



DEPARTMENT OF PHYSICS

"T3, Examination 2017-18"

Semester:IV

Subject:Condensed Matter -II

Branch: Physics

Course Type: Core

Time: 3 Hours

Max.Marks: 100

Date of Exam:18/05/2018

Subject Code:PHH621

Session:II

Course Nature:Hard

Program: M.Sc

Signature: HOD/Associate HOD:

Note: Part A: Attempt any two questions. Each question carry 10 marks.

Part B: Attempt any two questions. (Each question carry 20 marks).

Part c: Attempt any two questions. (Each question carry 20 marks).

PART-A (Attempt all)

Q1. Describe Huckel Molecular orbital model. What are its various assumptions? Apply Huckel molecular orbital theory to obtain energies and wave functions of an ethylene molecule. (10)

Q2. Consider butadiene in the lowest excited state.

(a) Calculate the π electron charge on each atom.

(b) Calculate the π bond order for each bond. (10)

Q3. Describe in detail, how Slater type orbital differs from Gaussian type orbital? (10)

PART-B (Attempt any Two)

Q4.What is a density matrix? Describe its various properties. Write down the density matrix in terms of basis set. For a two level system, using density operator, calculate the various density matrix elements.

(20)

Q5. Derive Hartree Fock theory in Density matrix form. (20)

Q6. Why Hartree Fock slater determinant is an inexact representation of the wave function, but the DFT determinant for a system of non-interacting electrons is exact for this particular wave function? Discuss in detail. (20)

PART-C (Attempt any Two)

Q7. State and prove Hohenberg-Kohn theorems. (20)

Q8. Derive the Expression for the Kohn Sham energy and the KS equations. (20)

Q9. Describe the formulation of density functional theory (DFT). Discuss various applications of DFT along with its strength and weakness. (20)
