DISCIPLINE SPECIFIC CORE COURSE – DSC - 14: QUANTUM MECHANICS – I

Course Title & Code	Credits	Credit distribution of the course			Eligibility Criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical		
Quantum Mechanics – I DSC – 14	4	3	0	1	Class XII pass with Physics and Mathematics as main subjects	Light and Matter, and Elements of Modern Physics papers of this course or their equivalents

LEARNING OBJECTIVES

The development of quantum mechanics has revolutionized the human life. In this course, the students will be exposed to the probabilistic concepts of basic non-relativistic quantum mechanics and its applications to understand the sub atomic world.

LEARNING OUTCOMES

After completing this course, the students will be able to,

- Understand the applications of the Schrodinger equation to different cases of potentials namely finite square potential well, harmonic oscillator potential.
- Solve the Schrodinger equation in 3-D.
- Understand the spectrum and eigen functions for hydrogen atom
- Understand the angular momentum operators in position space, their commutators, eigenvalues and eigen functions.
- In the laboratory course, the students will be able to use computational methods to
    - Solve Schrödinger equation for ground state energy and wave functions of various simple quantum mechanical one- dimensional potentials
    - Solve Schrödinger equation for ground state energy and radial wave functions of some central potentials

SYLLABUS OF DSC - 14

THEORY COMPONENT

Unit – I **(10 Hours)**

General discussion of bound states in an arbitrary potential: Continuity of wave function, boundary conditions and emergence of discrete energy levels. Application to energy eigen states for a particle in a finite square potential well, Momentum space wavefunction, Time evolution of Gaussian Wave packet, Superposition Principle, linearity of Schrodinger Equation, General solution as a linear combination of discrete stationary states, Observables as operators, Commutator of position and momentum operators, Ehrenfest's theorem.

Unit – II **(8 Hours)**

Harmonic oscillator: Energy eigen values and eigen states of a 1-D harmonic oscillator using algebraic method (ladder operators) and using Hermite polynomials. Zero point energy and uncertainty principle.

Unit – III **(15 Hours)**

Schrödinger Equation in three dimensions: Probability and probability densities in 3D. Schrödinger equation in spherical polar coordinates, its solution for Hydrogen atom solution using separation of angular and radial variables, Angular momentum operator, quantum numbers and spherical harmonics. Radial wave functions from Frobenius method; shapes of the probability densities for ground and first excited states; Orbital angular momentum quantum numbers l and m_l, s, p, d shells.

Unit – IV **(12 Hours)**

Angular momentum: Commutation relations of angular momentum operators; concept of spin and total angular momentum; ladder operators, eigenvalues, eigenvectors; Pauli matrices; addition of angular momenta

References:

Essential Readings:

1) Quantum Mechanics: Theory and Applications, A. Ghatak and S. Lokanathan, 6th edition, 2019, Laxmi Publications, New Delhi.
2) Introduction to Quantum Mechanics, D. J. Griffith, 2nd edition, 2005, Pearson Education.
3) A Text book of Quantum Mechanics, P. M. Mathews and K. Venkatesan, 2nd edition, 2010, McGraw Hill.
4) Quantum Mechanics, B. H. Bransden and C. J. Joachain, 2nd edition, 2000, Prentice Hall
5) Quantum Mechanics: Concepts and Applications, 2nd edition, N. Zettili, A John Wiley and Sons, Ltd., Publication
6) Atomic Physics, S. N. Ghoshal, 2010, S. Chand and Company

Additional Readings:

1) Quantum Mechanics for Scientists & Engineers, D. A. B. Miller, 2008, Cambridge University Press.
2) Introduction to Quantum Mechanics, R. H. Dicke and J. P. Wittke, 1966, Addison-Wesley Publications
3) Quantum Mechanics, L. I. Schiff, 3rd edition, 2010, Tata McGraw Hill.
4) Quantum Mechanics, R. Eisberg and R. Resnick, 2nd edition, 2002, Wiley
5) Quantum Mechanics, B. C. Reed, 2008, Jones and Bartlett Learning.
6) Quantum Mechanics, W. Greiner, 4th edition, 2001, Springer.
7) Introductory Quantum Mechanics, R. L. Liboff, 4th edition, 2003, Addison Wesley

PRACTICAL COMPONENT

(15 Weeks with 2 hours of laboratory session per week)

At least 4 programs must be attempted. The implementation may be done in C++/Scilab /Python. Use of available library functions may be encouraged. Similar programs may be added.

Unit 1

1) Visualize the spherical harmonics by plotting the probability density for various values of the quantum numbers (*l, m*)

2) Use the analytical solution for a particle in finite potential well. Numerically solve the transcendental equation one gets after putting the continuity and boundary conditions to determine the energy eigenvalues for various values of the potential width and depth. Plot the corresponding normalised eigen functions.

Unit 2

Solve the Schrödinger equation using shooting/finite difference or any other method for the following simple 1-D potentials and compare with the analytical solutions:

1) Particle in a box
2) Particle in a finite potential well
3) Harmonic Potential

Unit 3

Solve the s-wave Schrodinger equation for the following cases.

$$\frac{d^2u}{dr^2} = A(r)u(r), A(r) = \frac{2m}{\hbar^2}[V(r) - E],$$

1) Ground state and the first excited state of the hydrogen atom:

$$V(r) = \frac{-e^2}{r}$$

Here *m* is the reduced mass of the electron. Obtain the energy eigenvalues and plot the corresponding wave functions. Remember that the ground state energy of the hydrogen atom is ≈ -13.6 eV. Take e = 3.795 $(eVÅ)^{1/2}$, ħc = 1973 (eVÅ) and m = $0.511\text{x}10^6$ eV/c^2.

2) For an atom in the screened coulamb potential

$$V(r) = \frac{-e^2}{r}e^{\frac{-r}{a}}$$

Here *m* is the reduced mass of the system (which can be chosen to be the mass of an electron). Find the energy (in eV) of the ground state of the atom to an accuracy of three significant digits. Also, plot the corresponding wavefunction. Take e = 3.795 $(eVÅ)^{1/2}$, m = $0.511\text{x}10^6$ eV/c^2, and a = 3 Å, 5 Å, 7 Å. In these units ħc = 1973 (eVÅ). The ground state energy is expected to be above -12 eV in all three cases.

Unit 4

Solve the s-wave Schrodinger equation $\frac{d^2u}{dr^2} = A(r)u(r), A(r) = \frac{2m}{\hbar^2}[V(r) - E]$, for a particle of mass *m* for the following cases

1) Anharmonic oscillator potential

$$V(r) = \frac{1}{2}kr^2 + \frac{1}{3}br^3$$

for the ground state energy (in MeV) of particle to an accuracy of three significant digits. Also, plot the corresponding wave function. Choose m = 940 MeV/c^2, k = 100 MeV fm^{-2}, b= 0, 10, 30 MeV fm^{-3}. In these units, $c\hbar$ = 197.3 MeV fm. The ground state energy is expected to lie between 90 and 110 MeV for all three cases.

2) For the vibrations of hydrogen molecule with Morse potential

$$V(r) = D(e^{-2ar'} - e^{-ar'}), r' = \frac{r - r_0}{r}$$

Here m is the reduced mass of the two-atom system for the Morse potential

Find the lowest vibrational energy (in MeV) of the molecule to an accuracy of three significant digits. Also plot the corresponding wave function.

Take: $m = 940 \times 10^6$ eV/c^2, $D = 0.755501$ eV, $\alpha = 1.44$, $r_0 = 0.131349$ Å

References for laboratory work:

1) Schaum's Outline of Programming with C++, J. Hubbard, 2000, McGraw-Hill Education.
2) C++ How to Program, P. J. Deitel and Harvey Deitel, 2016, Pearson
3) Scilab (A Free Software to Matlab): H. Ramchandran, A. S. Nair, 2011, S. Chand and Co
4) Documentation at the Python home page (https://docs.python.org/3/) and the tutorials there (https://docs.python.org/3/tutorial/).
5) Documentation of NumPy and Matplotlib: https://numpy.org/doc/stable/user/ and https://matplotlib.org/stable/tutorials/
6) Computational Physics, Darren Walker, 1st edition, 2015, Scientific International Pvt. Ltd
7) An Introduction to Computational Physics, T. Pang, 2010, Cambridge University Press
8) A Guide to MATLAB, B. R. Hunt, R. L. Lipsman, J. M. Rosenberg, 3rd edition, 2014, Cambridge University Press