Exam.Code:1029
Sub. Code: 7542

2023

M. Tech. (Material Science and Technology)

First Semester

MT-102: Quantum Physics in Atoms and Molecules

Time allowed: 3 Hours Max. Marks: 50

NOTE: *Attempt five questions in all, including Question No. I which is compulsory and selecting two questions from each Part.*

x-x-x

1. Attempt the following: (This question is compulsory) (2x5=10)

(a) Why can't we observe Compton effect with visible light?

(b) Show that Quantum mechanical Harmonic oscillator problem is in accord with Correspondence principle.

(c) On what factors does thermionic emission from any metal depends?

(d) What is the difference between between ab-initio methods and DFT?

(e) Compare the ground state momentum of the particle in the two potential wells having same width such that one of the wells has finite height and other has infinite height.

PART A

2. (a) What are the salient features of Black body radiation spectrum? Show that R-J law failed but Planck's distribution law explains the blackbody radiation spectrum. (6)

(b) What effect on the scattering angle in the Davisson Germer experiment does increasing the electron energyhave? (2)

(c) In an experiment, tungsten cathode, which has a threshold wavelength 2300Å, is irradiated by ultraviolet light of wavelength 1800Å. Calculate the maximum energy of emitted photoelectrons and work function of tungsten. (2)

3. (a) Establish the time dependent and time independent form of Schrodinger equation. (5)

(b) Using Uncertainity Principle, show that electrons cannot reside inside the nucleus. (2)

(c) What are matter waves? Show that matter waves travel with the velocity of the body. (3)

4. (a) Show that there is a finite probability of finding the particles across the barrier even if the energy of particles E is less than barrier height. Also, determine the flux of incident particles, reflected particles, and the particles transmitted. Also plot the behaviour of wavefunction in various regions of barrier. (6)

(b) A particle limited to x axis has the wave function $\psi = ax$ between $x = 0$ and $x = 1$; $\psi = 0$ elsewhere. Findthe expectation value of x. (2)

(c) Find the commutator [x, H]. (2)

PART B

5. (a) Give basic postulates of free electron theory and tell what modifications have been considered in Kronig Penney (K-P) Model to remove the failures of classical free electron theory. Show that if $V = 0$, the energy spectrum proposed by K-P model becomes continuous and it is that of the free particle. Use physical arguments to justify this result. (7)

(b) Explain how resistivity of metals varies with composition and temperature. (3)

6. (a) Derive an expression for effective mass? Discuss its variation and that of group velocity in a band. (5)

(b) Discuss briefly the various theoretical models proposed to understand the specific heat of solids, citing clearly the basic assumptions and limitations of the models if any. (3)

(c) Calculate the relaxation time of electron in sodium if the Fermi energy of sodium is 3.1 eV and electrical conductivity is 2.1 x 10^7 S/m at 0 K. (2)

7. (a) What is Born Oppenheimer approximation? How does it simplify Schrodinger many body equation? (5)

(b) What do you mean by Local density approximation in DFT? How is it different from GGA? Give the name of any two software codes based on DFT. (5)

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