SEMESTER – II

		L T P C
17PHP202	**QUANTUM MECHANICS - I**	**4 - - 4**

Scope: Quantum mechanics is the most important branch of physics, as it has got application in any other branch of physics. This was developed at a time of crisis. It has revolutionized the whole science. It is important for any physics student to know the basics of quantum mechanics.

Objectives: This paper gives an idea about the development of quantum mechanics.

UNIT - I

Quantum Theory: Introduction – Limitation of classical physics – Origin of quantum theory – Planck's quantum hypothesis – Einstein's theory of Photoelectric effect –Bohr model of hydrogen atom – Inadequacy of quantum theory.

Wave Mechanics Matter waves – Uncertainty principle –Wave packet – Group and phase velocity – Time-dependent and Time-independent Schrodinger equations for a free particle and particle in a potential .

UNIT - II

One dimensional potential well: Square-well potential with rigid walls – Square-well potential with finite walls – Square-well potential barrier – Alpha emission – Bloch waves in a periodic potential – Linear harmonic oscillator (Schrodinger method and operator method) – Free particle.

UNIT - III

Three dimensional potential Well: Particle moving in a spherically symmetric potential – System of two interacting particles – Rigid rotator – Hydrogen atom –– Three-dimensional square-well potential - Deutron

Matrix mechanics: Matrix representation of wave function – Matrix representation of operator – Properties of matrix elements – Schroedinger equation in matrix form –Unitary Transformations – Linear harmonic oscillator.

UNIT - IV

Time-independent Perturbation theory: Basic concepts – Non-degenerate energy levels – First and Second order corrections for energy and wave functions – Ground state of Helium atom – Effect of electric field on the ground state of hydrogen atom (Stark effect) – Degenerate energy levels – Effect of electric field on the n=2 state of hydrogen atom

UNIT - V

Variational method &WKB Approximation: Variational principle – Variation method for excited states – Application of variation method to ground state of helium – The WKB method

Time dependent perturbation theory: Introduction – First-order perturbation – Harmonic perturbation – Transition to continuum states (Fermi's Golden rule) – Absorption and emission of radiation – Transition probability – Selection rules

TEXT BOOKS:

1. Aruldhas. G, 2009, Quantum Mechanics, 2nd Edition, Prentice-Hall of India, New Delhi.
2. Leonard I. Schiff, 2000, Quantum Mechanics, 3rd Edition, McGraw Hill International, Auckland

REFERENCES:

1. Gupta, Kumar and Sharma, 2002 – 2003, Quantum Mechanics, 22nd Edition, Jai Prakash Nath & Co, Meerut.
2. Satya Prakash, New Edition, 2003, Quantum Mechanics, Kedar Nath & Ram Nath & Co, Meerut.
3. Eugen Merzbacher,2013, Quantum Mechanics, 3rd Edition, Wiley, Weinheim
4. Mathews. P.M. and K. Venkatesan, 2nd Edition, 2013, Textbooks of Quantum Mechanics, McGraw Hill International, Weinheim.
5. Chatwal R.G. and Sk. Anand, 4th edition, 2004, Quantum Mechanics, Himalaya Publishing House, New Delhi

Thangappan. V. K., 2nd Edition,2013, Quantum Mechanics, Tata McGraw Hill, New Delhi

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KARPAGAM ACADEMY OF HIGHER EDUCATION

(Deemed to be University Established Under Section 3 of UGC Act 1956)

Coimbatore – 641 021.

LECTURE PLAN
DEPARTMENT OF PHYSICS

STAFF NAME: Dr. A. SARANYA
SUBJECT NAME: QUANTUM MECHANICS SUB.CODE: 17PHP202
SEMESTER: II CLASS: II M.Sc (PHY)

S.No	Lecture Duration Period	Topics to be Covered	Support Material/Page Nos
		UNIT-I	
1	1 hr	Introduction	T1 (1)
2	1 hr	Limitations of classical physics	T1 (1)
3	1 hr	Origin of quantum theory-Planck’s quantum hypothesis	T1 (4-5)
4	1 hr	Einstein’s theory of photoelectric effect	T1 (5-6)
5	1 hr	Bohr model of hydrogen atom	T1 (7-8)
6	1 hr	Inadequacy of quantum theory	T1 (16-17)
7	1 hr	Matter waves-Uncertainty principle	T1 (24-26)
8	1 hr	Wave packet	T1 (28-31)
9	1 hr	Group and phase velocity	T1 (31)
10	1 hr	Time-dependent Schrodinger equation	T1 (31-33)
11	1 hr	Time independent Schrodinger equations for a free particle and particle in a potential	T1 (38-39)
12	1 hr	REVISION	
	Total No of Hours Planned For Unit 1=12		
		UNIT-II	
1	1 hr	Square-well potential with rigid walls	T1 (81-83)

2	1 hr	Square-well potential with finite walls	T1 (83-86)
3	1 hr	Square-well potential barrier	T2 (87-89)
4	1 hr	Alpha emission	T1 (90)
5	1 hr	Bloch waves in a periodic potential	T2 (92)
6	1 hr	Linear harmonic oscillator(Schrodinger method)	T1 (95-100)
7	1 hr	Linear harmonic oscillator(operator method)	T1 (100-103)
8	1 hr	Free particle	T1 (103-104)
9	1 hr	REVISION	
10	1 hr	CLASS TEST	
	Total No of Hours Planned For Unit II=10		
		UNIT-III	
1	1 hr	Particle owing in a spherically symmetric potential	T1 (114-119)
2	1 hr	System of two interacting particles	T1 (119-122)
3	1 hr	Rigid rotator	T1 (122)
4	1 hr	Hydrogen atom	T1 (211)
5	1 hr	Three-dimensional square-well potential	T2 (133-135)
6	1 hr	Deuterons	T1 (134-135)
7	1 hr	Matrix representation of wave function	T1 (144)
8	1 hr	Matrix representation of operator	T1 (144)
9	1 hr	Properties of matrix elements	T1 (145)
10	1 hr	Schrodinger equation in matrix form	T1 (145)
11	1 hr	Unitary transformations	T1 (148-150)
12	1 hr	Linear harmonic oscillator	T1(150-154)
13	1hr	REVISION	
	Total No of Hours Planned For Unit III=13		

		UNIT-IV	
1	1 hr	Basic concepts	T1 (195-196)
2	1 hr	Non-degenerate energy levels	T1 (196-198)
3	1 hr	First order corrections for energy	T1 (199)
4	1 hr	Second order corrections for energy and wave functions	T1 (198)
5	1 hr	Ground state of helium atoms	T1 (199-201)
6	2 hr	Effect of electric field on the ground state of hydrogen atom(stark effect)	T1 (201-204)
7	1 hr	Degenerate energy levels	T1 (204-205)
8	2 hr	Effects of electric field on the n=2 state of hydrogen atom	T1 (205-207)
9	1 hr	REVISION	
	Total No of Hours Planned For Unit IV=11		
		UNIT-V	
1	1 hr	Variational principle	T1 (215-216)
2	1 hr	Variation method for excited state	T1 (216)
3	1 hr	Application of variation method to ground state of helium	T1 (217)
4	1 hr	The WKB method	T1 (229-231)
5	1 hr	Introduction-first order perturbation	TI (243-244)
6	1 hr	Harmonic perturbation	T1 (244-246)
7	1 hr	Transition to continuum states(Fermi Golden rule)	T1 (246-247)
8	1 hr	Absorption of radiation and Emission of radiation	T1 (247-251)
9	1 hr	Transition probability	T1(252)
10	1 hr	Selection rule	T1(253)
11	1 hr	REVISION	
12	1 hr	Question Paper discussion	
13	1 hr	Question Paper discussion	
14	1 hr	Question Paper discussion	

	Total no. of Hours planned for unit- V		14
Total Planned Hours	**60**		

TEXT BOOKS:

1. Aruldhas. G, 2009, Quantum Mechanics, 2nd Edition, Prentice-Hall of India, New Delhi.
2. Leonard I. Schiff, 2000, Quantum Mechanics, 3rd Edition, McGraw Hill International, Auckland

REFERENCES:

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2. Satya Prakash, New Edition, 2003, Quantum Mechanics, Kedar Nath & Ram Nath & Co, Meerut.
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UNIT-I

SYLLABUS

Quantum Theory: Introduction – Limitation of classical physics – Origin of quantum theory – Planck’s quantum hypothesis – Einstein’s theory of Photoelectric effect –Bohr model of hydrogen atom – Inadequacy of quantum theory.

Wave Mechanics Matter waves – Uncertainty principle –Wave packet – Group and phase velocity – Time-dependent and Time-independent Schrodinger equations for a free particle and particle in a potential .

Limitation of Classical Physics

Classical mechanics describe the motion of the macroscopic particle, such as star, planet, moon, lump of clay as well as microscopic particle such as motion of a bacteria, virus. It describe the motion of a particle in non-relativistic limit. i.e. V<<C

Newtonian mechanics is based on concept of

1. Absolute Space
2. Absolute Time
3. Absolute mass and it's contained

In Newton's law of motion ($\vec{F}=m\vec{a}$ $F_{\rightarrow}=ma_{\rightarrow}$). Due to certain limitation of classical mechanics and it's wrong assumption could not explain following physical phenomena.

1. It could not explain the spectrum of black body radiation.

The total energy density at temperature T comes out to be infinity but experimentally T total energy should be finite and measurable.

2. It could not explain the stability of atoms.

According to classical theory electron accelerate around nucleus of an atom less it's energy in the form of radiation ad it's energy continuously decreases. Radius of electronic orbit also decreases and electron jump inside nucleus and atom becomes unstable.

But in real atom is stable.

3. It could not explain discrete atomic spectrum:

According to classical theory of radiation, energy exchange between atom and radiation field must be continuous. But atoms absorbs and emits discrete energy in unit of (hνhν).

4. It could not explain photoelectric effect:

According to classical theory of radiation the kinetic energy of emitted electron (photoelectron) depends upon the intensity of radiation, independent of frequency.

5. It could not explain the phenomena of pair production ($E=mc^2E=mc^2$).

6. It could not explain the phenomena of Compton scattering.

According to classical theory of radiation the frequency of scattered radiation should be equal to frequency of oscillating charge (electron), which is equal to frequency of incident radiation. There should be no change in frequency.

7. It could not explain variation of electric conductivity of solid (supper conductivity).

8. Classical mechanics could not explain the phenomena associated with spinning motion of electron. (Ferromagnetism, Poulies exclusion principle).

9. Classical mechanics could not explain Zeeman effect, Stark effect, Raman effect.

10. It could not explain phenomena of radioactivity (ββ-decay, αα- decay)

11.Classical mechanics is based on the exact measurement of physical quantity but in real we can not measure a physical quantity exactly and preciously with out any error (uncertainity principle).

12. According to classical mechanics total energy of particles is always positive. But in Dirac theory negative energy state is also exit. (Existance of positron, antiparticle of electron). The energy of positron is negative before it's formation. So this can not explain by classical theory.

To sole above physically observable problem Scientists purposed, a new field of physics based on uncertainity principle and wave-matter duality of particles. This new field of physics is known as quantum mechanics.

Planck's Quantum hypothesis

Planck's formula for the distribution of energy in the radiation from a black body was the starting point of the quantum theory, which has been developed during the last 20 years and has borne a wealth of fruit in energy domain of physics. Since its publication in 1901 many methods for deriving this law have been proposed. It is recognized that basic assumptions of the quantum theory are irreconcilable with the laws of classical electrodynamics. All derivations up to now use the relation

$$E_n = -\frac{m_e e^4}{32\pi^2\epsilon_0^2\hbar^2}\frac{1}{n^2} = -\frac{e^2}{8\pi\epsilon_0 a_0}\frac{1}{n^2} = -\frac{E_1}{n^2},$$

that is, the relation between the radiation density and the mean energy of an oscillator, and they make assumptions about the number of degrees of freedom of the ether, which appear in the above formula (the first factor on the right– hand side). This factor, however, can be derived only from classical theory. This is the unsatisfactory feature in all derivations and it is therefore no wonder that attempts are being made to obtain a derivation that is free of this logical flaw.

Einstein has given a remarkably elegant derivation. He recognized the logical defect of all previous derivations and tried to deduce the formula independently of classical theory. From very simple assumptions about the
energy exchange between molecules and a radiation field he found the relation.

Matter waves

Photons are the particles of light. Matter is made of atoms, and atoms are made protons, neutrons and electrons. These are not macroscopic particles. Typical atomic dimensions are on the order of 10-10 m, nuclear dimensions are on the order of 10-15 m, and the electron seems to be a point particle with no size at all.

If a wave equation describes the behavior of photons, maybe a wave equation also describes the behavior of other microscopic particles.

In 1924, Luis deBroglie (Nobel Prize in Physics in 1929) proposed that a wave function is associated with all particles. Where this wave function has nonzero amplitude, we are likely to find the particle. The standard interpretation is that the intensity of the wave function of a particle at any point is proportional to the probability of finding the particle at that point. The wavelengths of the harmonic waves used to build the wave function let us calculate the most likely momentum of the particle and the uncertainty in the momentum. The wave function for a material particle is often called a matter wave.

Bohr model of hydrogen atom

To overcome the difficulty associated with the classical collapse of the electron into the nucleus, Bohr proposed that the orbiting electron could only exist in certain special states of motion - called stationary states, in which no electromagnetic radiation was emitted. In these states, the angular momentum of the electron L takes on integer values of Planck's constant divided by 2π, denoted by ~ = h/2π (pronounced h-bar). In these stationary states, the electron angular momentum can take on values ~, 2~, 3~, ..., but never non-integer values. This is known as quantization of angular momentum, and was one of Bohr's key hypotheses.

For circular orbits, the position vector of the electron r is always perpen- dicular to its linear momentum p. The angular momentum L = r × p has magnitude L = rp = me vr in this case. Thus Bohr's postulate of quantized angular momentum is equivalent to

me vr = n~,

The energy levels are indicated schematically. The electron energy is quantized, with only certain discrete values allowed. In the lowest energy level, known as the ground state, the electron has en- ergy E1 = 13.6 eV. The higher states, n = 2, 3, 4, with energies −3.6 eV, −1.5 eV, −0.85 eV, are called excited states. The integer, n that labels both the allowed radius and energy level, is known as the principle quantum number of the atom. It tells us what energy level the electron occupies.

When the electron and nucleus are separated by an infinite distance (n → ∞) we have E = 0. By bringing the electron in from infinity to a particular state n, we release energy E = −(Efinal − Einitial) = |En | (note the minus sign comes from the energy being released). Similarly, if we start with an atom in state n, we must supply at least |En | to free the electron. This energy is known as the binding energy of the state n. If we supply more energy than |En | to the electron, then the excess beyond the binding energy will appear as kinetic energy of the freed electron.

The excitation energy of an excited state n is the energy above the ground state, $E_n - E_1$. For the first excited state, n = 2, the excitation energy is

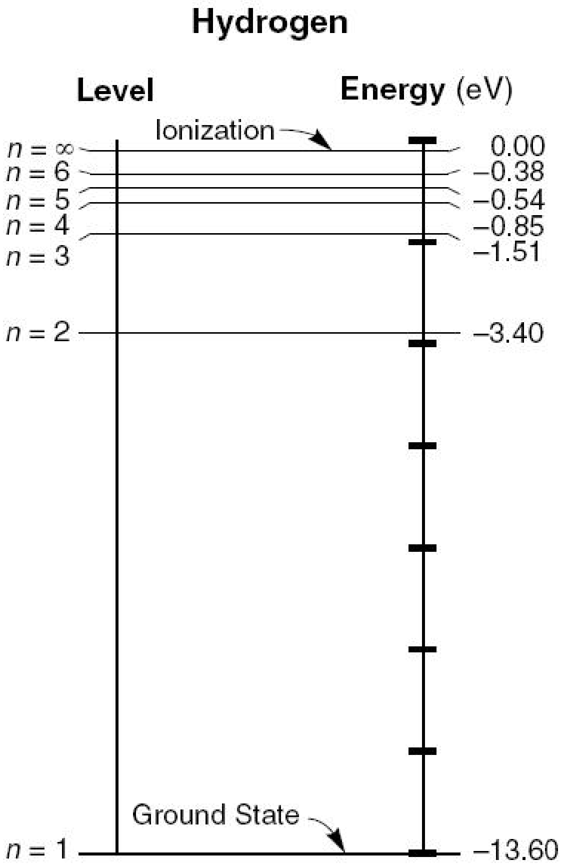
$\Delta E = E_2 - E_1 = -3.4$ eV − (−13.6 eV) = 10.2 eV.

Once Bohr had worked out that the energy levels of hydrogen were quantized, i.e. only allowed to take on discrete values, he was able to easily de- scribe the spectral lines observed for hydrogen if he were to posit a second postulate: radiation can only be emitted when the atom makes a transition from one energy level, say n, to another with lower energy, $m < n$. The energy of the emitted photon will thus be given by the difference in energy between these two levels

$$\Delta E = E_2 - E_1 = -3.4 \text{ eV} - (-13.6 \text{ eV}) = 10.2 \text{ eV}.$$

Comparison of this with Rydberg's empirical formula, , Bohr identified his ground state energy value, $E_1 = 13.6$ eV with the experimentally determined Rydberg constant, R = 13.6 eV. These two agreed well within experimental errors of the time.

Note that Bohr's second postulate, i.e. the energy of an emitted photon from an atom is given by the difference in energy level, contradicts the concepts of classical physics in which an oscillating charge emits radiation at its frequency of oscillation. For an electron in state n with energy E_n , its oscillation frequency is just $\nu_n = E_n /h$.



Energy Levels for the Hydrogen Atom

Schematic representation of the discrete allowed energy levels in the hydrogen atom.

Bohr's postulates

- Quantized angular momentum: $L = m_e vr = n$~.
- Radiation is only emitted when an atom makes transitions between stationary states: $E_{ph} = E_m - E_n$.

As we will see when we discuss the wave nature of matter and the de Broglie wavelength, the quantization of angular momentum, which leads to allowed orbits with radii rn = a0 n2 and momenta pn = ~/a0n = ~n/rn implies that the circumference of the allowed states is an integer multiple of the de Broglie wavelength λdB = h/p

nλdB = 2πrn

Uncertainty relations

A central aspect of the dual wave-particle nature of quantum systems is the indeterminism associated with measurement outcomes. This wave-particle duality is most pronounced when discussing the uncertainties associated with the simultaneous measurement of the position and momentum of a quantum particle. In classical physics, we think of uncertainty as a flaw in our measurement devices. For example, if we attempt to measure the position of a particle with respect to another particle using a ruler with millimeter scale divisions, we can at best quote the position to say the nearest half millimeter. The uncertainty in the position, which we denote by Δx, is limited by our measurement device. A further source of uncertainty in measurements arises from statistical fluctuations in the measurement pro- cess, for example, we might not quite line up the ruler origin at exactly the same point for repeated measurements. This type of random error can be eliminated by repeating the measurement many times and using the average value of the measurement outcomes and their standard deviation to estimate the true value of the position. Furthermore, if the particle is moving and we wanted to measure the position and momentum of the particle, there is nothing to stop us from doing both simultaneously to any level of precision.

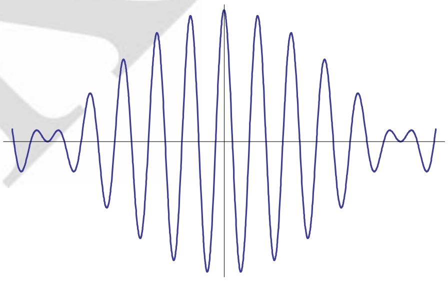
However, in quantum physics there are inherent uncertainties associ- ated with the values of measurements performed on quantum systems. The uncertainty principle (or Heisenberg uncertainty principle named after its discoverer) tells us that the product of uncertainties associated with posi- tion and momentum must be greater than or equal to the Planck constant divided by 4 π, i.e.,

$$\Delta x \Delta px \geq \sim ,\ \hbar$$

where ~ = h/2π as usual. We interpret this inequality by stating that the if we try to measure both position and momentum simultaneously, the product of their uncertainties must be larger than a very small, but finite value. In other words, it is not possible to simultaneously determine the position and momentum of a quantum system with unlimited precision. This uncertainty principle in x and px can be extended to other measurement outcomes including the two other spatial-momentum directions (y, py and z, pz) as well as other complementary observables, that is quantities that cannot be simultaneously determined to arbitrary precision (many, but not all, complementary observables turn out to be Fourier-transform pairs). For example, there is an uncertainty relation between energy and time.

Wave packets

A pure sine wave has a well-defined wavelength and thus frequency (energy) and momentum, but is completely delocalized in space, spreading infinitely throughout space. The same holds for plane waves as discussed in the pre- vious section. A classical particle, on the other hand is completely localized in space, has a well-defined position and therefore trajectory. An electron bound to an atom is localized in position to within an uncertainty on the order of the atomic diameter (given by twice the Bohr radius for example), but its precise position within the atom is not well defined. To describe such “quasi-localized” waves, physicists have at their disposal the concept of wave packets. A wave packet can be considered to the be the superposition of many waves that interfere constructively in the vicinity of the particle, giving a large amplitude where the particle is expected to be found, and interfere destructively far from where the particle is predicted to be found.

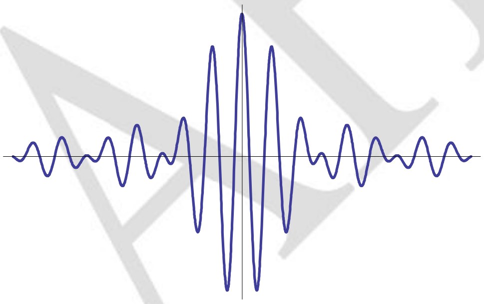


Two cosine waves with slightly different wavelengths (top) add constructively in superposition near zero displacement (bottom), but destructively further away. This leads to a beat pattern.

In one dimension, we can add two sine waves with different, but nearly equal, wave vectors, k1 and k2, which leads to a beat pattern with a spatial localization for part of the wave depicted. The associated wave is given by

$$\psi 2(x) = A(\sin(k1x) + \sin(k2\,x)),$$

where we have assumed equal amplitudes for both wave vector components. By adding more waves to this superposition, say N in total, with appropriate wave vectors and relative phases, we can create an increasingly localized wave packet



Wave packet constructed from ten different cosines, each with slightly different wavelengths.

Time dependent Schrodinger equation

According to Planck and Einstein the energy and frequency of light are related by E = ~ω. De Broglie extended this dualism to massive particles by relating in addition the momentum to the wave vector p = ~k. It was Erwin Schr¨odinger who reconsidered de Broglie’s matter waves and discovered in 1926 a wave equation, the equation of motion corresponding to the wave nature of particles, which fits the physical observations. This differential equation is a fundamental equation and cannot be derived from first principles but we can make its form plausible. Let us consider plane waves or rather wave packets which are of the form

$$\begin{aligned} \psi(t,x) &= e^{i(kx-\omega t)} \\ \psi(t,x) &= \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \tilde{\psi}(k)\, e^{i(kx-\omega t)} \quad . \end{aligned}$$

We differentiate these waves with respect to t and x and recall the relations of wave and particle properties,

$$\begin{aligned} i\hbar \frac{\partial}{\partial t}\, \psi(t,x) &= \underbrace{\hbar\omega}_{E}\, \psi = E\,\psi \quad \rightarrow \quad \int \frac{dk}{\sqrt{2\pi}}\, \underbrace{\hbar\omega}_{E}\, \tilde{\psi}(k)\, e^{i(kx-\omega t)} \\ -i\hbar \nabla\, \psi(t,x) &= \underbrace{\hbar k}_{p}\, \psi = p\,\psi \quad \rightarrow \quad \int \frac{dk}{\sqrt{2\pi}}\, \underbrace{\hbar k}_{p}\, \tilde{\psi}(k)\, e^{i(kx-\omega t)} \\ -\hbar^2 \Delta\, \psi(t,x) &= \underbrace{(\hbar k)^2}_{p^2}\, \psi = p^2\,\psi \quad \rightarrow \quad \int \frac{dk}{\sqrt{2\pi}}\, \underbrace{(\hbar k)^2}_{p^2}\, \tilde{\psi}(k)\, e^{i(kx-\omega t)} \quad . \end{aligned}$$

The nonrelativistic energy–momentum relation for massive particles, where we assume for simplicity that the potential V = V (x) is independent of time

$$E = \frac{p^2}{2m} + V(x)\,,$$

then provides a differential equation for ψ which Schr¨odinger assumed to hold quite generally for massive particles in an external potential V (x) 1 .

$$i\hbar \frac{\partial}{\partial t}\, \psi(t,x) \;=\; \left(-\frac{\hbar^2}{2m}\Delta + V(x)\right) \psi(t,x) \;=\; H\,\psi(t,x)$$

The operator H = − ~ 2 2m ∆ + V (x) is called the Hamiltonian of the system, ~ is Planck's constant and m is the mass of the particle. The solution ψ(t, x) of the Schrodinger equation is called the wave function. It contains all the information about a physical system.

Time independent equation

The time dependence entered into the wave function via a complex exponential factor exp[−iEt/ħ]. This suggests that to 'extract' this time dependence we guess a solution to the Schr¨odinger wave equation of the form Ψ(x,t) = ψ(x)e−iEt/ ħ i.e. where the space and the time dependence of the complete wave function are contained in separate factors1. The idea now is to see if this guess enables us to derive an equation for ψ(x), the spatial part of the wave function.

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}e^{-iEt/\hbar} + V(x)\psi(x)e^{-iEt/\hbar} = i\hbar. - iE/\hbar e^{-iEt/\hbar}\psi(x) = E\psi(x)e^{-iEt/\hbar}.$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + (E - V(x))\psi(x) = 0$$

which is the time independent Schr¨odinger equation. We note here that the quantity E, which we have identified as the energy of the particle, is a free parameter in this equation. In other words, at no stage has any restriction been placed on the possible values for E. Thus, if we want to determine the wave function for a particle with some specific value of E that is moving in the presence of a potential V (x), all we have to do is to insert this value of E into the equation with the appropriate V (x), and solve for the corresponding wave function. In doing so, we find, perhaps not surprisingly, that for different choices of E we get different solutions for ψ(x). We can emphasize this fact by writing ψE(x) as the solution associated with a particular value of E. But it turns out that it is not all quite as simple as this. To be physically acceptable, the wave function ψE(x) must satisfy two conditions, one of which we have seen before namely that the wave function must be normalizable, and a second, that the wave function and its derivative must be continuous. Together, these two requirements, the first founded in the probability interpretation of the wave function, the second in more esoteric mathematical necessities which we will not go into here and usually only encountered in somewhat artificial problems, lead to a rather remarkable property of physical systems described by this equation that has enormous physical significance: the quantization of energy.

Possible 4 mark question

1. Explain the postulates of Bohr with regard to hydrogen atom.
2. Obtain Eigen values and Eigen functions.
3. Give a note on (i) Planck quantum hypothesis
4. Write a note on Einstein's theory of photoelectric effect.
5. Derive Schrödinger's time –dependent equation for matter waves.
6. Derive Schrödinger's time-independent equation for matter waves.
7. Give an informative account of dual nature of matter.
8. List out the limitations of classical mechanics and inadequacy of quantum mechanics.

Possible 10 mark question

1. Calculate the maximum wavelength that hydrogen in its ground state can absorb. What would be the next maximum wavelength?
2. Calculate the velocity and frequency of revolution of the electron of the Bohr hydrogen atom in its ground state?
3. Derive an expression for dependent equation of schrodingers.

KARPAGAM UNIVERSITY

DEPARTMENT OF PHYSICS

I M.Sc., PHYSICS

QUANTUM MECHANICS -I (17PHP202)

MULTIPLE CHOICE QUESTIONS

QUESTION	OPTION 1	OPTION 2	OPTION 3	OPTION 4	ANSWER
UNIT I					
The operator for energy is ____	iħ∂/∂t	-iħ∂/∂t	iħ∂/∂x	–iħv	iħ∂/∂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
If |P> = |A> + |B> then <P| is given by	<A|B>	<A| + |B>	<A| + <B|	|A> + |B>	<A| + <B|
The sum of the two bras is defined by its scalar product with any ket vector, as {<R|+<S|}|Q> which is given by	<R|Q|S>	<R|Q> + <S|Q>	<R|S|Q>	<R|S> <Q|	<R|Q> + <S|Q>
A state function can be expressed by a ____ in an infinite dimensional space by imagining an axis for each function ψ_i	row vector	state vector	column vector	ket vector	column vector
If the vector A and B are orthogonal, <A|B> =	0	1	-1	Infinity	0
If C is a complex number, and if |R> = C|A> then <R| is given by	C<A|	C|A>	C^*<A|	C^*|A>	C^*<A|
The set of eigen kets {|ψ_1>, |ψ_2>, |ψ_3> ….|ψ_n>….|ψ_m>} will be an orthonormal set of eigen kets if	<ψ_n|ψ_m> = 0	<ψ_n|ψ_m> = δ_{mn}	<ψ_n|ψ_m> = 1	|ψ_m><ψ_n| = 0	<ψ_n|ψ_m> = δ_{mn}
An operator A, which represents a dynamic variable, is said to be Hermitian, if, for two square integrable functions ψ and φ we have < φ | Aψ> equal to	<A|φ|ψ>	<φA|ψ>	< ψ|φ>A	<φ|ψ>A	<A|φ|ψ>
In Schrodinger picture, the state vector and operator are respectively	time dependent and time independent	time independent and time dependent	both time independent	both time dep	time independent and time dependent
In Heisenberg picture, the state vector and operator are	time dependent and time independent	time independent and time dependent	both time independent	both time dep	both time dependent
In interaction picture the state vector and operator are	time dependent and time independent	time independent and time dependent	both time independent	both time dependent	time independent and time dependent
The value of $[a, a^\dagger]$ is	zero	1	ħω	i ħ	zero
ket vectors are	column vectors	row vectors	rectangular vectors	square vectors	row vectors
Multiplying |Q><R| by an arbitrary |A> on the right, we get	<Q|R><A|	|Q><R|A>	<Q|R|A>	|Q><A|R>	|Q><A|R>
Every operator representing a dynamical variable must be a	column matrix	unit matrix	unitary	Hermitian	unitary
The operator for velocity is	i ħ∇/m	-i ħm∇	-i ħ∇/m	i ħm∇	-i ħm∇

The Hamiltonian operator in one dimension for the harmonic oscillator is	$H = p/2m + \frac{1}{2} k_x^2$	$H = p^2/2m + \frac{1}{2} k_x^2$	$H = p/2m + \frac{1}{2} k_x$	$H = p/2m - \frac{1}{2} k_x^2$	$H = p/2m + \frac{1}{2} k_x$
The zero point energy of a linear harmonic oscillator is	$\frac{1}{4} \hbar\omega$	$1/3\ \hbar\omega$	$\frac{1}{2} \hbar\omega$	$\hbar\omega$	$1/3\ \hbar\omega$
Discrete energy values of harmonic oscillator is given by	$E_n = (n - \frac{1}{2}) \hbar\omega_0$	$E_n = (n + \frac{1}{2}) \hbar\omega_0$	$E_n = n\hbar\omega_0$	$E_n = (n + 1) \hbar\omega_0$	$E_n = (n + \frac{1}{2}) \hbar\omega_0$
In Hilbert space, all infinite series occurring are	divergent	convergent	unchange	none of the above	none of the above
$\langle A\|B\rangle$ is equal to	$\langle B\|A\rangle$	$B\|A\rangle$	$A\langle B\|$	$\langle B\|A\rangle^*$	$\langle B\|A\rangle$
A ket vector $\|A\rangle$ is said to be ____ if $\langle A\|A\rangle = 1$	normalized	orthogonal	orthonormal	linear	orthogonal
The commutation relation $[x,P_x]$ yields	$\hbar$	$i\ \hbar$	$-i\ \hbar$	$\frac{1}{2} \hbar$	$i\ \hbar$
The operator is Hermitian if ____	$\int upv^* d\tau = \int puv^* d\tau$	$\int u^* pv d\tau = \int (pu)^* v d\tau$	$\int upv d\tau = \int pu^* v^* d\tau$	$\int u^* pv^* d\tau = \int puv d\tau$	$\int upv^* d\tau = \int puv^* d\tau$
The quantum mechanical operator for momentum is	$P = - i\hbar\nabla$	$P = i\hbar\nabla$	$P = \hbar\nabla$	$P = - \hbar\nabla$	$P = i\hbar\nabla$
The operator for kinetic energy is	$(\hbar^2 \nabla^2)/2m$	$-(\hbar^2 \nabla^2)/2m$	$(h^2\nabla^2)/2m$	$-(h^2\nabla^2)/2m$	$(h^2\nabla^2)/2m$
A bra and a ket vector are said to be orthogonal if their scalar product is	one	two	zero	infinity	zero
The relation for parity operator $\pi\psi(x)$ is	$\psi(x)$	$\pi\psi(x)$	$\psi(-x)$	$\pi\psi(-x)$	$\psi(x)$
Hermitian operators have ____ eigen values	real	imaginary	complex	infinity	complex
If two Hermitian operators operators commute, then their product is	unitary	inverse	Hermitian	Identity	Identity
The commutation relation $[x,H]$ yields	$-i\hbar p$	$i\hbar p$	$(-i\hbar/m)p$	$(i\hbar/m)p$	$-i\hbar p$
The commutation relation $[p,H]$ yields	$- i\hbar k_x$	$i\hbar k_x$	$(-i\hbar/m)k_x$	$(i\hbar/m)k_x$	$i\hbar k_x$
If a is lowering operator and $a^\dagger$ raising operator then $aa^\dagger$ is	$H/\hbar\omega_o - \frac{1}{2}$	$H/\hbar\omega_o + \frac{1}{2}$	1	0	$H/\hbar\omega_o - \frac{1}{2}$
If a is lowering operator and $a^\dagger$ raising operator then $a^\dagger a$ is	$H/\hbar\omega_o - \frac{1}{2}$	$H/\hbar\omega_o + \frac{1}{2}$	1	0	$H/\hbar\omega_o + \frac{1}{2}$
If $\|a\rangle$ and $\|b\rangle$ are arbitrary kets then $[\|a\rangle\langle b\|]^*$ is	$\langle a\|b\rangle$	$\|b\rangle\langle a\|$	$[\|a\rangle\langle b\|]^*$	$\|a\rangle\langle b\|$	
If A and B are unitary operators, then the product is	Hermitian	Unitary	Hamiltonian	Inverse	Hermitian
The expectation value of observable p in state ψ is	$\langle p\rangle = \int \psi^* p\psi d\tau$	$\langle p\rangle = \int \psi p\psi^* d\tau$	$\langle p\rangle = \int \psi^* \psi d\tau$	$\langle p\rangle = \int \psi p\psi^* d\tau$	$\langle p\rangle = \int \psi p\psi^* d\tau$
In bra and ket space, any complete bracket expression denotes a	vector	number	operator	space	vector
In bra and ket space, any incomplete bracket expression denotes a	vector	number	operator	space	operator
The development of classical mechanics is mainly based on	Planck's radiation law	Bohr's quantum theory of H atom	Newton's three laws of motion	Kepler's laws	Kepler's laws
Classical mechanics could not explain	Spectrum of black body radiation	Stability of atoms	Intensity of Stokes and Anti Stokes lines of Raman lines	All the above	Spectrum of black body radiation
Old quantum theory explains _____	particle in a box	Pauli's exclusion principle	Spectral lines of hydrogen molecule	Spin of the electrons	Spectral lines of hydrogen molecule
The quantum concept was introduced by ____	Schrodinger	Bohr	Planck	Einstein	Planck
The idea of dual nature of light was proposed by	Plank	De Broglie	Einstein	Maxwell	Einstein
The value of Plank's constant is	$6.62 \text{ X } 10^{-34}\ JS^2$	$6.62 \text{ X } 10^{-31}\ JS$	$6.62 \text{ X } 10^{-34}\ JS$	$6.62 \text{ X } 10^{-31}\ JS^2$	$6.62 \text{ X } 10^{-31}\ JS^2$

Wave mechanics described the behaviour of	atomic system	interaction with other particles	electromagnetic radiation	all the above	atomic system
The wave equation for a moving particle is represented by	$\nabla^2\psi + (1/v^2)\ \partial^2 \psi/\partial t = 0$	$\nabla^2\psi - (1/v^2\ \partial^2\psi/\partial t^2 = 0$	$\nabla^2\psi + (v^2\ \partial^2\psi/\partial t^2 = 0$	$\nabla^2\psi - (v^2\ \partial^2\psi/\partial t^2 = 0$	$\nabla^2\psi - (1/v^2)\ \partial^2\psi/\partial t^2 = 0$
The equation which describes the motion of a non-relativistic material particle is	$H\psi + E\psi = 0$	$H\psi = E\psi$	$H\psi = -i\hbar\partial\psi/\partial t$	$H\psi = (1/i\hbar)\partial\psi/\partial t$	$H\psi = -i\hbar\partial\psi/\partial t$
The state functions in the Hilbert space are called as	linear vectors	state vectors	basis vectors	complex vectors	linear vectors
The state functions in the Hilbert space are represented by	column vector	basis vector	linear vector	all the above	linear vector
The change of basis from one ortho-normal set to another in Dirac notation is expressed as	$\langle p\vert = \langle n\vert\langle n\vert p\rangle$	$\langle p\vert = \langle n\vert p\rangle$	$\vert p\rangle = \vert n\rangle\langle n\vert p\rangle$	$\vert p\rangle = \langle n\vert p\rangle$	$\langle p\vert = \langle n\vert\langle n\vert p\rangle$
If the condition pc = cp is satisfied then the operator p is said to be	Hermitian	Unitary	Inverse	Linear	Hermitian
The eigen functions of Hermitian operators belonging to different eigen values are	orthogonal	normalized	orthogonal and normalized	neither orthogonal nor normalized	orthogonal and normalized
The expectation value of operator in Schrödinger picture is such that	$\partial/\partial t \langle A_s\rangle = 0$	$\partial/\partial t \langle A_s\rangle = 1$	$\partial/\partial t \langle A_s\rangle = H$	$\partial/\partial t \langle A_s\rangle = -1$	$\partial/\partial t \langle A_s\rangle = 0$
In harmonic oscillator problem, the matrix for ‘a’ contains	only upper diagonal elements	only lower diagonal elements	only diagonal elements	both upper and lower diagonal elements	only lower diagonal elements
In harmonic oscillator problem, the matrix for ‘$a^\dagger$’ contains	only upper diagonal elements	only lower diagonal elements	only diagonal elements	both upper and lower diagonal elements	only diagonal elements
In harmonic oscillator problem, the matrix for H contains	only upper diagonal elements	only lower diagonal elements	only diagonal elements	both upper and lower diagonal elements	only upper diagonal elements

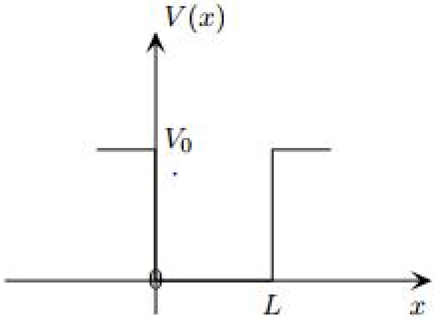
UNIT-II

SYLLABUS

One dimensional potential well: Square-well potential with finite walls – Square-well potential with rigid walls- Square-well potential barrier – Alpha emission – Bloch waves in a periodic potential – Linear harmonic oscillator (Schrodinger method and operator method) – Free particle.

The Finite Potential Well

The infinite potential well is a valuable model since, with the minimum amount of fuss, it shows immediately the way that energy quantization as potentials do not occur in nature. However, for electrons trapped in a block of metal, or gas molecules contained in a bottle, this model serves to describe very accurately the quantum character of such systems. In such cases the potential experienced by an electron as it approaches the edges of a block of metal, or as experienced by a gas molecule as it approaches the walls of its container are effectively infinite as far as these particles are concerned, at least if the particles have sufficently low kinetic energy compared to the height of these potential barriers. But, of course, any potential well is of finite depth, and if a particle in such a well has an energy comparable to the height of the potential barriers that define the well, there is the prospect of the particle escaping from the well. This is true both classically and quantum mechanically, though, as you might expect, the behaviour in the quantum mechanical case is not necessarily consistent with our classical physics based expectations. Thus we now proceed to look at the quantum properties of a particle in a finite potential well.



Square-well potential with rigid walls

In quatum mechanics, the particle in a box model (also known as the infinite potential well or the infinite square well) describes a particle free to move in a small space surrounded by impenetrable barriers. The model is mainly used as a hypothetical example to illustrate the differences between classical and quantum systems. In classical systems, for example, a ball trapped inside a large box, the particle can move at any speed within the box and it is no more likely to be found at one position than another. However, when the well becomes very narrow (on the scale of a few nanometers), quantum effects become important. The particle may only occupy certain positive energy levels. Likewise, it can never have zero energy, meaning that the particle can never "sit still". Additionally, it is more likely to be found at certain positions than at others, depending on its energy level. The particle may never be detected at certain positions, known as spatial nodes.

The particle in a box model is one of the very few problems in quantum mechanics which can be solved analytically, without approximations. Due to its simplicity, the model allows insight into quantum effects without the need for complicated mathematics. It serves as a simple illustration of how energy quantization, which are found in more complicated quantum systems such as atoms and molecules, come about. It is one of the first quantum mechanics problems taught in undergraduate physics courses, and it is commonly used as an approximation for more complicated quantum systems.

The simplest form of the particle in a box model considers a one-dimensional system. Here, the particle may only move backwards and forwards along a straight line with impenetrable barriers at either end. The walls of a one-dimensional box may be visualised as regions of space with an infinitely large potential energy. Conversely, the interior of the box has a constant, zero potential energy. This means that no forces act upon the particle inside the box and it can move freely in that region. However, infinitely large forces repel the particle if it touches the walls of the box, preventing it from escaping. The potential energy in this model is given as

$$V(x) = \begin{cases} 0, & x_c - \frac{L}{2} < x < x_c + \frac{L}{2}, \\ \infty, & \text{otherwise,} \end{cases}$$

where L is the length of the box, x_c is the location of the center of the box and x is the position of the particle within the box. Simple cases include the centered box ($x_c = 0$) and the shifted box ($x_c = L/2$).

Position wave function

In quantum mechanics, the wavefunction gives the most fundamental description of the behavior of a particle; the measurable properties of the particle (such as its position, momentum and energy) may all be derived from the wavefunctionThe wavefunction can be found by solving the Schrödinger equation for the system

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t)$$

where is the reduced Planck constant, is the mass of the particle, is the imaginary unit and is time.

Inside the box, no forces act upon the particle, which means that the part of the wavefunction inside the box oscillates through space and time with the same form as a free particle

$$\psi(x,t) = [A\sin(kx) + B\cos(kx)]\mathrm{e}^{-i\omega t}.$$

where and are arbitrary complex numbers. The frequency of the oscillations through space and time is given by the wavenumber and the angular frequency respectively. These are both related to the total energy of the particle by the expression

$$E = \hbar\omega = \frac{\hbar^2 k^2}{2m},$$

which is known as the dispersion relation for a free particle.[1] Here one must notice that now, since the particle is not entirely free but under the influence of a potential (the potential *V* described above), the energy of the particle given above is not the same thing as where *p* is the momentum of the particle, and thus the wavenumber *k* above actually describes the energy states of the particle, not the momentum states (i.e. it turns out that the momentum of the particle is not given) In this sense, it is quite dangerous to call the number *k* a wavenumber, since it is not related to momentum like "wavenumber" usually is. The rationale for calling *k* the wavenumber is that it enumerates the number of crests that the wavefunction has inside the box, and in this sense it is a wavenumber. This discrepancy can be seen more clearly below, when we find out that the energy spectrum of the particle is discrete (only discrete values of energy are allowed) but the momentum spectrum is continuous (momentum can vary continuously) and in particular, the relation for the energy and momentum of the particle does not hold. As said above, the reason this relation between energy and momentum does not hold is that the particle is not free, but there is a potential *V* in the system, and the energy of the particle is E=T+V where *T* is the kinetic and *V* the potential energy.

Particle Scattering by a Barrier

It is manifestly an eigenvalue problem since the solution can be found only at discrete values of E. The electron is trapped inside the box. However, in an open region problem where the electron is free to roam, the energy of the electron E can be arbitrary. We can assume that the potential pro_le is such that V (x) = 0 for x < 0 while

$$V(x) = V_o$$

for x > 0. The energy of the electron is such that 0 < E < V. On the left side, we assume an electron coming in from with the wavefunction described by Aexp(ik_{1x}). When this wavefunction hits the potential barrier, a reected wave will be present, and the general solution on the left side of the barrier is given by

$$\psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$$

E is the kinetic energy of the incident electron. On the right side, however, the Schrodinger equation to be satisfied is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi_2(x) = (E - V_0)\psi_2(x)$$

The solution of the transmitted wave on the right is

$$\psi_2(x) = A_2 e^{ik_2 x}$$

$$k_2 = \sqrt{2m(E - V_0)}/\hbar$$

Given the known incident wave amplitude A_1,we can match the boundary conditions at x = 0 to find the reacted wave amplitude B_1 and the transmitted wave amplitude A_1, By eyeballing the Schrodinger equation we can arrive at the requisite boundary conditions, continuous at x = 0.is pure imaginary, and the wave is evanescent and decays when x .This effect is known as tunneling.

The electron as a nonzero probability of being found inside the barrier, albeit with decreasing probability into the barrier. The larger V, Since E < $V_{0,}$ k_2 is compared to E, the more rapidly decaying is the wavefunction into the barrier. However, if the electron is energetic enough so that

E > V_o,k_2 becomes real, and then the wavefunction is no more evanescent. It penetrates into the barrier; it can be found even long way from the boundary. It is to be noted that the wavefunction in this case cannot be normalized as the above represents situation of an electron roaming over infinite space. The above example illustrates the wave physics at the barrier., k becomes real, and then the wavefunction is no more evanescent. It penetrates into the barrier; it can be found even a long way from the boundary.

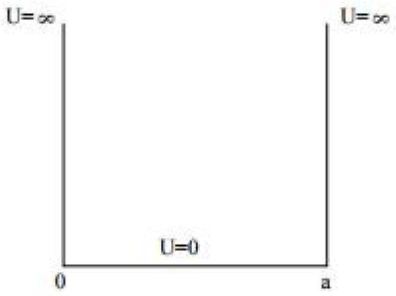
Square-well potential with finite walls

As a first application of the Schrödinger equation, we use it to redeliver the allowed energies of a particle in a rigid box and check that we get the same answers as before. We start by identifying the potential energy function U(x). Inside the box the potential energy is zero, and outside the box it is infinite. Thus

$$U(x) = \begin{cases} 0 & \text{for } 0 \le x \le a \\ \infty & \text{for } x < 0 \text{ and } x > a \end{cases}$$

This potential energy function is often described as an infinitely deep square well because a graph of U(x) looks like a well with infinitely high sides and square corners

Since U(x) = ∞ outside the box, the particle can never be found there, so ψ(x) must be zero outside the box, i.e., when x < 0 and when x > a. The continuity of ψ(x) requires



that

$$\psi(0) = \psi(a) = 0$$

Inside the box, where $U(x) = 0$, the Schroedinger equation reduces to

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \qquad \text{for } 0 \leq x \leq a$$

Introducing the shorthand notation:

$$\psi' = \frac{d\psi}{dx} \qquad and \qquad \psi'' = \frac{d^2\psi}{dx^2}$$

yields

$$\psi''(x) = -\frac{2mE}{\hbar^2}\psi(x)$$

Show that no solutions have negative energy: If $E < 0$, the coefficient

$$\alpha = \frac{\sqrt{-2mE}}{\hbar}$$

$$\psi''(x) = \alpha^2\psi(x)$$

This is a second order differential equation which has the solutions exp(αx) and exp(−αx) or any combination of these:

$$\psi(x) = Ae^{\alpha x} + Be^{-\alpha x}$$

is also a solution for any constants A and B. In addition, given 2 independent solutions, ψ1(x) and ψ2(x), every solution can be expressed as a linear combination of the form . So, if by any means, we can spot 2 independent solutions, we are assured that every solution is a linear combination of these two. Having 2 arbitrary constants, A and B, comes from the following consideration. The differential equation has a second derivative ψ ″(x). To find ψ(x), one has to effectively do 2 integrations which produces 2 constants of integration. The 2 arbitrary constants correspond to these 2 constants of integration. Since e αx and e −αx are independent solutions of , it follows that the most general

$$\psi(x) = A\psi_1(x) + B\psi_2(x)$$

$$A + B = 0$$

while ψ(a) = 0 implies that

$$Ae^{\alpha a} + Be^{-\alpha a} = 0$$

The only way to satisfy these 2 conditions is A = B = 0. So if E < 0, then the only solution of the Schroedinger equation is ψ = 0. So if E < 0, then there can be no standing waves and so negative values of the energy E are not allowed. A similar argument gives the same conclusion for E = 0.

Alpha emission

In a series of seminal experiments Ernest Rutherford and his collaborators established the important features of alpha decay. The behavior of the radiations natural sources of uranium and thorium and their daughters was studied in magnetic and electric fields. The least penetrating particles, labeled "α-rays" because they were the first to be absorbed, were found to be positively charged and quite massive in comparison to the more penetrating egatively charged "β--rays" and the most penetrating neutral "γ--rays." In a subsequent experiment the α--rays from a needle--like source were collected in a very small concentric discharge tube and the emission spectrum of helium was observed in the trapped volume. Thus, alpha rays were proven to be energetic helium nuclei. The α particles are the most ionizing radiation emitted by natural sources (with the extremely rare exception of the spontaneous fission of uranium) and are stopped by as little as a sheet of paper or a few centimeters of air. The particles are quite energetic, (E_o =4-9MeV), but interact very strongly with electrons as they penetrate into material and stop within 100 μm in most materials.

Understanding these features of α decay allowed early researchers to use the emitted α--particles to probe the structure of nuclei in scattering experiments and later, by reaction with beryllium, to produce neutrons. In an interesting dichotomy, the α--particles from the decay of natural isotopes of uranium, radium and their daughters have sufficient kinetic energies to overcome the Coulomb barriers of light elements and induce nuclear reactions but are not energetic enough to induce reactions in the heaviest elements.

$$^{A}_{Z}(Z)_{N} \rightarrow {}^{A-4}_{Z-2}(X)^{2-}_{N-2} + {}^{4}_{2}He^{2+}_{2} + Q_{\alpha}$$

where we have chosen to write out all of the superscripts and subscripts.

Thus the α-decay of 238U can be written

$$^{238}U \rightarrow {}^{234}Th^{2-} + {}^{4}He^{2+} + Q$$

The Qα-value is positive (exothermic) for spontaneous alpha decay. The helium nucleus emerges with a substantial velocity and is fully ionized, and the atomic electrons on the daughter are disrupted by the sudden change but the whole process conserves electrical charge. We can rewrite the equation in terms of the masses of the neutral atoms: and then calculate the Qα---value because the *net* change in the atomic binding energies (~65.3 Z7/5 --- 80 Z2/5 eV) is very small compared to the nuclear decay energy.

The semi-empirical mass equation, the emission of an α---particle lowers the Coulomb energy of the nucleus, which increases the stability of heavy nuclei while not affecting the overall binding energy per nucleon because the tightly bound α---particle has approximately the same binding energy/nucleon as the original nucleus.

Two important features of alpha decay are that the energies of the alpha particles known to generally increase with the atomic number of the parent but energy of the emitted particle is less than that of the Coulomb barrier in the reverse reaction between the α---particle and the daughter nucleus. In addition, all nuclei with mass numbers greater than A»150 are thermodynamically unstable against alpha emission (Qα is positive) but alpha emission is the dominant decay process only for the heaviest nuclei, A>210. The energies of the emitted α---particles can range from 1.8 MeV (144Nd) to 11.6 MeV (212Pom) with the half---life of 144Nd being 5x1029 times as long as that of 212Pom. Typical heavy element alpha decay energies are in the range from 4---9 MeV, as noted earlier.

In general, alpha decay leads to the ground state of the daughter nucleus so that the emitted particle carries away as much energy as possible and as little angular momentum as possible. The ground state spins of even---even parents and daughters (including the alpha particle, of course) are zero which makes alpha particle emission the most likely process for these nuclei. Small branches are seen to higher excited states but such processes are strongly suppressed. Some decays of odd---A heavy nuclei populate low---lying excited states that match the spin of the parent so that the orbital angular momentum of the α particle can be zero. For example, the strongest branch (83%) of the alpha decay of

249Cf goes to the 9th excited state of 245Cm because this is the lowest lying state with the same spin and parity as that of the parent. Alpha decay to several different excited states of a daughter nucleus is called *fine structure*; α---decay from an excited state of a parent nucleus to the ground state of the daughter nucleus is said to be *long range alpha emission* because these α---particles are more energetic and thus have longer ranges in matter. The most famous case of long range α---emission is that of 212Pom where a 45 s isomeric level at 2.922 MeV decays to the ground state of 208Pb by emitting a 11.65 MeV α-particle.

We will consider the general features of alpha emission and then we will describe them in terms of a simple quantum mechanical model. It turns out that α emission is a beautiful example of the quantum mechanical process of tunneling through a barrier that is forbidden in classical mechanics. Alpha particles played an important role in nuclear physics before the invention of charged particle accelerators and were extensively used in research. Therefore, the basic features of alpha decay have been known for some time.

Bloch waves in a periodic potential:

The eigenstates ψ of the Hamitonian Hˆ above can be chosen to have the form of a plane wave times a function with the periodicity of the Bravais lattice

$$\psi_{n}k\,(r) = e^{ik\cdot r}u_{n}k\,(r)$$

$$u_{n}k\,(r + R) = u_{n}k\,(r)$$

The quantum number n is called the band index and takes numbers n = 1, 2, 3, . . . This quantum number corresponds to the appearance of independent eigenstates of different energies but with the same k, as will be shown later.

An alternative formulation of Bloch's theorem is that the eigenstates of Hˆ can be chosen so that associated with each ψ is a wave vector k such that

$$\psi(r + R) = e^{ik\cdot R}\psi(r)$$

Born – von Karman boundary condition

Apply boundary condition of macroscopic periodicity. Generalize to volume commensurate with underly- ing Bravais lattice:

$\psi(r + N_i a_i) = \psi(r), \qquad i = 1, 2, 3$

where a_i are the primitive vectors and N_i are integers of order $N^{1/3}$ where $N = N_1 N_2 N_3$ is the total number of primitive cells in the crystal. The quantum number k can be composed from the reciprocal lattice vectors with (non-integer) coefficients

$$x_i ,k = x_1 b_1 + x_2 b_2 + x_3 b_3$$

Since $a_i \cdot b_j = 2\pi\delta_{ij}$ the Bloch theorem then gives $e^{i/2xiNi} = 1$. Thus, $x_i = m_i/N_i$ and the allowed Bloch wave vectors are given by

with m_i integers. For a simple cubic Bravais lattice, the allowed wave vector components reduce to the earlier $k_X = 2\pi m_X/L$ etc., since $N_i = L/a$ and $b_X = (2\pi/a)\hat{x}$ etc.

Linear Harmonic Oscillator

The linear harmonic oscillator is described by the Schrodinger equation

$$i\hbar\,\partial_t\,\psi(x,t) \;=\; \hat{H}\,\psi(x,t)$$

for the Hamiltonian

$$\hat{H} \;=\; -\,\frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial x^2} \;+\; \frac{1}{2}m\,\omega^2 x^2\;.$$

It comprises one of the most important examples of elementary Quantum Mechanics. There are several reasons for its pivotal role. The linear harmonic oscillator describes vibrations in molecules and their counterparts in solids, the phonons. Many more physical systems can, at least approximately, be described in terms of linear harmonic oscillator models. However, the most eminent role of this oscillator is its linkage to the boson, one of the conceptual building blocks of microscopic physics. For example, bosons describe the modes of the electromagnetic field, providing the basis for its quantization. The linear harmonic oscillator, even though it may represent rather non-elementary objects like a solid and a molecule, provides a window into the most elementary structure of the physical world. The most likely reason for this connection with fundamental properties of matter is that the harmonic oscillator Hamiltonian.

Its propagator, the motion of coherent states, and its stationary states. In the present the approach the harmonic oscillator in the framework of the Schrodinger equation. The important role of the harmonic oscillator certainly justifies an approach from two perspectives, i.e., from the path integral (propagotor) perspective and from the Schrodinger equation perspective. The path integral approach gave us a direct route to study time-dependent properties, the Schrodinger equation approach is suited particularly for stationary state properties. Both approaches, however, yield the same stationary states and the same propagator, as we will demonstrate below. The Schrodinger equation approach will allow us to emphasize the algebraic aspects of quantum theory. This Section will be the first in which an algebraic formulation will assume center stage. In this respect the material presented provides an important introduction to later Sections using Lie algebra methods to describe more elementary physical systems. Due to the pedagodical nature of this Section we will link carefully the algebraic treatment with the differential equation methods used so far in studying the Schrodinger equation description of quantum systems. In the following we consider first the stationary states of the linear harmonic oscillator and later consider the propagator which describes the time evolution of any initial state. The stationary states of the harmonic oscillator have been considered already in Chapter 2 where the corresponding wave functions

$$\hat{H}\,\varphi_E(x) = E\,\varphi_E(x)$$

Due to the nature of the harmonic potential which does not allow a particle with finite energy to move to arbitrary large distances, all stationary states of the harmonic oscillator must be bound states and, therefore, the natural boundary conditions apply

$$\lim_{x \to \pm\infty} \phi_E(x) = 0 .$$

can be solved for any $E \in R$ however, only for a discrete set of E values can the boundary conditions, be satisfied.

Free particle

Free particle is a particle that, in some sense, is not bound by an external force, or equivalently not in a region where its potential energy varies. In classical physics, this means the particle is present in a "field-free" space. In quantum mechanics, it means a region of uniform potential, usually set to zero in the region of interest since potential can be arbitrarily set to zero at any point (or surface in three dimensions) in space.

A free particle in non-relativistic quantum mechanics is described by the free Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\ \psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)$$

where ψ is the wavefunction of the particle at position **r** and time *t*. The solution for a particle with momentum **p** or wave vector **k**, at angular frequency ω or energy *E*, is given by the complex plane wave

$$\psi(\mathbf{r},t) = Ae^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} = Ae^{i(\mathbf{p}\cdot\mathbf{r}-Et)/\hbar}$$

with amplitude *A*. As for *all* quantum particles free *or* bound, the Heisenberg uncertainty principles

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}, \quad \Delta E \Delta t \geq \hbar$$

$$\mathbf{p} = \hbar\mathbf{k}, \quad E = \hbar\omega$$

Since the potential energy is (set to) zero, the total energy *E* is equal to the kinetic energy, which has the same form as in classical physics

$$E = T \ \rightarrow\ \frac{\hbar^2 k^2}{2m} = \hbar\omega$$

Possible 6 marks

1. Explain alpha emission in detail.
2. Derive the Schrödinger relation for a linear harmonic oscillator. Discuss the significance of zero Point energy.
3. Obtain the solution of wave equation in one dimension for a particle moving in a constant potential field with finite walls.
4. Explain the concept free particle.
5. Explain square well potential barrier.
6. Explain the Bloch waves in a periodic potential.

Possible 10 marks

1. Calculate the maximum wavelength that hydrogen in its ground state can absorb. What would be the next maximum wavelength?
2. Solve the time-independent Schrödinger equation for a three dimensional harmonic oscillator whose potential energy is $V= \frac{1}{2} (k_1x^2 + k_2y^2+ k_3z^2)$.
3. Write the Schrödinger equation and the form of the wave function in the different regions of a square well with rigid rotator.
4. Briefly discuss how the particles are interacting in a system.

KARPAGAM UNIVERSITY
DEPARTMENT OF PHYSICS
I M.Sc., PHYSICS
QUANTUM MECHANICS -I (17PHP202)
MULTIPLE CHOICE QUESTIONS

UNIT II

QUESTION	OPTION 1	OPTION 2	OPTION 3	OPTION 4	ANSWER
The eigen value of a Hamiltonian is important because it gives of the system	energy	position	momentum	acceleration	energy
The Hamiltonian is a	energy operator	momentum operator	position operator	none	momentum operator
Which of the following statement is not true?	According to classical mechanics,	According to classical mechani	According to quantum mechani	All the statements are wrong	According to quantum mechanics a particle can penetrate a barrier
In a one dimensional square well potential, the wave function of the particle in the level n has ----	n^2 nodes	n-1 nodes	n nodes	only one node.	n-1 nodes
According to classical theory, a particle confined in a box _____	cannot have zero energy	can have zero energy	can have only a fixed non zero	can have any value of energy	cannot have zero energy
According to quantum mechanics, a particle confined in a box _____	cannot have zero energy	can have zero energy	can have only a fixed non zero	can have any value of energy	cannot have zero energy
Zero point energy is the energy of the particle -----	when it is in the ground state	when the particle is at rest	when the particle is in the botto	particle in excited state	when the particle is at rest
The wave function of particle in a square potential well with infinite wall is ____ at the boundary	Infinity	zero	some non-zero finite value	can be anything	some non-zero finite value
The wave function of a particle in a square potential well with finite wall is ____ at the boundary	infinity	zero	some non-zero finite value	can be anything	some non-zero finite value
Non-zero wave function in the boundary means ____	There is no chance of finding the p	There is infinite probability tha	there is a finite probability that	does not have any physical signifi	There is infinite probability that the particle is in the barrier
The probability of finding the particle inside the potential barrier, when the particle is in a potential well with f	barrier penetration	quantum mechanical tunneling	uncertainty of the particle’s spa	zero point energy	uncertainty of the particle’s space coordinates
For a given particle in a square potential well, the number of bound states depend on the	height of the potential well only	width of the potential well alon	height and width of the potentia	completely independent of the hei	height of the potential well only
The probability that a particle may penetrate through a potential barrier, which is higher than its energy E, is c	quantum mechanical tunneling	barrier penetration	uncertainty principle	zero point energy	barrier penetration
Quantum mechanical tunneling can be explained only with ____	particle nature of matter	wave nature of matter	mass of the particle	volume of the particle.	mass of the particle
Emission of alpha particle from the nucleus is explained using	uncertainty principle	particle nature of matter	quantum mechanical tunneling	schroedinger equation	None of the above
It is estimated that the alpha particle moves inside a nucleus with velocity of the order of ____	10^{-7} m/s	10^{21}m/s	10^{-21} m/s	10^{7} m/s	10^{-21} m/s
Bloch theory gives explanation of	a single one dimensional potential	a single three dimensional poter	a single square potential barrier	periodic potential barrier, which r	a single one dimensional potential well
The approximation of a periodic potential well to that of a series of square potential barrier is called	Kronig Pennie model	Bloch equation	Quantum mechanical tunneling	Fermi golden rule	Bloch equation
The potential energy of a linear harmonic oscillator is ___	kx^2	$\frac{1}{2} kx^2$	$–kx^2$	$-1/2\ kx^2$	$-1/2\ kx^2$
In the case of linear harmonic oscillator the potential is ___	a constant	a linearly increasing quantity	a linearly decreasing quantity	proportional to x^2	proportional to x^2
The energy eigen value of a linear harmonic oscillator, according to quantum mechanics is ____	$E_n = n \hbar\omega$	$E_n = (n-1/2) \hbar\omega$	$E_n = (n+1) \hbar\omega$	$E_n = (n+1/2) \hbar\omega$	$E_n = (n+1/2) \hbar\omega$
The energy of a linear harmonic oscillator according to quantum theory is ___	$E_n = n \hbar\omega$	$E_n = (n-1/2) \hbar\omega$	$E_n = (n+1) \hbar\omega$	$E_n = (n+1/2) \hbar\omega$	$E_n = n \hbar\omega$
The difference between the energy of the linear harmonic oscillator, in the case of quantum theory and quantun	the energy possessed by the partic	the energy possessed by the par	the energy possessed by the par	the energy possessed by the partic	the energy possessed by the particle by virtue of its motion
The zero point energy of a linear harmonic oscillator is given by	$\hbar\omega$	$– \hbar\omega$	$\frac{1}{2} \hbar\omega$	$- \frac{1}{2} \hbar\omega$	$\hbar\omega$
If $y^2 = (m\omega/\hbar^2).x^2$, the Hermite polynomial for n=0, for a linear harmonic oscillator is ---	1	2y	$4y^2 – 2$	$8y^3 – 12y$	2y
If $y^2 = (m\omega/\hbar^2).x^2$, the Hermite polynomial for n=1, for a linear harmonic oscillator is ---	1	2y	$4y^2 – 2$	$8y^3 – 12y$	$4y^2 – 2$
If $y^2 = (m\omega/\hbar^2).x^2$, the Hermite polynomial for n=2, for a linear harmonic oscillator is ---	1	2y	$4y^2 – 2$	$8y^3 – 12y$	$8y^3 – 12y$
If $y^2 = (m\omega/\hbar^2).x^2$, the Hermite polynomial for n=3, for a linear harmonic oscillator is ---	1	2y	$4y^2 – 2$	$8y^3 – 12y$	1
The commutation relation between the position coordinate x and the momentum p is given by	$i\hbar$	$- i\hbar$	$\frac{1}{2} i\hbar$	$-1/2\ i\hbar$	$i\hbar$
An annihilation operator *a* _______ the energy of the particle by ___	reduces, by $\hbar\omega$	increases, by $- \hbar\omega$	increases, by $\hbar\omega$	reduces, by $– \hbar\omega$	increases, by $\hbar\omega$
A creation operator $a^\dagger$ _____ the energy of the particle by ___	reduces, by $\hbar\omega$	increases, by $- \hbar\omega$	increases, by $\hbar\omega$	reduces, by $– \hbar\omega$	reduces, by $– \hbar\omega$
An electron is in the ground state (lowest energy level) of an infinite well where its energy is 5.00 eV. In the next high	20 eV	1.25 eV	12.5 eV	125 eV	20 eV
An electron is in an infinite square well that is 9.6-nm wide. The electron makes the transition from then = 14 to then	3400 nm	4100 nm	2800 nm	4700 nm	4100 nm
An electron is in an infinite square well that is 8.9-nm wide. The ground state energy of the electron is closest to	0.0066 eV	0.0085 eV	0.0057 eV	0.0047 eV	0.0047 eV
The wave function for a particle must be normalizable because	the particle’s charge must be conserv	the particle’s momentum must be	the particle cannot be in two plac	the particle must be somewhere	the particle must be somewhere

Which of the following terms refers to the molecular modelling computational method that uses equations obeying the	Quantum mechanics	Molecular calculations	Molecular mechanics	Quantum theory	Molecular mechanics
Which of the following terms refers to the molecular modelling computational method that uses quantum physics?	Quantum mechanics	Molecular calculations	Molecular mechanics	Quantum theory	Quantum mechanics
Which of the following statements is true?	Energy minimisation is carried out u	Energy minimisation is used to fi	Energy minimisation is carried ou	Energy minimisation stops when a s	Energy minimisation is used to find a stable conformation for a molecule.
Which of the following is a limitation of the Bohr Model of the atom?	It does not explain atomic spectra	It successfully predicts the intensi	The model only applies to Hydrog	The model only applies to light ator	The model only applies to Hydrogen like atoms
The Compton Effect supports which of the following theories?	Special Theory of Relativity	Light is a wave	Thomson model of the atom	Light is a particle	Light is a particle

UNIT-III

SYLLABUS

Three dimensional potential Well: Particle moving in a spherically symmetric potential – System of two interacting particles – Rigid rotator – Hydrogen atom –– Three-dimensional square-well potential - Deutron

Matrix mechanics: Matrix representation of wave function – Matrix representation of operator – Properties of matrix elements – Schroedinger equation in matrix form –Unitary Transformations – Linear harmonic oscillator.

Particle moving in a spherically symmetric potential – System of two interacting particles

An important problem in quantum mechanics is that of a particle in a spherically symmetric potential, i.e., a potential that depends only on the distance between the particle and a defined center point. In particular, if the particle in question is an electron and the potential is derived from Coulomb's law, then the problem can be used to describe a hydrogen-like (one-electron) atom (or ion).

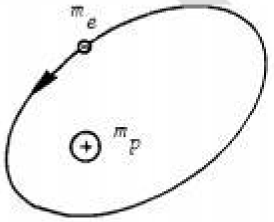
In the general case, the dynamics of a particle in a spherically symmetric potential are governed by a Hamiltonian of the following form:

$$\hat{H} = \frac{\hat{p}^2}{2m_0} + V(r)$$

where is the mass of the particle, is the momentum operator, and the potential depends only on, the modulus of the radius vector r. The quantum mechanical wavefunctions and energies (eigenvalues) are found by solving the Schrödinger equation with this Hamiltonian. Due to the spherical symmetry of the system, it is natural to use spherical coordinates and When this is done, the time-independent Schrödinger equation for the system is separable, allowing the angular problems to be dealt with easily, and leaving an ordinary differential equation in to determine the energies for the particular potential

Hydrogen Atom

The simplest of all atoms is the Hydrogen atom, which is made up of a positively charged proton with rest mass mp = 1.6726231 × 10−27 kg, and a negatively charged electron with rest mass me = 9.1093897 × 10−31 kg. Therefore, the hydrogen atom is the only atom which consists of only two particles. This makes an analytical solution of both the classical as well as the quantum mechanical dynamics of the hydrogen atom possible. All other atomes are composed of a nucleus and more than one electron. According to the Bohr-Somerfeld model of hydrogen, the electron circles the proton on a planetary like orbit, see Figure 4.8.The stationary Schroedinger Equation for the Hydrogen atom is



$$\Delta\psi(\vec{r}) + \frac{2m_0}{\hbar^2}\left(E - V(\vec{r})\right)\ \psi(\vec{r}) = 0$$

The potential is a Coulomb potential between the proton and the electron such that

$$V(\vec{r}) = -\frac{e_0^2}{4\pi\varepsilon_0\ |\vec{r}|}$$

and the mass is actually the reduced mass

$$m_0 = \frac{m_p\ \cdot\ me}{m_p + m_e}$$

that arises when we transform the two body problem between electron and proton into a problem for the center of mass and relative coordinate motion. Due to the large, but finite, mass of the proton, i.e. the proton mass is 1836 times the electron mass, both bodies circle around a common center of mass. The center of mass is very close to the position of the proton and the reduced mass is almost identical to the proton mass. Due to the spherical symmetry of the potential the use of spherical coordinates is advantageous

$$\Delta\psi = \frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial\psi}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2\psi}{\partial\varphi^2}\right]$$

We will derive separate equations for the radial and angular coordinates by assuming trial solutions which are products of functions only depending on one of the coordinates r , ϑ , or ϕ

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(\frac{2m_0E}{\hbar^2} + \frac{m_0e_0^2}{2\pi\varepsilon_0\hbar^2 r} - \frac{\alpha}{r^2}\right)R = 0 \quad ,$$

the azimuthal equation

$$\frac{1}{\sin\vartheta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\theta}{d\vartheta}\right) + \left(\alpha - \frac{m^2}{\sin^2\vartheta}\right)\theta = 0 \quad ,$$

and the polar equation

$$\frac{d^2\phi}{d\varphi^2} + m^2\phi = 0 \quad ,$$

where α and m are constants yet to be determined. The polar equation has the complex solutions

$$\phi(\varphi) = \text{const.}\ e^{jm\varphi},\ \text{with}\ m = \ldots -2, -1, 0, 1, 2 \ldots$$

because of the symmetry of the problem in the polar angle ϕ, i.e. the wavefunction must be periodic in ϕ with period 2π.

Rigid Rotor

The rigid rotor is a mechanical model that is used to explain rotating systems. An arbitrary rigid rotor is a 3-dimensional rigid object, such as a top. To orient such an object in space, three angles known as Euler angles, are required. A special rigid rotor is the linear rotor which requires only two angles to describe its orientation. An example of a linear rotor is a diatomic molecule. More general molecules like water (asymmetric rotor), ammonia (symmetric rotor), or methane (spherical rotor) are 3-dimensional, see classification of molecules.

Particle in an infinite-wall box.

* useful insights into "valence states" of diatomic and conjugated polyatomic molecules. The system size is related to the energy of the HOMO → LUMO electronic transition.

Harmonic Oscillator

* *all* molecular vibrations for diatomic molecules and "normal modes" in polyatomic molecules
* almost all particle-in-a-well situations are harmonic near equilibrium
* perturbation theory used to account for diagonal and inter-mode effects (anharmonicity in the energy level spacing and Intramolecular Vibrational Redistribution) of anharmonicity in the potential energy function To deal with the rigid rotor.
* All molecules have rotational energy levels that are rigid-rotor like.

All central force systems (electronic structure of atoms, rotational structure of molecules, nuclear spins) may be separated into a *universal* spherical problem, described by angular momenta, and a *system-specific* radial problem.

The properties of angular momenta are universally described by spherical harmonics and by a set of commutation rules by which an angular momentum
may be defined, even when the angular momentum cannot be defined by the usual vector equation

$$IA = \hat{r} \times \hat{p}.$$

The electron spin is an example of an angular momentum that must be defined by commutation rules because there is no spatial coordinate associated with spin.

The Hydrogen atom. This provides a different (from particle-in-a-box) and more useful template for understanding "electronic structure" and is directly relevant to the

"Rydberg" electronic states of all molecules. * Many-electron systems. We will use LCAO-MO to provide a qualitative picture of molecular "valence states", the evil 1 rij inter-electron repulsion (that spoils all of the individual electron angular momentum, quantum numbers), and the necessity to "anti-symmetrise" many-electron wavefunctions (the Pauli Exclusion Principle) because electrons are "fermions". There are two quite different approaches to angular momentum.

Three-dimensional square-well potential

In quantum mechanics, the **particle in a box** model (also known as the **infinite potential well** or the **infinite square well**) describes a particle free to move in a small space surrounded by impenetrable barriers. The model is mainly used as a hypothetical example to illustrate the differences between classical and quantum systems. In classical systems, for example, a ball trapped inside a large box, the particle can move at any speed within the box and it is no more likely to be found at one position than another. However, when the well becomes very narrow (on the scale of a few nanometers), quantum effects become important. The particle may only occupy certain positive energy levels. Likewise, it can never have zero energy, meaning that the particle can never "sit still". Additionally, it is more likely to be found at certain positions than at others, depending on its energy level. The particle may never be detected at certain positions, known as spatial nodes.

The particle in a box model is one of the very few problems in quantum mechanics which can be solved analytically, without approximations. Due to its simplicity, the model allows insight into quantum effects without the need for complicated mathematics. It serves as a simple illustration of how energy quantization (energy levels), which are found in more complicated quantum systems such as atoms and molecules, come about. It is one of the first quantum mechanics problems taught in undergraduate physics courses, and it is commonly used as an approximation for more complicated quantum systems.

Deutron

The nucleus of the hydrogen atom isotope deuterium; mass number, 2. It is designate D, or d. A deuteron consists ofone proton and one neutron. Its mass is 2.014102 atomic mass units; its nucleon binding energy, 2.22452 ± 0.00010 MeV; itsspin, 1 (in ħ units); its magnetic moment, 0.857411 ± 0.000019 nuclear magnetons; and its nuclear electrical quadrupolemoment, $(2.738 \pm 0.014)10^{-27}$ cm^2.

Since the deuteron is the simplest nucleus containing more than one nucleon, the study of its properties has made it possibleto determine the action radius of nuclear forces and to conclude that the interaction between a proton and a neutron in thenucleus does not have the character of a central force but depends on the mutual orientation of their spins. The nucleonspins in the deuteron are parallel. Deuterons (in contrast to protons) absorb neutrons poorly and, at the same time, owing tothe closeness in their respective masses, strongly decelerate them. Deuterons are widely used in experimental nuclearphysics as bombarding particles and as targets (for example, in the studies of nuclear reactions).

The large difference between the masses of D and ‘H leads to significant differences in their properties (forexample, the boiling point of normal hydrogen is 20.39°K, whereas the boiling point of deuterium is 23.57°K; the rates ofsome chemical reactions differ by a factor of 5–10 for substances containing D and ^{1}H).

In industry deuterium is isolated by using isotopic exchange between water and hydrogen sulfide (deuterium is distributedunevenly between these compounds, concentrating in H^2O), by the distillation of liquid hydrogen, and by the multistepelectrolysis of water. Deuterium is used as a component of the hydrogen bomb, and in the future it may become athermonuclear fuel in energetics. In scientific research it is used as an isotope tracer. Heavy water D_2O serves as a neutronmoderator in atomic reactors. Deuterium was discovered spectrally in 1932 by the American scientist H. Urey and his co-workers.

Matrix representation of wave function

A function is actually an equivalence of a vector. In linear algebra, we denote a vector as $v = [v_1, v_2, v_3, \ldots v_N]^t$. A short-hand notation for this vector is v_j where $j = 1, \ldots, N$. But for a function $f(x)$, the countably finite index j in v_j is now replaced by an uncountably infinite (nondenumerable) set of indices denoted by x. Hence, we can think of $f(x)$ as a vector in an infinite dimensional vector space. An inner product in linear algebra is written as

$$\mathbf{V}^{\dagger}\cdot\mathbf{U}=\sum_{j=1}^{N}V_j^{*}U_j$$

The analogue of the above for functions is

$$\langle f|g\rangle=\int_{-\infty}^{\infty}dx\,f(x)^{*}g(x)$$

The above is the inner product between two functions which are actually vectors.[1] The left- hand side is the compact notation for the inner product between two state vectors known as Dirac's bra-ket notation. The <f| is the "bra" while |g> is the "ket". The "bra" can be thought of as the conjugate transpose of a vector, while the "ket" is analogous to an ordinary vector.

Matrix representation of operator

An operator equation can be written as

$$|g\rangle=\hat{A}|f\rangle$$

We can convert the above into a matrix equation by inserting an identity operator on the right-hand side to give

$$|g\rangle=\sum_{n}\hat{A}|\psi_n\rangle\langle\psi_n|f\rangle$$

Furthermore, we can multiply the above from the left by the basis vector $\langle\psi_m|$, $m = 1, \ldots, \infty$

The above is an infinite dimensional matrix equation which can be written as

$$\mathbf{g} = \overline{\mathbf{A}} \cdot \mathbf{f}$$

$$\begin{aligned} [\mathbf{A}]_{mn} &= \langle\psi_m|\hat{A}|\psi_n\rangle \\ [\mathbf{g}]_m &= \langle\psi_m|g\rangle \\ [\mathbf{f}]_n &= \langle\psi_n|f\rangle \end{aligned}$$

The matrix equation can be solved approximately by truncating its size to N ×N , or without truncation, it can be solved iteratively.

The matrix denoted by

$$A_{mn} = \langle\psi_m|\hat{A}|\psi_n\rangle$$

is the matrix representation of the operator $\hat{A}$. By the same token, $\langle\psi_m|g\rangle$ and $\langle\psi_n|f\rangle$ are the vector representations of the functions g and f respectively.

In the above, we have assumed that the range space and the domain space of the operator are the same, and hence, they can be spanned by the same basis set. For a Hermitian operator, this is usually the case. However, for some operators where the range space and the domain space are different, we may choose to with a different set of basis functions.

Properties of matrix elements

Property	**Example**

Commutativity of Addition	**$A + B = B + A$**
Associativity of Addition	**$A + (B + C) = (A + B) + C$**
Associativity of Scalar Multiplication	**$(cd) A = c (dA)$**
Scalar Identity	**$1A = A(1) = A$**
Distributive	**$c (A + B) = cA + cB$**
Distributive	**$(c + d) A = cA + dA$**
Additive Identity	**$A + O = O + A = A$**
Associativity of Multiplication	**$A (BC) = (AB) C$**
Left Distributive	**$A (B + C) = AB + AC$**
Right Distributive	**$(A + B) C = AC + BC$**
Scalar Associativity / Commutativity	**$c (AB) = (cA) B = A (cB) = (AB) c$**
Multiplicative Identity	**$IA = AI = A$**

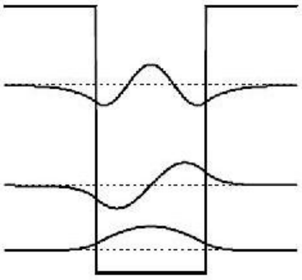
Schroedinger equation in matrix form

Linear harmonic oscillator

The pendulum, a particle attached to a spring, or many vibrations in atoms and molecules can be described as a harmonic oscillator. Hence, the harmonic oscillator is one of the most important examples in quantum mechanics. Its quantum mechanical version can be described by the 1D Schrodinger equation.

The classical equation for a harmonic oscillator is given by

$$\frac{\mathrm{d}^2 z}{\mathrm{d}t^2} = -\omega^2 z$$



where K is the spring constant, and m is the mass of the particle. The potential energy of a particle attached to a spring is given by

$$V(z) = \frac{1}{2}m\omega^2 z^2$$

Consequently, the above potential energy can be used in the Schrodinger equation to describe the trapping of wave modes. The kinetic energy of the particle is described by a term propor- tional to the square of the momentum operator. Hence, the corresponding 1D Schrodinger equation is

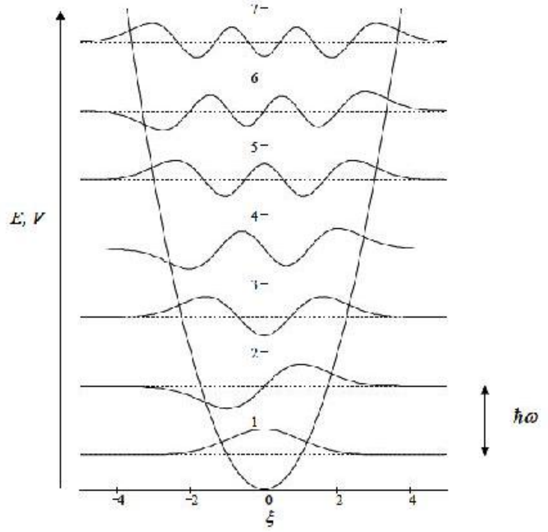
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\omega^2 z^2\right]\psi_n(z) = E_n\psi_n(z)$$

with a parabolic potential well. It turns out that this equation has closed-form solutions, yielding the wavefunction for an eigenstate given by

$$\psi_n(z) = \sqrt{\frac{1}{2^n n!}\sqrt{\frac{m\omega}{\pi\hbar}}}e^{-\frac{m\omega}{2\hbar}z^2}H_n\left(\sqrt{\frac{m\omega}{\hbar}}z\right)$$

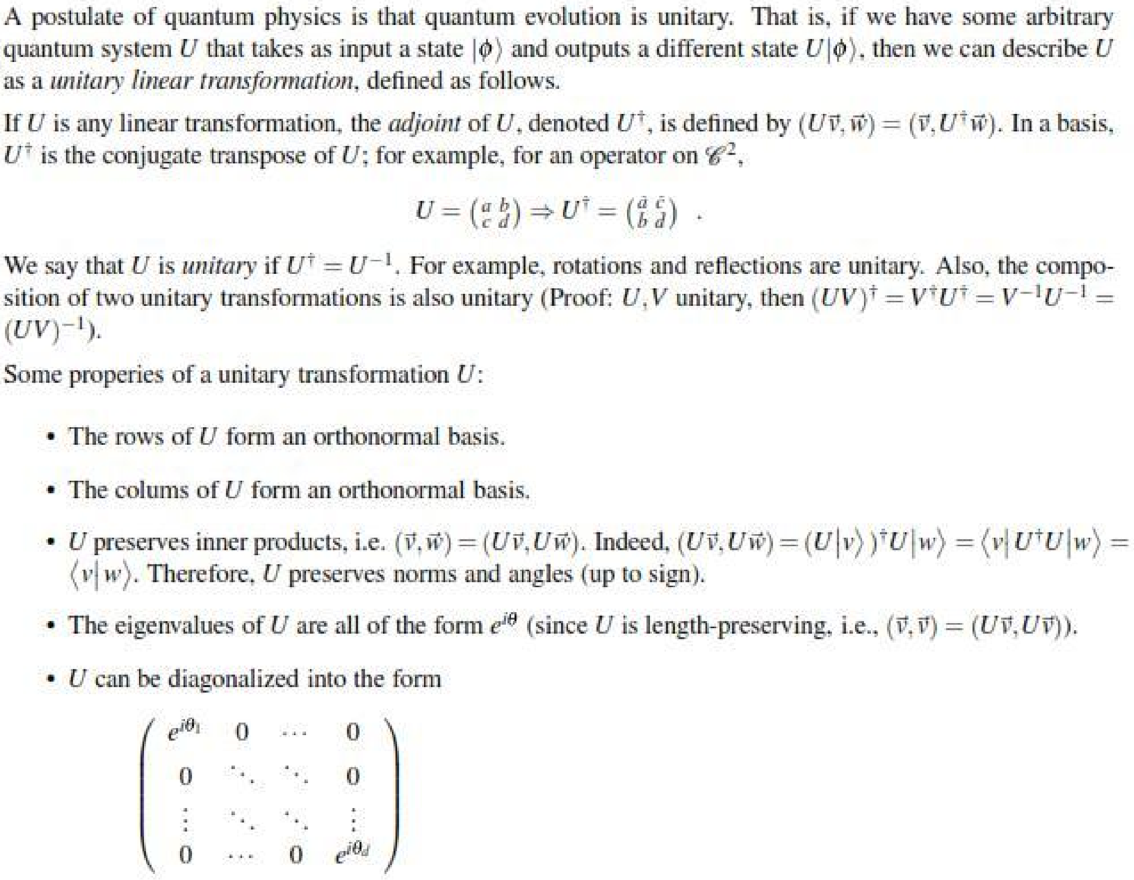
where Hn (x) is a Hermite polynomial, and the wavefunction is Gaussian tapered. The energy of the eigenstate is given by

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



The energy levels are equally spaced ~ω apart. Even the lowest energy state, the ground state, has a nonzero energy of ~ω/2. The higher energy states correspond to larger amplitudes of oscillation, and vice versa for the lower energy states. In order to kick the quantum harmonic oscillator from the low energy state to a level above, it needs a packet of energy of ~ω, the quantization energy of a photon. The physics of quantized electromagnetic oscillations (pho- tons) and quantized mechanical oscillations (phonons) is intimately related to the quantum harmonic oscillator.

Unitary Transformations



A postulate of quantum physics is that quantum evolution is unitary. That is, if we have some arbitrary quantum system U that takes as input a state $|\phi\rangle$ and outputs a different state $U|\phi\rangle$, then we can describe U as a *unitary linear transformation*, defined as follows.

If U is any linear transformation, the *adjoint* of U, denoted $U^\dagger$, is defined by $(U\vec{v},\vec{w}) = (\vec{v},U^\dagger\vec{w})$. In a basis, $U^\dagger$ is the conjugate transpose of U; for example, for an operator on $\mathscr{C}^2$,

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow U^\dagger = \begin{pmatrix} \bar{a} & \bar{c} \\ \bar{b} & \bar{d} \end{pmatrix} \quad .$$

We say that U is *unitary* if $U^\dagger = U^{-1}$. For example, rotations and reflections are unitary. Also, the composition of two unitary transformations is also unitary (Proof: U,V unitary, then $(UV)^\dagger = V^\dagger U^\dagger = V^{-1}U^{-1} = (UV)^{-1}$).

Some properies of a unitary transformation U:

- The rows of U form an orthonormal basis.
- The colums of U form an orthonormal basis.
- U preserves inner products, i.e. $(\vec{v},\vec{w}) = (U\vec{v},U\vec{w})$. Indeed, $(U\vec{v},U\vec{w}) = (U|v\rangle)^\dagger U|w\rangle = \langle v|U^\dagger U|w\rangle = \langle v|w\rangle$. Therefore, U preserves norms and angles (up to sign).
- The eigenvalues of U are all of the form $e^{i\theta}$ (since U is length-preserving, i.e., $(\vec{v},\vec{v}) = (U\vec{v},U\vec{v})$).
- U can be diagonalized into the form

$$\begin{pmatrix} e^{i\theta_1} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & e^{i\theta_d} \end{pmatrix}$$

Possible 4 Marks

1. Obtain the radial equation, energy Eigen value and radial wave function of hydrogen atom.
2. Obtain the Schrödinger equation in matrix from.
3. Describe the concept of deuteron.
4. What is a unitary transformation? Show that (i) the operator equation remains unchanged (ii) the Hermition operator is unchanged.
5. How a particle moving with a spherically symmetrical potential? Explain it.
6. What are the properties of Matrix elements? How to represent the matrix of operator and wave function?

Possible 10 Marks

1. Solve the time-independent Schrödinger equation for a three dimensional harmonic oscillator whose potential energy is V= ½ ($k_1x^2 + k_2y^2 + k_3z^2$).
2. A rigid rotator is constrained to rotate about a fixed axis. Find out its normalized eigen function and eigen values.
3. Show that the three 2-p eigen function of hydrogen atom are orthogonal to each other.

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MULTIPLE CHOICE QUESTIONS					
QUESTION	**OPTION 1**	**OPTION 2**	**OPTION 3**	**OPTION 4**	**ANSWER**
UNIT III					
The value of the magnetic quantum number can be	0,1,2,3, …	1,2,3,4, …	±1, ±2, ±3, ±4, ±5 ….	0, ±1, ±2, ±3, ±4 …	1,2,3,4, …
Which of the following statements is correct?	A linear combination of degenerate eigenfunctions	A linear combination of degenerate eig	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	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 ____	lh	lħ	[l(l+1)ħ]	$[l(l+1)]^{1/2}$ ħ.	$[l(l+1)]^{1/2}$ ħ.
The quantum number l is referred to as _____	angular momentum quantum number	spin angular momentum quantum num	orbital angular momentum quantum number	momentum	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	radial probability function	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 = a constant	dP_{10}-/dr = θ	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 electron's probability density distribution for the ____ state of a Hydrogen atom remains spherically symmetric	nth	1st	2nd	10th	1st
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 eigen value of the even function of the parity operator is	λ = 0	λ = 1	λ = ±1	λ = - 1	λ = - 1
The eigen value of the odd function of the parity operator is	λ = 0	λ = 1	λ = ±1	λ = -1	λ = 0
The eigen functions corresponding to the eigen value λ = ±1 of the parity operator are the	odd function	even function	can be even or odd	neither even nor odd	odd function
The eigen function corresponding to the eigen value λ = - 1 of the parity operator are the	odd function	even function	can be even or odd	neither even nor odd	even function
Hydrogen atom as a system of ________ interacting point charges	single	two	three	no	two
In quantum mechanics, the infinite square well can be regarded as the prototype of	all bound system	all unbound system	prometheus unbound	neither bound nor unbound	all bound system
In the infinite square well problem, the wave function and its first spatial derivative are:	both continuous at the boundaries	continuous and discontinuous at the bo	both discontinuous at the boundaries.	discontinuous and continuous at the	continuous and discontinuous at the boundaries, respectively
Meeting the boundary conditions of bound quantum mechanical systems imposes:	Heisenberg's uncertainty principle.	Schr¨odinger's equation	quantization	a vector potential.	quantization
At energies higher than the bound stationary states there	are between one and several tens of unbound state	are only two unbound states	is a continuum of unbound states	is a single unbound state	is a continuum of unbound states
How does the probability of an electron tunneling through a potential barrier vary with the thickness of the barrier?	It decreases inversely with thickness	It decreases sinusoidally with thickness	It decreases linearly with thickness	It decreases exponentially with thick	It decreases exponentially with thickness
Reduced mass of the system is represented as	θ	μ	ν	γ	μ
Which term represent radial quantum number?	k	μ	ν	γ	k

UNIT-IV

SYLLABUS

Time-independent Perturbation theory: Basic concepts – Non-degenerate energy levels – First and Second order corrections for energy and wave functions – Ground state of Helium atom – Effect of electric field on the ground state of hydrogen atom (Stark effect) – Degenerate energy levels – Effect of electric field on the n=2 state of hydrogen atom

Non-degenerate energy levels

In quantum physics, the quantum state of a given system is described by probability wavefunction, which depends on a set of quantum coordinates. The absolute square of the wavefunction determines the probability of finding the particle in the given quantum state. Each quantum state has a specific energy. For example, if we look at the particle in a box of width L, problem the particle energy can be expressed as

$$E_n = \frac{\hbar^2\pi^2}{2mL^2}(n^x + n^y + n^z)$$

For the ground state we have n=1

$$E_{100} = \frac{\hbar^2\pi^2}{2mL^2}(1+0+0) = \frac{\hbar^2\pi^2}{2mL^2}$$

$$E_{010} = \frac{\hbar^2\pi^2}{2mL^2}(0+1+0) = \frac{\hbar^2\pi^2}{2mL^2}$$

$$E_{001} = \frac{\hbar^2\pi^2}{2mL^2}(0+0+1) = \frac{\hbar^2\pi^2}{2mL^2}$$

There are three quantum states here ((100), (010), (001)) which are having same energy and these states are commonly referred as degenerate states. But each level is described by a specific wave function. In quantum mechanical words if two or more eigen functions correspond to the same eigen value they are said to be degenerate.

First and Second order corrections for energy and wave functions

Time-independent perturbation theory is one of two categories of perturbation theory, the other being time-dependent perturbation (see next section). In time-independent perturbation theory the perturbation Hamiltonian is static (i.e., possesses no time dependence). Time-independent perturbation theory was presented by Erwin Schrödinger in a 1926 paper,[2] shortly after he produced his theories in wave mechanics. In this paper Schrödinger referred to earlier work of Lord Rayleigh, who investigated harmonic vibrations of a string perturbed by small inhomogeneities. This is why this perturbation theory is often referred to as **Rayleigh–Schrödinger perturbation theory**.

First order corrections

Unperturbed Hamiltonian H_0, which is also assumed to have no time dependence. It has known energy levels and eigenstates, arising from the time-independent Schrödinger equation:

$$H_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle, \qquad n = 1, 2, 3, \cdots$$

For simplicity, we have assumed that the energies are discrete. The (0) superscripts denote that these quantities are associated with the unperturbed system. Note the use of bra–ket notation.

Let V be a Hamiltonian representing a weak physical disturbance, such as a potential energy produced by an external field. (Thus, V is formally a Hermitian operator.) Let λ be a dimensionless parameter that can take on values ranging continuously from 0 (no perturbation) to 1 (the full perturbation). The perturbed Hamiltonian is

$$H = H_0 + \lambda V$$

The energy levels and eigenstates of the perturbed Hamiltonian are again given by the Schrödinger equation

$$(H_0 + \lambda V)\,|n\rangle = E_n|n\rangle.$$

Our goal is to express in terms of the energy levels and eigenstates of the old Hamiltonian. If the perturbation is sufficiently weak, we can write them as a (Maclaurin) power series in *λ*

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$$
$$|n\rangle = \left|n^{(0)}\right\rangle + \lambda\left|n^{(1)}\right\rangle + \lambda^2\left|n^{(2)}\right\rangle + \cdots$$

When *k* = 0, these reduce to the unperturbed values, which are the first term in each series. Since the perturbation is weak, the energy levels and eigenstates should not deviate too much from their unperturbed values, and the terms should rapidly become smaller as we go to higher order.

Substituting the power series expansion into the Schrödinger equation, we obtain

$$(H_0 + \lambda V)\left(\left|n^{(0)}\right\rangle + \lambda\left|n^{(1)}\right\rangle + \cdots\right) = \left(E_n^{(0)} + \lambda E_n^{(1)} + \cdots\right)\left(\left|n^{(0)}\right\rangle + \lambda\left|n^{(1)}\right\rangle + \cdots\right)$$

Expanding this equation and comparing coefficients of each power of *λ* results in an infinite series of simultaneous equations. The zeroth-order equation is simply the Schrödinger equation for the unperturbed system. The first-order equation is

$$H_0\left|n^{(1)}\right\rangle + V\left|n^{(0)}\right\rangle = E_n^{(0)}\left|n^{(1)}\right\rangle + E_n^{(1)}\left|n^{(0)}\right\rangle$$

Second -order and higher corrections

The higher-order deviations by a similar procedure, though the calculations become quite tedious with our current formulation. Our normalization prescription gives that

$$2\left\langle n^{(0)}\middle|n^{(2)}\right\rangle + \left\langle n^{(1)}\middle|n^{(1)}\right\rangle = 0.$$

Up to second order, the expressions for the energies and (normalized) eigenstates are

$$E_n(\lambda) = E_n^{(0)} + \lambda \left\langle n^{(0)} \right| V \left| n^{(0)} \right\rangle + \lambda^2 \sum_{k \neq n} \frac{\left| \left\langle k^{(0)} \right| V \left| n^{(0)} \right\rangle \right|^2}{E_n^{(0)} - E_k^{(0)}} + O(\lambda^3)$$

$$\begin{aligned} |n(\lambda)\rangle = \left| n^{(0)} \right\rangle &+ \lambda \sum_{k \neq n} \left| k^{(0)} \right\rangle \frac{\left\langle k^{(0)} \right| V \left| n^{(0)} \right\rangle}{E_n^{(0)} - E_k^{(0)}} + \lambda^2 \sum_{k \neq n} \sum_{\ell \neq n} \left| k^{(0)} \right\rangle \frac{\left\langle k^{(0)} \right| V \left| \ell^{(0)} \right\rangle \left\langle \ell^{(0)} \right| V \left| n^{(0)} \right\rangle}{\left(E_n^{(0)} - E_k^{(0)} \right) \left(E_n^{(0)} - E_\ell^{(0)} \right)} \\ &- \lambda^2 \sum_{k \neq n} \left| k^{(0)} \right\rangle \frac{\left\langle n^{(0)} \right| V \left| n^{(0)} \right\rangle \left\langle k^{(0)} \right| V \left| n^{(0)} \right\rangle}{\left(E_n^{(0)} - E_k^{(0)} \right)^2} - \frac{1}{2} \lambda^2 \left| n^{(0)} \right\rangle \sum_{k \neq n} \frac{\left\langle n^{(0)} \right| V \left| k^{(0)} \right\rangle \left\langle k^{(0)} \right| V \left| n^{(0)} \right\rangle}{\left(E_n^{(0)} - E_k^{(0)} \right)^2} + O(\lambda^3). \end{aligned}$$

Extending the process further, the third-order energy correction can be shown to be

$$E_n^{(3)} = \sum_{k \neq n} \sum_{m \neq n} \frac{\langle n^{(0)} | V | m^{(0)} \rangle \langle m^{(0)} | V | k^{(0)} \rangle \langle k^{(0)} | V | n^{(0)} \rangle}{\left(E_n^{(0)} - E_m^{(0)} \right) \left(E_n^{(0)} - E_k^{(0)} \right)} - \langle n^{(0)} | V | n^{(0)} \rangle \sum_{m \neq n} \frac{|\langle n^{(0)} | V | m^{(0)} \rangle|^2}{\left(E_n^{(0)} - E_m^{(0)} \right)^2}.$$

Ground state of Helium atom

One important application of quantum mechanics is to explain the structure of atoms. Here we will look at two simple approaches to understand an atom with two electrons. This atom is helium.

The Hamiltonian for two electrons, each of charge e, orbiting a nucleus of charge Ze is

$$H = \frac{\mathbf{p}_1^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{r_1} + \frac{\mathbf{p}_2^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{r_2} + \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|}$$

If we ignore the final term, then this Hamiltonian is easy to solve: it simply consists of two independent copies of the hydrogen atom. The eigenstates would be

$$(x_1, x_2) = \quad {}_{n_1, l_1, m_1}(x_1) \quad {}_{n_2, l_2, m_2}(x_2)$$

where ${}_{n,l,m}(r)$ are the usual energy eigenstates of the hydrogen atom. We should remember that the electrons are fermions so we can’t put them in the same state. However, electrons also have a spin degree of freedom which we have neglected above. This means that two electrons can have the same spatial wavefunction as long as one is spin up and the other spin down.

Effect of electric field on the ground state of hydrogen atom (Stark effect)

The Stark effect is the shifting and splitting of spectral lines of atoms and molecules due to presence of an external electric field. The amount of splitting or shifting is called the Stark splitting or Stark shift. In general, one distinguishes first- and second-order Stark effects. The first-order effect is linear in the applied electric field, while the second-order effect is quadratic in the field.

The Stark effect is responsible for the pressure broadening (Stark broadening) of spectral lines by charged particles. When the split/shifted lines appear in absorption, the effect is called the inverse Stark effect.

The Stark effect is the electric analogue of the Zeeman effect where a spectral line is split into several components due to the presence of a magnetic field.

The Stark effect can be explained with fully quantum-mechanical approaches, but it has also been a fertile testing ground for semiclassical methods.

The Stark effect originates from the interaction between a charge distribution (atom or molecule) and an external electric field. Before turning to quantum mechanics we describe the interaction classically and consider a continuous charge distribution $\rho(\mathbf{r})$. If this charge distribution is non-polarizable its interaction energy with an external electrostatic potential $V(\mathbf{r})$ is

$$E_{\text{int}} = \int \rho(\mathbf{r}) V(\mathbf{r}) d\mathbf{r}^3.$$

If the electric field is of macroscopic origin and the charge distribution is microscopic, it is reasonable to assume that the electric field is uniform over the charge distribution. That is, $V$is given by a two-term Taylor expansion,

$$V(\mathbf{r}) = V(\mathbf{0}) - \sum_{i=1}^{3} r_i F_i \text{, with the electric field: } F_i \equiv -\left(\frac{\partial V}{\partial r_i}\right)\Big|_{\mathbf{0}},$$

where we took the origin **0** somewhere within ρ. Setting *V*(0) as the zero energy, the interaction becomes

$$E_{\text{int}} = -\sum_{i=1}^{3} F_i \int \rho(\mathbf{r}) r_i \, d\mathbf{r} \equiv -\sum_{i=1}^{3} F_i \mu_i = -\mathbf{F} \cdot \boldsymbol{\mu}.$$

Here we have introduced the dipole moment **μ** of ρ as an integral over the charge distribution. In case ρ consists of *N* point charges q_j this definition becomes a sum

$$\boldsymbol{\mu} \equiv \sum_{j=1}^{N} q_j \mathbf{r}_j.$$

Degenerate energy levels

In quantum mechanics, an energy level is degenerate if it corresponds to two or more different measurable states of a quantum system. Conversely, two or more different states of a quantum mechanical system are said to be degenerate if they give the same value of energy upon measurement. The number of different states corresponding to a particular energy level is known as the degree of degeneracy of the level. It is represented mathematically by the Hamiltonian for the system having more than one linearly independent eigenstate with the same energy eigenvalue. In classical mechanics, this can be understood in terms of different possible trajectories corresponding to the same energy.

Degeneracy plays a fundamental role in quantum statistical mechanics. For an *N*-particle system in three dimensions, a single energy level may correspond to several different wave functions or energy states. These degenerate states at the same level are all equally probable of being filled. The number of such states gives the degeneracy of a particular energy level.

Particle in a rectangular plane

Consider a free particle in a plane of dimensions L_x and L_y in a plane of impenetrable walls. The time-independent Schrödinger equation for this system with wave function , can be written as

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right)=E\psi$$

The permitted energy values are

$$E_{n_x,n_y}=\frac{\pi^2\hbar^2}{2m}\left(\frac{n_x^2}{L_x^2}+\frac{n_y^2}{L_y^2}\right)$$

The normalized wave function is

$$\psi_{n_x,n_y}(x,y)=\frac{2}{\sqrt{L_xL_y}}\sin\left(\frac{n_x\pi x}{L_x}\right)\sin\left(\frac{n_y\pi y}{L_y}\right)$$

where n_x, n_y=1,2,3...

So, quantum numbers nx, ny are required to describe the energy eigenvalues and the lowest energy of the system is given by

$$E_{1,1}=\pi^2\frac{\hbar^2}{2m}\left(\frac{1}{L_x^2}+\frac{1}{L_y^2}\right)$$

Effect of electric field on the n=2 state of hydrogen atom

Electric field in a hydrogen atom is a sum of electric field produced by the charge of electron and electric field produced by the charge of proton, $E = E_e + E_p$. The energy of this field is the energy of the field produced by electron plus the energy of the field produced by proton plus interaction energy. As was mentioned before, in quantum mechanics the energy of any electron and any proton are equal to zero. So the energy of the electric field in a hydrogen atom in quantum mechanics consists of the interaction energy only. This interaction energy is negative, because the two particles have charges of the opposite signs. The value of the electrostatic (me–energy of the electric field in a hydrogen atom in the ground state is $U_0 = me^4/\hbar^2$. Anyway, the energy of the electric field is negative in any stationary state of a hydrogen atom

Possible 4 marks

1. Write the second-order correction to wave function on non-degenerate energy levels.
2. What is quadratic Stark-effect
3. Discuss in detail non degenerate energy levels.
4. Explain the basic concepts of time-independent perturbation theory.
5. Explain the effect of electric field on the n=2 state of hydrogen atom
6. Discuss the ground state of helium atom.
7. Describe the effect of electric field on the ground state of hydrogen atom.

Possible 10 marks

1. Based on non-degenerate energy level, explain the first-order correction for energy and wave function.
2. Calculate the maximum wavelength that hydrogen in its ground state can absorb. What would be the next maximum wavelength?
3. Calculate the velocity and frequency of revolution of the electron of the Bohr hydrogen atom in its ground state?

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MULTIPLE CHOICE QUESTIONS					
QUESTION	**OPTION 1**	**OPTION 2**	**OPTION 3**	**OPTION 4**	**ANSWER**
UNIT IV					
The value of second order perturbed energy $E_n^{(2)}$ is	$(E_n^0 - E_m \Sigma_m<m\vert H^{(1)}\vert n>$	$\Sigma_m [<m\vert H^{(1)}\vert n>]^2 - E_m^0)]$	$\Sigma_n [<n\vert H^{(1)}\vert n>/(E_n^0 - E_m^0)]$	$\Sigma_m [<m\vert H^{(1)}\vert n>]$	$\Sigma_m [<m\vert H^{(1)}\vert n>]^2/(E_n^0 - E_m^0)]$
Total energy of helium atom, (if E_H is ground state energy of H atom) is	$-(2Z^2 + (5/4)Z)E_H$	$-(2Z^2 - (5/4)Z)E_H$	$(2Z^2 + (3/2)Z)E_H$	$(2Z^2 - (3/2)Z)E_H$	$-(2Z^2 - (5/4)Z)E_H$
The perturbation term in normal helium atom is	e/r	e^2/r	e^2/r_{12}	Ze^2/r	e^2/r_{12}
The method of molecular wave functions as a linear combination of atomic orbitals is called as	combination method	LCAO method	Bohr method	Dirac method	LCAO method
The first order time independent perturbed energy for the non-degenerate case is	$\int\psi_n^{(1)}H^{(2)}\psi_n^{(1)}d\tau$	$\int\psi_n^{(1)}H^{(1)}\psi_n^{(1)}d\tau$	$\int\psi_n^{(0)}H^{(1)}\psi_n^{(0)}d\tau$	$\int\psi_n^{(0)}H^{(0)}\psi_n^{(0)}d\tau$	$\int\psi_n^{(0)}H^{(1)}\psi_n^{(0)}d\tau$
The value of the perturbation parameter λ is	0 to 0.5	0.5 to 1	0 to 1	0 to infinity	0 to 1
If E_n is the ground state energy of hydrogen atom, the first order perturbed energy of helium atoms is given by	$(5/4)ZE_H$	$(5/4)E_H$	$(5/3)Z$	$(5/3)E_H$	$(5/4)ZE_H$
The first excited state of hydrogen will have total degenerate level of	3	2	4	1	4
First order perturbed energy $E_k`$ is	$\hbar H_{kk}`$	$H_{kk}`$	$-H_{kk}`$	$i\hbar H_{kk}`$	$\hbar H_{kk}`$
The potential energy of helium atom V is	$-Ze^2/r_1 - Ze^2/r_2 + e^2/r_{12}$	$Ze^2/r_1 + Ze^2/r_2$	$Ze^2/r_1 + Ze^2/r_2 + e^2/r_{12}$	$Ze^2/r_1 + Ze^2/r_2 - e^2/r_{12}$	$-Ze^2/r_1 - Ze^2/r_2 + e^2/r_{12}$
Unperturbed Hamiltonian for hydrogen atom is	$(\hbar^2/2\mu)\nabla^2 + e^2/r$	$(\hbar^2/2\mu)\nabla^2 - e^2/r$	$-(\hbar^2/2\mu)\nabla^2 - e^2/r$	$-(\hbar^2/2\mu)\nabla^2 + e^2/r$	$-(\hbar^2/2\mu)\nabla^2 - e^2/r$
For a ground state of hydrogen atom, the first order perturbation energy correction due to stark effect is	positive	negative	zero	infinity	negative
The wave mechanical perturbation theory was developed by	Dirac	Heisenberg	Schrodinger	De Broglie	Schrodinger
First order stark effect for the ground state of hydrogen atom is	finite	infinite	zero	positive	zero
The first order perturbation energy $E_n`$ given by	$\sum_m [<H_{mn}`>\psi_m^o]/(E_n^0 - E_m^0)$	$\sum_m [<H_{mm}`>\psi_m^o]/(- E_m^0)$	$\sum_m [<H_{mn}`>]/\psi_m(E_n^0 - E_m^0)$	$\sum_m [\psi_m^o(E_n^0 - E_m^0)]/<H_{mn}`>$	$\sum_m [\psi_m^o(E_n^0 - E_m^0)]/<H_{mn}`>$
The effective nuclear charge Z\` and the nuclear charge Z for helium atom are related due to time independent perturbation theory by	$Z` = Z - 5/16$	$Z` = Z + 5/16$	$Z` = (5/16)Z$	$Z` = 1.1 Z$	$Z` = (5/16)Z$
If the function ψ is not normalized, the expectation value of energy $<E>$ is	$\int\psi^*H\psi d\tau$	$\int\psi^*\psi d\tau$	$\{\int\psi^*H\psi d\tau\}/\int\psi^*\psi d\tau$	$\{\int\psi^*\psi d\tau\}/\int\psi^*H\psi d\tau$	$\{\int\psi^*H\psi d\tau\}/\int\psi^*\psi d\tau$
The de Broglie wave length associated with a particle moving with energy E in a region of potential V is	$h/[2m(E - V)]^{1/2}$	$h/[2m(E - V)]^{-1/2}$	$(E - V)^{1/2}$	$(E - V)^{-1/2}$	$h/[2m(E - V)]^{1/2}$
Assuming that nucleus is at rest, the Hamiltonian for H atom is	$p^2/2m + e^2/r$	$p^2/2m + e^2/r^2$	$p^2/2m - e^2/r$	$p^2/2m - e^2/r^2$	$p^2/2m + e^2/r$

Eigen value of hydrogen atom in ground state is	$– e^2/2\ a_o$	$e^2/2\ a_o$	$– e/2\ a_o$	$e/2\ a_o$	$– e/2\ a_o$
Eigen function of hydrogen atom in ground state is	$\psi_{1s} = [1/\sqrt{(\pi a_o{}^3)}]\exp(r/a_o)$	$\psi_{1s} = [1/\sqrt{(\pi a_o{}^3)}]\exp(r/a_o)$	$\psi_{1s} = [-1/\sqrt{(\pi a_o{}^3)}]\exp(r/a_o)$	$\psi_{1s} = [-1/\sqrt{(\pi a_o{}^3)}]$ $r/a_o)$	$\psi_{1s} = [1/\sqrt{(\pi a_o{}^3)}]$ex $r/a_o)$
The energy of Helium atom by perturbation method is	$2.75\ e^2/a_o$	$2.75\ e^2$	$- 2.75\ e^2/a_o$	$- 2.75\ e^2$	$- 2.75\ e^2/a_o$
The energy of Helium atom without perturbation in ground state is	$– 4e^2/a_o$	$4e^2/a_o$	e^2/a_o	$– 2.75e^2/a_o$	$– 4e^2/a_o$
The application for first order perturbation theory for a non-degenerate system is	Zeeman effect	Stark effect	Particle in a box	Stationary Harmonic oscillator	Stark effect
First order Stark effect in first excited state of H atom has the wave function ψ_{nlm} is	Zero-fold degenerate	Four-fold degenerate	Three-fold degenerate	Two-fold degenerate	Four-fold degenerate
The equation H = L + T represents the total energy system in	motion	stationary	motion or stationary	motion with respect to time	motion with respect to time
Equation of motion of a wave particle is	$– i\hbar\ \partial\psi/\partial t = (-\hbar^2/2m)/\ \nabla\psi$	$i\hbar\ \partial\psi/\partial t = (-\ \hbar^2\ /2m)$ $\nabla^2\psi$	$i\hbar\ \partial\psi/\partial t = (\hbar^2\ /2n$ $\nabla\psi$	$i\hbar\ \partial\psi/\partial t = (-\ \hbar^2/2m)/\ \nabla\psi$	$i\hbar\ \partial\psi/\partial t = (-\ \hbar^2\ /2n$ $\nabla^2\psi$
The Schrodinger equation can be solved exactly for which the Hamiltonian is	small	large	both small and large	unperturbed	unperturbed
If the ____ energy of the system is disturbed by the influence of additional forces, the energy levels are shifted	total	kinetic	potential	either potential or kinetic	potential
In non-degenerate system there is one eigen function corresponding to	one eigen value	many eigen values	two eigen values	three eigen values	one eigen value
Ortho-normalization condition is given by	$\int\psi_i{}^{(0)*}\psi_j{}^{(0)}d\tau = 0$	$\int\psi_i{}^{(0)*}\psi_j{}^{(0)}d\tau = 1$	$\int\psi_i{}^{(0)*}\psi_j{}^{(0)}d\tau = \delta_{ij}$	$\int\psi_i{}^{(0)*}\psi_i{}^{(0)}d\tau = 0$	$\int\psi_i{}^{(0)*}\psi_j{}^{(0)}d\tau = \delta_{ij}$
The second order perturbation energy eigen value for non-degenerate case is	$\sum_m C_m\psi_m{}^{(0)}H^{(1)}\psi_n{}^{(0)*}d\tau$	$\sum_m C_m\psi_n{}^{(0)}\ {}^*H\ {}^{(1)}\ \psi$ $d\tau$	$\sum_m C_m\psi_n{}^{(0)}H^{(1)}\psi_m{}^{(0)}d\tau$	$\int C_m\psi_n{}^{(0)}H^{(1)}\psi_m{}^{(0)}d\tau$	$\sum_m C_m\psi_n{}^{(0)\,*}H^{(1)}\psi_m{}^{(0)}\ d\tau$
The first order time independent perturbed wave function for the non-degenerate case is	$\{[\int\psi_m{}^{(0)*}H^{(1)}\psi_n{}^{(0)}d\tau]/(E_m{}^0 – E_n{}^0)\}\psi_m{}^{(0)}$	$–\{[\int\psi_m{}^{(0)*}H^{(1)}\psi_n{}^{(0)}d\tau]/(E_m{}^0 – E_n{}^0)\}\psi_m{}^{(0)}$	$\{[\int\psi_n{}^{(0)*}H^{(1)}\psi_m{}^{(0)}d\tau]/(E_m{}^0 – E_n{}^0)\}\psi_m{}^{(0)}$	$–\{[\int\psi_n{}^{(0)*}H^{(1)}\psi_m{}^{(0)}d\tau]/(E_m{}^0 – E_n{}^0)\}\psi_m{}^{(0)}$	$–\{[\int\psi_m{}^{(0)*}H^{(1)}\psi_n{}^{(0)}d\tau]/(E_m{}^0 – E_n{}^0)\}\psi_m{}^{(0)}$
In ground state of Helium atom, to make approximate solution the nucleus is considered as at	random motion	uniform motion	rest	either uniform or rest	rest
The eigen value of ground state of helium atom is Z^2E_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	$2Z^2E_H$	$2ZE_H$	$–\ 2ZE_H$	$– 2Z^2E_H$	$– 2Z^2E_H$
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 φ_o, φ_1, φ_2, …… 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	zero	anti-parallel
Non-degenerate perturbation method was developed by	Dirac	Schrödinger	WKB	Bohr	Schrödinger
The final type of approximation method is	WKB	Variation	Perturbation degenerate	Perturbation non-degenerate	WKB
When a small disturbance is applied to a system, there may be change in	eigen values	eigen functions	either a or b	both a and b	eigen functions
Problems of one dimension and also of three dimension reducible to one dimension are solved by	variation method	WKB method	Perturbation degenerate method	Perturbation non-degenerate method	WKB method
Mathematically slowly varying potential can be expressed by	$\lvert(1/k_2)dk/dx\rvert < 1$	$\lvert(1/k_2)dk/dx\rvert > 1$	$\lvert(k_2)dk/dx\rvert < 1$	$\lvert(k_2)dk/dx\rvert > 1$	$\lvert(1/k_2)dk/dx\rvert < 1$
The ionization energy for hydrogen atom is 13.6 eV. The ionization energy for	13.6 eV	27.2 eV	40.8 eV	122.4eV	122.4eV
The lowest excited state of the helium atom has the term symbol	1S0	3S1	He+	1S2	3S1
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
A hydrogen atom radiates a photon as it falls from a 2p level to the 1s level. Th	22.8	91.2	121.6	182.4	121.6
For the hydrogen atom, which of the following orbitals has the lowest energy	4s	4p	4f	all have same energy	all have same energy
The orbital degeneracy (excluding spin) of hydrogen atom energy levels equals	n-1	n^2	n+1	2n+1	n^2
For real atomic orbitals with quantum numbers n, `, the total number of nodal s	n	n-1	n+1	2l+1	n-1
Which of the following statements about the hydrogen atom ground state is IN	It is described by th	The electron’s angular	The wavefunction is s	The wavefunction decreas	The electron’s angular momentum equals ¯h.

UNIT-V

SYLLABUS

Variational method &WKB Approximation: Variational principle – Variation method for excited states – Application of variation method to ground state of helium – The WKB method

Time dependent perturbation theory: Introduction – First-order perturbation – Harmonic perturbation – Transition to continuum states (Fermi's Golden rule) – Absorption and emission of radiation – Transition probability – Selection rules

Variational principle

The variational method provides a simple way to place an upper bound on the ground state energy of any quantum system and is particularly useful when trying to demonstrate that bound states exist. In some cases, it can also be used to estimate higher energy levels too.
The variational method does not tell us how far above the ground state E0 lies. It would be much better if we could also get a lower bound for E0 so that we can say for sure that ground state energy sits within a particular range. However, for particles moving in a general potential V (x), the only lower bound that is known is E0 > min V (x). Since we're often interested in potentials like V (x) ⇠ 1/r, which have no lower bound this is not particularly useful.

Variation method for excited states

For our trial wavefunction we pick (x1, x2) = (x1) (x2) where

$$\psi(\mathbf{x};\alpha) = \sqrt{\frac{\alpha^3}{\pi a_0^3}}\, e^{-\alpha r/a_0}$$

There's one last bit of physics hidden in this calculation. The optimum trial wave- function that we ended up using was that of an electron orbiting a nucleus with charge (Z 5/16)e, rather than charge Ze. This has a nice interpretation: the charge of the nucleus is screened by the presence of the other electron.

Application of variation method to ground state of helium

The hydrogen atom wavefunctions and energies, we have seen, are determined as a combination of the various quantum "dynamical" analogues of classical motions (translation, vibration, rotation) and a central-force interaction (i.e, the Coulomb interaction between an electron and a nucleus). Now, we consider the Helium atom and will see that due to the attendant 3-body problem for which we cannot determine a closed-form, first-principles analytic solution, we will have to find recourse in approximate methods. The Helium atom has 2 electrons with coordinates r1 and r2 as well as a single nucleus with coordinate R. The nucleus carries a Z = +2e charge.

The Schrodinger equation is

$$\left(-\frac{\hbar^2}{2M}\nabla^2 - \frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{\hbar^2}{2m_e}\nabla_2^2\right)\psi(\mathbf{R},\mathbf{r_1},\mathbf{r_2}) +$$

$$\left(-\frac{2e^2}{4\pi\epsilon_o\,|R-r_1|} - \frac{2e^2}{4\pi\epsilon_o\,|R-r_2|} + \frac{e^2}{4\pi\epsilon_o\,|r_1-r_2|}\right)\psi(\mathbf{R},\mathbf{r_1},\mathbf{r_2}) = E\psi(\mathbf{R},\mathbf{r_1},\mathbf{r_2})$$

where the symbol ”nabla”, when squared, is given by

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Keep in mind that the R, r_1, and r_2 represent the Cartesian coordinates of each paticle. This is a 3-body problem and such problems are not solved exactly. Thus, the problem will be reformulated in terms of coordinates of two particles, the electrons. The first approximation: M >> me , fix the nucleus at the origin (R) = 0. This is more rigorously shown by transforming the origin to the center of mass of the system. For the two electron-nucleus coordinates, this is much like what we have seen for the hydrogen atom electron-nucleus formulation from earlier discussion. Thus, the Schrodinger equation in relative variables is

$$\frac{\hbar^2}{2m_e}\left(-\nabla_1^2 - \nabla_2^2\right)\psi(\mathbf{r_1},\mathbf{r_2}) - \frac{2e^2}{4\pi\epsilon_o}\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{4\pi\epsilon_o\,|r_2-r_1|}\psi(\mathbf{r_1},\mathbf{r_2}) = E\psi(\mathbf{r_1},\mathbf{r_2})$$

The ∇^2 terms represent the kinetic energy of the two electrons. The $\frac{1}{r1}$ and $\frac{1}{r2}$ terms represent the nucleus-electron Coulomb interaction. The last term on the left hand side of the equation represents the electron-electron repulsion taken as a Coulomb interaction based on the absolute value of the electron-electron separation.

The WKB method

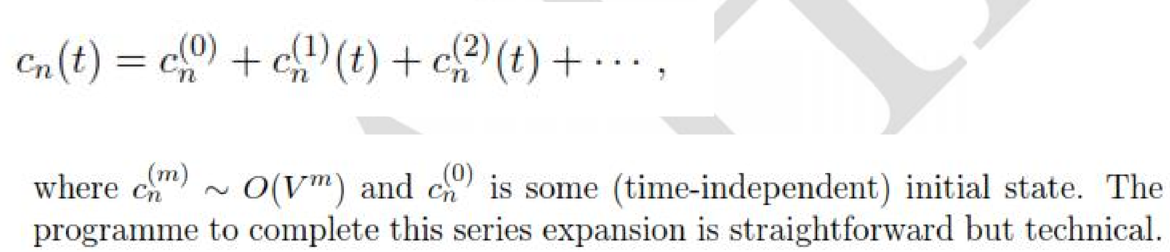
The WKB approximation is a method for solving the one-dimensional Schro¨dinger equation. The approximation is valid in situations where the potential changes slowly compared to the de Broglie wavelength = 2ħ/p of the particle. The basic idea is that the wavefunction will be approximately that of a free particle, but with an amplitude and phase that vary to compensate the changes in the potential.

The method is named after the physicists Wentzel, Kramers and Brillouin. It is sometimes called the WKBJ approximation, with Harold Jeffreys' name tagged on the end to recognise the fact that he discovered before any of the other three. The main applications of the method are in estimating bound state energies and computing tunnelling rates.

First-order perturbation – Harmonic perturbation

First-order perturbation

Time-dependent Hamiltonian for which an analytical solution is unavailable – sadly the typical situation. In this case, we must turn to a perturbative analysis, looking for an expansion of the basis coefficients $c_n(t)$ in powers of the interaction,



$$c_n(t) = c_n^{(0)} + c_n^{(1)}(t) + c_n^{(2)}(t) + \cdots ,$$

where $c_n^{(m)} \sim O(V^m)$ and $c_n^{(0)}$ is some (time-independent) initial state. The programme to complete this series expansion is straightforward but technical.

Time-dependent perturbation theory, developed by Paul Dirac, studies the effect of a time-dependent perturbation $V(t)$ applied to a time-independent Hamiltonian H_0.

Since the perturbed Hamiltonian is time-dependent, so are its energy levels and eigenstates. Thus, the goals of time-dependent perturbation theory are slightly different from time-independent perturbation theory. One is interested in the following quantities:

- The time-dependent expectation value of some observable A, for a given initial state.
- The time-dependent amplitudes of those quantum states that are energy eigenkets (eigenvectors) in the unperturbed system.

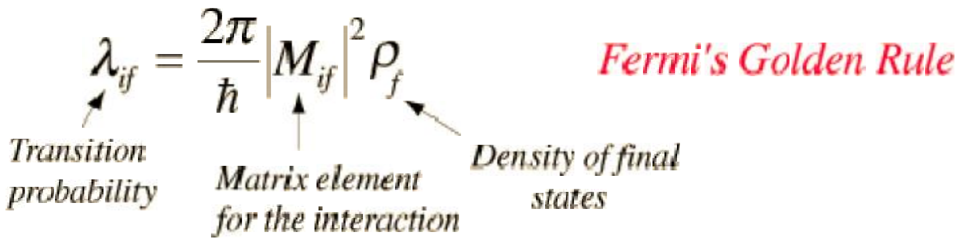
The first quantity is important because it gives rise to the classical result of an A measurement performed on a macroscopic number of copies of the perturbed system. For example, we could take A to be the displacement in the x-direction of the electron in a hydrogen atom, in which case the expected value, when multiplied by an appropriate coefficient, gives the time-dependent dielectric polarization of a hydrogen gas. With an appropriate choice of perturbation (i.e. an oscillating electric potential), this allows one to calculate the AC permittivity of the gas. The second quantity looks at the time-dependent probability of occupation for each eigenstate. This is particularly useful in laser physics, where one is interested in the populations of different atomic states in a gas when a time-dependent electric field is applied. These probabilities are also useful for calculating the "quantum broadening" of spectral lines (see line broadening) and particle decay in particle physics and nuclear physics

Harmonic perturbation – Transition to continuum states (Fermi's Golden rule)

In quantum physics, **Fermi's golden rule** is a formula that describes the transition rate (probability of transition per unit time) from one energy eigen state of a quantum system into other energy eigen states in a continuum, affected by a weak perturbation.

One of the prominent failures of the Bohr model for atomic spectra was that it couldn't predict that one spectral line would be brighter than another. From the quantum theory came an explanation in terms of wavefunctions, and for situations where the transition probability is constant in time, it is usually expressed in a relationship called Fermi's golden rule.

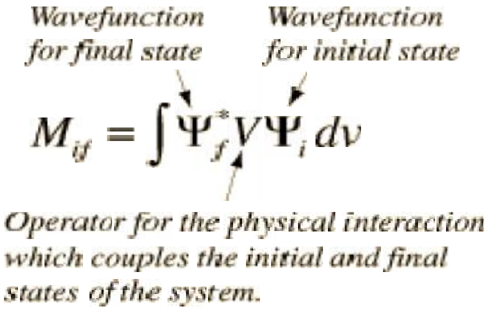
In general conceptual terms, a transition rate depends upon the strength of the coupling between the initial and final state of a system and upon the number of ways the transition can happen (i.e., the density of the final states). In many physical situations the transition probability is of the form



$$\lambda_{if} = \frac{2\pi}{\hbar}\left|M_{if}\right|^2 \rho_f$$

The transition probability l is also called the decay probability and is related to the mean lifetime t of the state by l = 1/t. The general form of Fermi's golden rule can apply to atomic transitions, nuclear decay, scattering ... a large variety of physical transitions.

A transition will proceed more rapidly if the coupling between the initial and final states is stronger. This coupling term is traditionally called the "matrix element" for the transition: this term comes from an alternative formulation of quantum mechanics in terms of matrices rather than the differential equations of the Schrodinger approach. The matrix element can be placed in the form of an integral where the interaction which causes the transition is expressed as a potential V which operates on the initial state wavefunction. The transition probability is proportional to the square of the integral of this interaction over all of the space appropriate to the problem.



$$M_{if} = \int \Psi_f^* V \Psi_i \, dv$$

This kind of integral approach using the wavefunctions is of the same general form as that used to find the "expectation value" or expected average value of any physical variable in quantum mechanics. But in the case of an expectation value for a property like the system energy, the integral has the wavefunction representing the eigenstate of the system in both places in the integral.

The transition probability is also proportional to the density of final states r_f. It is reasonably common for the final state to be composed of several states with the same energy such states are said to be "degenerate" states. This degeneracy is sometimes expressed as a "statistical weight" which will appear as a factor in the transition probability. In many cases there will be a continuum of final states, so that this density of final states is expressed as a function of energy.

Absorption and emission of radiation

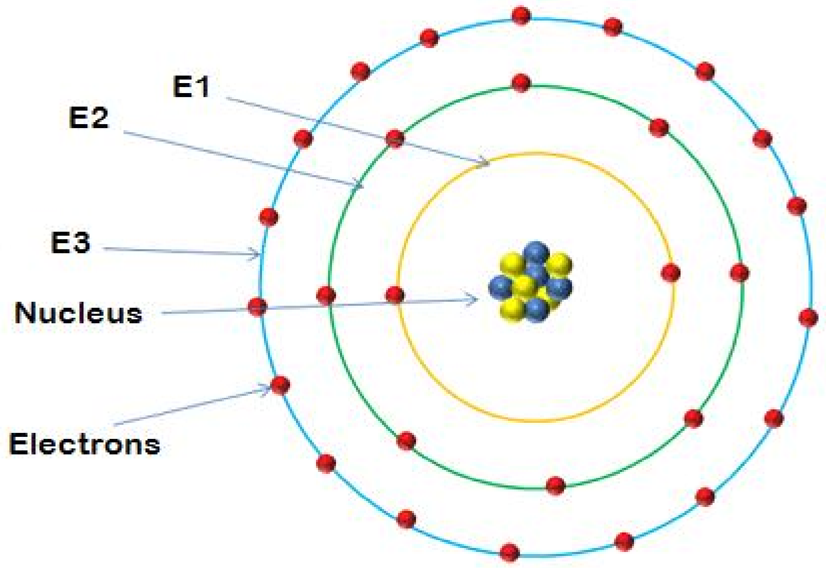
Every object in the universe is made up of atoms. Atoms are made up of extremely small particles such as electrons, protons, and neutrons. Electrons are the negatively charged particles and protons are the positively charged particles. Neutrons have no charge. Hence, neutrons are referred as neutral particles.

The strong nuclear force between the protons and neutrons makes them stick together to form the nucleus. Neutrons have no charge. so the overall charge of the nucleus is positive because of the protons.

The electrostatic force of attraction between the nucleus and electrons causes electrons to revolve around the nucleus.

The electrons revolving around the nucleus have different energy levels based on the distance from the nucleus.

The electrons revolving very close to the nucleus have lowest energy level whereas the electrons revolving at the farthest distance from nucleus have highest energy level.



The electrons in the lower energy state (E_1) needs extra energy to jump into next higher energy state (E_2). This energy can be supplied in the form of the electric field, heat or light.

When the electrons in the lower energy state (E_1) gains sufficient energy from photons, they jump into next higher energy state (E_2).

The electrons in the higher energy state do not stay for long period. After a short period, they again fall back to the lower energy level by losing their energy. The electrons in the higher energy level or higher energy state lose energy in the form of light before they fall back to the lower energy state.

The electrons in the higher energy state are known as excited electrons whereas the electrons in the lower energy state are known as ground electrons.

In lasers, the way light or photons interact with atoms plays an important role in its operation. The photons interact in three ways with the atoms:

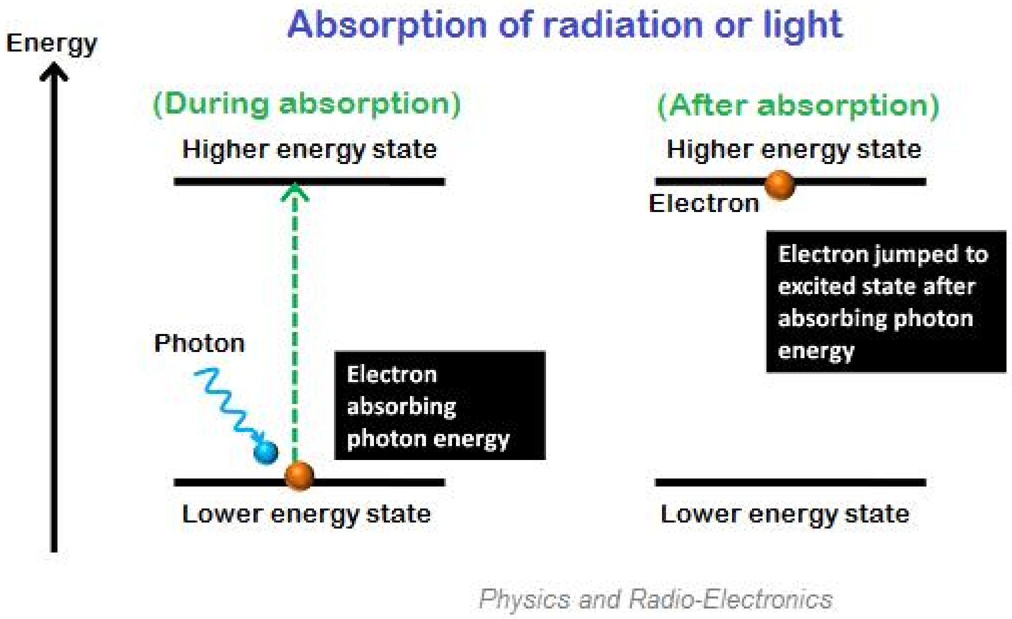
- Absorption of radiation or light
- Spontaneous emission
- Stimulated emission

Absorption of radiation or light

The process of absorbing energy from photons is called absorption of radiation.

It is well known that there are different energy levels in an atom. The electrons that are very close to the nucleus have lowest energy level. These electrons are also known as ground state electrons.

Let us consider that the energy level of ground state electrons or lower energy state electrons is E_1 and the next higher energy level or higher energy state is E_2.



When ground state electrons or lower energy state electrons (E_1) absorbs sufficient energy from photons, they jump into the next higher energy level or higher energy state (E_2). In other words, when the ground state electrons absorb energy which is equal to the energy difference between the two energy states ($E_2 – E_1$), the electrons jumps from ground state (E_1) to the excited state or higher energy level (E_2). The electrons in the higher energy level are called excited electrons.

The light or photons energy applied to excite the electrons can be mathematically written as

$hv = E_2 – E_1$

Where h = Planck's constant

V = Frequency of photon

E_1 = Lower energy level electrons or ground state electrons

E_2 = Higher energy level electrons or excited state electrons

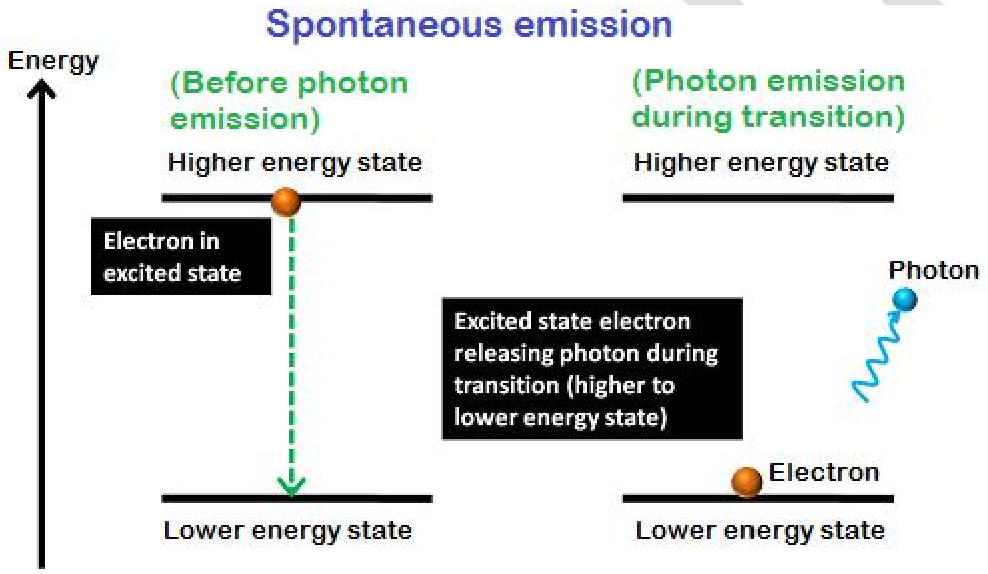
Absorption occurs only if the energy of photon exactly matches the difference in energy between the two electron shells or orbits.

Spontaneous emission

The process by which excited electrons emit photons while falling to the ground level or lower energy level is called spontaneous emission.

Electrons in the atom absorb energy from various sources such as heat, electric field, or light. When the electrons in the ground state or lower energy state (E1) absorb sufficient energy from photons, they jump to the excited state or next higher energy state (E_2).

The electrons in the excited state do not stay for a long period because the lifetime of electrons in the higher energy state or excited state is very small, of the order of 10^{-8} sec. Hence, after a short period, they fall back to the ground state by releasing energy in the form of photons or light.



The energy of the emitted photon is directed proportional to the energy gap of the material. The materials with large energy gap will emit high-energy photons or high-intensity light whereas the materials with small energy gap will emit low energy photons or low-intensity light.

The energy of released photon is equal to the difference in energies between the two electron shells or orbits.

The energy of the excited electrons can also be released in other forms such as heat. If the excited state electrons release energy in the form of photons or light while falling to the ground state, the process is called spontaneous emission.

In spontaneous emission, the electrons changing from one state (higher energy state) to another state (lower energy state) occurs naturally. So the photon emission also occurs naturally or spontaneously.

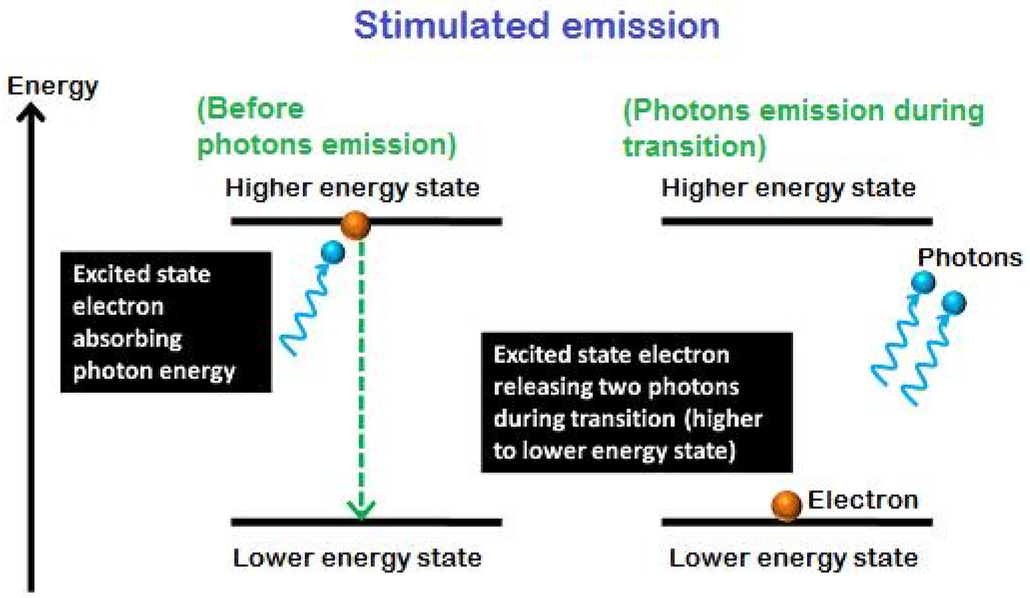
The photons emitted due to spontaneous emission do not flow exactly in the same direction of incident photons. They flow in the random direction.

Stimulated emission

The process by which electrons in the excited state are stimulated to emit photons while falling to the ground state or lower energy state is called stimulated emission.

Unlike the spontaneous emission, in this process, the light energy or photon energy is supplied to the excited electrons instead of supplying energy to the ground state electrons.

The stimulated emission is not a natural process it is an artificial process. In stimulated emission, the electrons in the excited state need not wait for natural spontaneous emission to occur. An alternative method is used to stimulate excited electron to emit photons and fall back to ground state.



The incident photon stimulates or forces the excited electron to emit a photon and fall into a lower state or ground state.

The energy of a stimulating or incident photon must be equal to the energy difference between the two electron shells.

In this process, the excited electron releases an additional photon of same energy (same frequency, same phase, and in the same direction) while falling into the lower energy state. Thus, two photons of same energy are released while electrons falling into the ground state.

In stimulated emission process, each incident photon generates two photons.

The photons emitted in the stimulated emission process will travel in the same direction of the incident photon.

Many ways exist to produce light, but the stimulated emission is the only method known to produce coherent light (beam of photons with the same frequency).

All the photons in the stimulated emission have the same frequency and travel in the same direction.

Selection rules

Selection rule or **transition rule**, formally constrains the possible transitions of a system from one quantum state to another. Selection rules have been derived for electromagnetic transitions in molecules, in atoms, in atomic nuclei, and so on. The selection rules may differ according to the technique used to observe the transition. The selection rule also plays a role in chemical reactions, where some are formally spin forbidden reactions, that is, reactions where the spin state changes at least once from reactants to products.

Possible 4 marks

1. What is called WKB approximation?
2. State and briefly explain Fermi's golden rule?
3. Discuss in detail the absorption and emission of radiation.
4. Explain the variational principle.
5. Explain the application of variation method of helium.
6. Write short notes on absorption of radiation.
7. Write short notes on emission of radiation.
8. Discuss the ground state of heluim atom.

Possible 10 marks

1. Explain (i) The variation principle (ii) variation method for excited states
2. Explain the Harmonic perturbation.
3. Evaluate $\langle x^2 \rangle$, $\langle p^2 \rangle$, $\langle V \rangle$ and $\langle T \rangle$ for the states of a harmonic oscillator.
4. A rotator having a moment of inertia I and an electric dipole moment μ executes rotational motion in a plane. Estimate the first-and second-order corrections to the energy levels when the rotator is acted on by an electric field ε in the plane of rotation.
5. A system in an unperturbed state n is suddenly subjected to a constant perturbation H'(r) which exist during time 0 to t. Find the probability for transition from state n to state k and show that it varies simple harmonically with,

   Angular frequency $=\frac{E_{k-E_n}}{2h}$ and amplitude = $4\frac{|H'_{kn}|^2}{(E_k-E_n)^2}$.
6. Obtain the selection rule for electric dipole transition of a linear harmonic oscillator.

KARPAGAM UNIVERSITY
DEPARTMENT OF PHYSICS
I M.Sc., PHYSICS
QUANTUM MECHANICS -I (17PHP202)
MULTIPLE CHOICE QUESTIONS

QUESTION	OPTION 1	OPTION 2	OPTION 3	OPTION 4	ANSWER
UNIT-V					
The expectation value of 1/r in the ground state of the hydrogen atom equals	a0	3/2a0	a0/4π	1/a0	1/a0
Oscillating electric and magnetic field associated with light can induce transition is an example of	time independent theory	variation theory	harmonic perturbation	WKB approximation	harmonic perturbation
Transition probability per unit time when transitions are extended to continuum is given by τ, where τ is equal to	$2\pi\lvert H_{ml}'\rvert^2\rho(E_m)$	$i\hbar\lvert H_{ml}'\rvert^2\rho(E_m)$	$\lvert H_{ml}'\rvert\rho(E_m)$	$(2\pi/\hbar)\lvert H_{ml}'\rvert^2\rho(E_m)$	$(2\pi/\hbar)\lvert H_{ml}'\rvert^2\rho(E_m)$
The time dependent theory was developed by	Einstein	Schrödinger	Pauli	Dirac	Dirac
The transition probability per unit time is proportional to	density of final states	$\lvert H_{ml}'\rvert$	Time ‘t’	t^2	density of final states
The validity of adiabatic approximation requires	smallness of $(\partial H/\partial t)$ but $E_m - E_s$ not too small	smallness of $(\partial H/\partial t)$ but $E_m - E_s$ large	large value of $(\partial H/\partial t)$ but $E_m - E_s$ small	large value of $(\partial H/\partial t)$ but $E_m - E_s$ not too small	smallness of $(\partial H/\partial t)$ but $E_m - E_s$ not too small
In sudden approximation, perturbation changes	at slow rate at narrow interval of time	at rapid rate in a very small interval of time	at rapid rate in large interval of time	at slow rate in large interval of time	at rapid rate in a very small interval of time
Frequency of radiation emitted during transition from m level to n level is	$E_m - E_n$	$(E_m - E_n)/\hbar$	$(E_m - E_n)/h$	$(E_n - E_m)/\hbar$	$(E_m - E_n)/h$
While calculating the first order perturbation the constant of integration is taken as zero in order that dm(t) to be zero at	$t = \infty$	$t = -\infty$	$t = 0$	$t = 2\pi$	$t = 0$
Height of the main curve in time dependent perturbation theory increase in proportion to	t^2	t	t^{-1}	t^3	t^2
The maximum value of $\mathrm{Sin}^2[(\omega_{ml}/2)/\omega_{ml}^2]$ occurs when ω_{ml} is	infinity	negative	zero	one	zero
The example for time dependent perturbation is	particle in a box	nuclear reactions and disintegration	harmonic oscillator	Stark effect	harmonic oscillator
Example for adiabatic approximation is	collision of gas molecules	harmonic oscillator	spectral analysis	interaction of electromagnetic waves	collision of gas molecules
Before the perturbation is applied to the system the first order transition constant $a_m^{(1)}$ be zero at	$t = \infty$	$t = 0$	$t = -\infty$	$t = t^2$	$t = 0$
In adiabatic approximation the Hamiltonian varies slowly with	position	time	position and time	velocity and distance	time
The molecular velocities and electron velocities in atoms are respectively	10^6 m/s and 10^2 m/s	10^2 m/s and 10^6 m/s	10^4 m/s and 10^8 m/s	10^8 m/s and 10^4 m/s	10^2 m/s and 10^6 m/s
A most common way of inducing transitions between stationary states of quantum system is by applying	sudden perturbation	constant perturbation	harmonic perturbation	adiabatic perturbation	harmonic perturbation
The transition probability per unit time is proportional to	$\lvert H_{ml}'\rvert$	$\lvert H_{ml}'\rvert^2$	t	t^2	$\lvert H_{ml}'\rvert^2$
Time dependent perturbation theory is often called	harmonic perturbation	constant perturbation	variation of constants	sudden approximation	harmonic perturbation
In case of time dependent perturbation theory, H′ might be zero except during the period	$t_1 < t < t_2$	$0 < t < \infty$	$t_1 \le t \le t_2$	$t_1 < t \le t_2$	$t_1 < t \le t_2$
In time dependent theory, perturbation is effective during the period	$0 < t < \infty$	$t_1 < t < t_2$	$t_1 \le t < t_2$	$t_1 < t \le t_2$	$t_1 < t \le t_2$
In time dependent theory, perturbation is effective, when H′ might be	negative	zero	one	infinite	one
The Schrödinger time equation for the system, in case of time dependent perturbation theory	$(H + H')\psi = (h/2\pi i)\partial\omega/\partial t$	$(H + H')\psi = (\hbar/2\pi i)\partial\omega/\partial t$	$(H + H')\psi = -(h/2\pi i)\partial\omega/\partial t$	$(H + H')\psi = -(\hbar/2\pi i)\partial\omega/\partial t$	$(H + H')\psi = -(h/2\pi i)\partial\omega/\partial t$

Breadth of the main curve in time dependent perturbation theory decreases inversely as	t^2	$–t$	$–t^2$	t	$–t$
Example for transition between stationary states in atoms is	oscillating electric and magnetic fields	electric field	magnetic field	harmonic oscillator	harmonic oscillator
The energy is transferred from the perturbing source to the system, this process is known as	absorption	emission	approximation	transformation probability	absorption
The energy is transferred to the perturbing source from the system, this process is known as	absorption	emission	approximation	transmission	emission
In adiabatic approximation the perturbation is turned on	fast	slowly	very slowly	very fast	very slowly
During the collision of gas molecules, the molecular velocities are low about	10 m/s	10^3 m/s	1 m/s	10^2 m/s	10^2 m/s
The gas molecules collide or approach each other, the process may be regarded as	adiabatic	isothermal	sudden approximation	perturbation	adiabatic
The condition of sudden approximation, by the help of uncertainty relation $\Delta E . \Delta T = \hbar$, is expressed as	$\Delta x . \Delta p \approx \hbar$	$\hbar / \Delta E >> t_0$	$\Delta x . \Delta t \approx \hbar$	$\Delta p . \Delta t \approx \hbar$	$\hbar / \Delta E >> t_0$
In sudden approximation the probability of transition from state k to state f will be given by	$\lvert a_f \rvert^2 = \lvert \langle f \vert H' \vert k \rangle \rvert^2 / \hbar^2 \omega_{fk}^2$	$\lvert a_f \rvert^2 = \lvert \langle f \vert H' \vert k \rangle \rvert / \hbar^2 \omega_{fk}^2$	$\lvert a_f \rvert^2 = \lvert \langle f \vert H' \vert k \rangle \rvert / \hbar \omega_{fk}$	$\lvert a_f \rvert^2 = \lvert \langle f \vert H' \vert k \rangle \rvert^2 / \hbar \omega_{fk}$	$\lvert a_f \rvert^2 = \lvert \langle f \vert H' \vert k \rangle \rvert^2 / \hbar^2 \omega_{fk}^2$
There is no transition between the states of the system then,	$\langle f \vert H(t) k \rangle = \infty$	$\langle f \vert H(t) k \rangle = 1$	$\langle f \vert H(t) k \rangle = 0$	$\langle k \vert H(t) f \rangle = 0$	$\langle f \vert H(t) k \rangle = 0$
The velocity of electrons in atoms are about	10^8 m/s	10^4 m/s	10^2 m/s	10^6 m/s	10^6 m/s
A particle executes a harmonic motion along x-axis and possesses a charge +e, dipole moment is	– ex	Ex	eE	– eE	eE
In WKB approximation, when V(x) is a constant, then the waves become	spherical	cylindrical	plane	circle	plane
In WKB approximation, the value of propagation constant k is	$[2m(E – V)]/\hbar$	$[2m(E – V)]^{1/2} /\hbar$	$[2m(E – V)]/\hbar^2$	$[2m(E – V)]^{1/2} /\hbar^2$	$[2m(E – V)]^{1/2} /\hbar$
The variation method is applicable for the system of	lowest energy state	highest energy state	both lowest and highest energy state	first excited state	lowest energy state
The validity of WKB approximation is	$[\lambda \lvert \partial V/\partial x \rvert]/4\pi(E – V) < 1$	$[\lambda \lvert \partial V/\partial x \rvert]/4\pi(E – V) > 1$	$4\pi(E – V)/ [\lambda \lvert \partial V/\partial x \rvert] < 1$	$4\pi(E – V)/ [\lambda \lvert \partial V/\partial x \rvert] > 1$	$[\lambda \lvert \partial V/\partial x \rvert]/4\pi(E – V) < 1$
WKB approximation is applied to only situation in which the potential energy is slowly varying function of	time	position	position and time	constant	position
In time dependent perturbation theory Hamiltonian is divided into	3 parts	2 parts	5 parts	4 parts	2 parts
Which term represent simple unperturbed hamiltonian?	H	H0	H'	H'0	H0
Which term represent small time dependent perturbed hamiltonian?	H	H0	H'	H'0	H'
In adiabatic approximation H contains the parameter change	very slow wrt to time	very fast wrt to time	very slow wrt to height	very fast wrt to time	very slow wrt to time
In sudden approximation H is _______________ in time	0	infinite	constant	vary	constant
Hamiltonian of the system is _________	H=H0+H^2	H=H0+H^3	H=H'0+H^2	H=H0+H'	H=H0+H'
The adiabatic approximation occurs in the collision of _____________ molecules	solid	liquid	quasi	gas	gas
The molecular velocities are usually low about	10^2 m/s	10^3 m/s	10^-2 m/s	10^-3 m/s	10^2 m/s
The transition probability of emission per unit time is proportional to	intensity of radiation present	radiation	scattering	dispersion	intensity of radiation present
The transition probability of absorption and emission between any pair of states are	0	infinite	positive	same	same