JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2023

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

COURSE CODE (CREDITS): 24P1WPH132 (3)

COURSE NAME: Electronic Structure Theory

COURSE INSTRUCTORS: Dr. Santu Baidya

MAX. MARKS: 15

MAX. TIME: 2 Hours

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

Q1. What is the Born-Oppenheimer approximation? Write down the total Hamiltonian of a material with N_e number of electrons and N_A number of nucleus. **[CO-1] [2+3]**

Q2. What is the Hartree product? State the Hartree approximation? **[CO-2] [2+3]**

Q3. Use the Hartree approximation to show the ground state energy of a He atom has discrepancy from original ground state energy. **[CO-3] [5]**