JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATION- 2023

B.Tech-I Semester (CSE/IT/ECE/CE/BT/BI)

COURSE CODE (CREDITS):22B1WPH731 MAX. MARKS: 25

COURSE NAME: Computational Nanotechnology

COURSE INSTRUCTORS: Dr. Santu Baidya MAX. TIME: 1 Hour 30 Minutes

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Note: *(a)All questions are compulsory.*

(b)Marks are indicated against each question in square brackets.

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

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Q1) Write down the Hamiltonian for a material with N_e number of electrons and N_I number of ions and explain each term in the Hamiltonian. Write the eigenvalue equation (Schrodinger equation) for this Hamiltonian. **[CO-3] [2+1]**

Q2) What is Born-Oppenheimer approximation (explain from Hamiltonian)? Why is it called adiabatic approximation? **[CO-3] [2+1]**

Q3) Write down the Hartree approximation and explain how does it help to solve many-electron problem in materials? What is the disadvantage of the Hartree approximation to explain quantum state of electrons in a material. **[CO-5] [2+1]**

Q4) Write down the Slater determinant form of wave function for a 2-electron system (e.g., He). Show that a Slater determinant wave function represents correctly electronic wave function properties, such as Pauli exclusion principle and anti-symmetric property. **[CO-3] [1+2]**

Q5) What is exchange energy in Hartree-Fock approximation? Write the koopman's theorem from Hartree-Fock approximation. **[CO-3] [1+2]**

Q6) Write down the second order differential equation (Schrodinger equation) for an electron in a one dimensional infinite quantum potential well where potential function is defined as $V(x) = 0$ for $0 \leq x \leq a$ (a is the potential well width along x axis) and $V(x) = \infty$ for $x \geq a$ and $x \leq 0$. What is the eigenvalue for the n^{th} quantum state for this electron. Then write down the python code to solve the second order differential equation for the solution to this quantum mechanical problem. **[CO-2] [2+3+5]**