



**Q.1. Answer the following short questions:**

**(6x5=30)**

- a) What is Born-Oppenheimer approximation? Explain it briefly. Also, write Hamiltonian term and Schrödinger equation involving assumptions/variables of Born-Oppenheimer approximation.
- b) Explain free electron gas model. Write assumptions of classical free-electron theory.
- c) State Bloch theorem. Explain the concept of Bloch electron and Bloch wave-functions.
- d) Explain at least two physical phenomenon's which cannot be explained on the basis of free electron model.
- e) Explain the concept of effective mass of an electron. What are the factors which make the consideration of effective mass important?
- f) Discuss electron-electron interactions in solids. How screening the Hartree-Fock approximation reduces the importance of electron-electron interactions.

**Answer the following questions.**

**(3x10=30)**

- Q. 2** Describe nearly free electron model and explain how this model helps in forming the energy band gaps in solids.
- Q. 3** Explain an augmented-plane wave (APW) method in detail. Solve Schrödinger wave-equation and explain the limitations of APW method in calculating the band structure of solids.
- Q. 4** Define the term pseudopotential. Assume plane-wave like function,  $f_n(k,r)$  and establish orthogonality condition for acceptable wave-functions. For a monoatomic crystal, write Hamiltonian with pseudopotential term and establish Schrödinger equation involving atomic pseudopotentials.