a consistent explanation for the negative energy.

b. Derive Dirac's relativistic equation.

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

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

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:

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

The latter form becomes the Klein–Gordon equation provided that the μ 's satisfy the Clifford algebra 2×3

$$\{\mu_i, \mu_j\} = \mu_i \mu_j + \mu_j \mu_i = -2 \mu_i \mu_j. \quad (3)$$

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 $x_0' = \gamma(x_0 - \beta x_1)$ with $\gamma = 1/\sqrt{1-\beta^2}$. 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

$$\begin{aligned} 0 &= i \gamma^\mu \partial_\mu \psi - m \psi \quad \psi(x) = S(\Lambda) \psi(x) \\ &= i S \gamma^\mu \partial_\mu \psi - S m \psi(x) \\ &= S i \gamma^\mu \partial_\mu \psi - i \gamma^\mu \partial_\mu \psi(x) \\ &= S i \gamma^\mu \partial_\mu \psi - i \gamma^\mu \partial_\mu \psi(x). \end{aligned} \quad (2)$$

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

$$\gamma^\mu = (\Lambda^{-1})^\mu_\nu \gamma^\nu, \quad (3)$$

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

$$\gamma^\mu = \gamma^\mu. \quad (4)$$

This condition relates S to the Lorentz transformation Λ . The infinitesimal form of the invariance condition reads

$$[S, \gamma^\mu] = -i \gamma^\mu \omega_{\mu\nu} \gamma^\nu = 0. \quad (5)$$

This implies that S must be proportional to γ^μ . The latter carries two vector indices, while S carries none. The only possibility is to contract the vector indices by S from the left, co-spinors by the S^{-1} from the right.

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

$$[\gamma^\mu, \gamma^\nu] = \{\gamma^\mu, \gamma^\nu\} - \{\gamma^\mu, \gamma^\nu\}, \quad (6)$$

we arrive at $(2 - 1) \gamma^\mu \gamma^\mu = 0$. We conclude that a Lorentz transformation for spinors is given by the matrix

the Dirac spinor $\psi = (\psi_L, \psi_R)$ transforms in the direct sum of two (irreducible) representations of the Lorentz group. The 2-spinors ψ_L and ψ_R are called left-chiral and right-chiral spinors. The massive Dirac equation, however, mixes these two representations

$$i \gamma^\mu \partial_\mu \psi_R - m \psi_L = 0, \\ i \gamma^\mu \partial_\mu \psi_L - m \psi_R = 0. \quad (7)$$

It is therefore convenient to use Dirac spinors for massive spinor particles whereas massless spinor particles can also be formulated using 2-spinors; we shall discuss the massless case later on.

25. a. Obtain the relativistic Lagrangian and Hamiltonian of a charged particle in electromagnetic field.

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

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

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

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

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 $\delta(r, r') = \frac{1}{\Delta\tau} \delta\tau$ 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 $i\hbar$ 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.

b.Explain classical theory of electromagnetic fields, and obtain the electromagnetic field four-tensor.

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:

$$\nabla \cdot E = \rho \quad \dots\dots(1)$$

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

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

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

Here $\rho(x, t)$ is the charge density and current density $j(x, t)$ 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 :

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

$$\text{.....(6)}$$

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

$$\nabla \times (\nabla \times A) + \frac{\partial}{\partial t} \left(\frac{\partial A}{\partial t} + \nabla \varphi \right) = j$$

$$\nabla(\nabla \cdot A) - \nabla^2 A + \nabla \frac{\partial \varphi}{\partial t} = j$$

$$\nabla^2 A - \frac{\partial^2 A}{\partial t^2} - \nabla(\nabla \cdot A + \frac{\partial \varphi}{\partial t}) = -j \quad \dots(9)$$

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

$$A \rightarrow A' = A + \nabla \chi$$

$$\dots(10)$$

$$\varphi \rightarrow \varphi' = \varphi -$$

$$\frac{\partial \chi}{\partial t}$$

$$\dots\dots(11)$$

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

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

$$E = \frac{\partial}{\partial t} (A + \nabla \chi) - \nabla \left(\varphi - \frac{\partial \chi}{\partial t} \right)$$

$$= - \frac{\partial A}{\partial t} - \nabla \varphi$$

$$\nabla \cdot A + \frac{\partial \varphi}{\partial t} = 0 \quad (12)$$

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:

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

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

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

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

$$\mathbf{j} = (\mathbf{j}, i\rho) \quad \text{.....(14)}$$

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

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

From eq we have

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

$$B_2 = \frac{\partial A_1}{\partial x_3} - \frac{\partial A_2}{\partial x_1} \quad \text{.....(17)}$$

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

From eq

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

$$iE_1 = \frac{\partial A_1}{\partial x_4} - \frac{\partial A_4}{\partial x_1} = F_{41} \quad \text{.....(19)}$$

$$iE_2 = \frac{\partial A_2}{\partial x_4} - \frac{\partial A_4}{\partial x_2} = F_{42} \quad \text{.....(20)}$$

$$iE_3 = \frac{\partial A_3}{\partial x_4} - \frac{\partial A_4}{\partial x_3} = F_{43} \quad \text{.....(21)}$$

In general

$$F_{\mu\nu} = \frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu}, \quad F_{\mu\nu} = -F_{\nu\mu} \quad \text{.....(22)}$$

$$F_{k4} = -iE_k, \quad F_{ij} = \epsilon_{ijk} B_k \quad \text{.....(23)}$$

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

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

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

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

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

$$\begin{bmatrix} iE_{x/c} & iE_{y/c} & iE_{z/c} & 0 \end{bmatrix}$$

Which is the electromagnetic field four tensor.

26.a. Discuss Quantisation of non-relativistic Schroedinger 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:

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

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

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

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

$$= -\frac{i\hbar}{2m} \nabla \cdot \nabla - \frac{i}{\hbar} V \Psi \quad \dots\dots\dots(6)$$

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

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

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

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

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

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

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

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 \mathcal{H} 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^* .

$$[\Psi(r,t), \Psi^*(r',t)] = \delta(r-r').$$

b. Discuss second Quantisation

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_i must be a non-negative integer; for fermions, the Pauli exclusion principle restricts n_i 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

$$N = \sum n_i.$$

There is a unique vacuum or no-particle state:

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

The single-particle states can be represented

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

Bosonic operators. Let us define the bosonic creation operator a_i^\dagger by

$$|n_1, n_2, \dots, n_{i-1}, n_i, n_{i+1}, \dots\rangle =$$

$$a_i^\dagger |n_1, n_2, \dots, n_{i-1}, n_i, n_{i+1}, \dots\rangle, \quad (1)$$

and the corresponding annihilation operator a_i by

$$a_i |n_1, n_2, \dots, n_{i-1}, n_i, n_{i+1}, \dots\rangle = \sqrt{n_i} |n_1, n_2, \dots, n_{i-1}, n_i - 1, n_{i+1}, \dots\rangle. \quad (2)$$

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

and

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

$$N = \sum_i N_i$$

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

$$|0\rangle_i = |i\rangle, \quad a_i |i\rangle = 0,$$

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