JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2025

Ph.D. Course Work (PMS)

COURSE CODE (CREDITS): 24P1WPH133 (3)   MAX. MARKS: 35

COURSE NAME: Electronic Structure Theory

COURSE INSTRUCTORS: Dr. Santu Baidya   MAX. TIME: 2 Hours

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 assumptions for Thomas-Fermi model. What is equation for Thomas-Fermi model?	CO-1	3+2
Q2	What is Free electron approximation and Independent electron approximation? What is Hubbard U? Explain Hubbard model for one dimensional hydrogen atom chain.	CO-3	2+1+2
Q3	What interaction is ignored in Hartree-Fock approximation? Write down integral form of exhange interaction for a many-electron system.	CO-5	1+1+3
Q4	State two Hohenberg-Kohn theorems. Prove the two theorems.	CO-1	4+6
Q5	What is Kohn-Sham approximation. Write down the computational flow chart to carry out Kohn-sham calculation. Why is it called self-consistent method?	CO-3	2+2+1
Q6	What is principle behind classical molecular dynamics? Write down the flow chart.	CO-2	3+2