

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATION- 2024

B.Tech-VII Semester (CSE/BT/BI)

COURSE CODE (CREDITS): 22B1WPH731(3)

MAX. MARKS: 25

COURSE NAME: Computational Nanotechnology

COURSE INSTRUCTORS: Dr. Santu Baidya

MAX. TIME: 1 Hour 30 Minutes

Note: (a) All questions are compulsory.

(b) The candidate is allowed to make Suitable numeric assumptions wherever required for solving problems

Q.No	Question	CO	Marks
Q1	Write down total Hamiltonian for any material with N electrons and Z number of atoms and explain each term. What is Born-Oppenheimer Hamiltonian?	CO-1	3+2
Q2	Using Taylor series expansion, find y at x=0.1, 0.2 correct to three significant digit given $\frac{dy}{dx} - 2y = 3e^x$, $y(0) = 0$.	CO-3	3
Q3	What is Hartree approximation and Hartree product? How does Hartree approximation solve many-electron problem in materials? State the disadvantages of Hartree approximation theory.	CO-5	2+3+2
Q4	What is N electron Slater determinant for many electrons wave function in Hartree-Fock approximation? Prove that Pauli exclusion principle and fermion anti-symmetry properties hold true with Slater determinant wave function.	CO-1	2+3
Q5	Write the numerical methods for solving eigenvalues and eigenstates of a particle inside a 1d infinite potential quantum well $V(x) = 0; 0 \leq x \leq a$ and $V(x) = \infty; elsewhere$, where a is the width of the well. Write a python code to plot probability density for a particle inside a quantum well.	CO-3	2+3