This question paper contains 3 printed pages

6991 *Your Roll No*

M.Tech. / II Sem.

NANO SCIENCE AND NANO TECHNOLOGY
Paper :NSNT – 201 : Quantum Mechanics

J

Time 3 hours Maximum Marks 38

(Write your Roll No on the top immediately on receipt of this question paper)
Attempt any 5 questions in all
($h=6.626 \times 10^{-34}$ J s) Some useful integrals can be found at the end of the question paper

1 Attempt any *four* parts

(a) Show that if the eigenfunctions of an operator are to be real, the operator should be Hermitian

(b) For a particle in a one-dimensional box, show that

$$\sigma_{p_x}\sigma_x \geq \frac{\hbar}{2}$$

(c) Why is it necessary to functionalize CdSe quantum dots with groups such as organic acids to make them useful in bioanalytical applications?

(d) The 3s band of solid Na will have as many orbitals (each delocalized over the entire solid) as the number of 3s orbitals from Na atoms in the sample If each orbital of the sample can hold two spin-paired 3s valence electrons, to what extent will the band be filled?

(e) Scanning tunnelling microscopy depends on the flow of electricity (current) between a surface and an atomically sharp probe tip Plot the current versus tip to surface distance

(f) Prove that the kinetic energy operator is hermitian

8

2 (a) Consider the problem of a particle of mass *m* in a cubic box of length *L* If one side of the box is distorted by a small distance *dL* in one direction, the degeneracy of the first triply degenerate level is lifted Derive the expression for the energies of the first excited state (2,1,1), (1,2,1) and (1,1,2) of the particle in the distorted box

(b) Calculate the energy difference between the resulting two sets of levels in Joules, if the particle has a mass 1.5×10^{-27} kg, the box of length 0.1 nm is distorted by 0.008 nm

100

(c) An electron (charge e) is confined to a cubic box of length L. Find the first order correction to the first excited energy level (which is triply degenerate) if an electric field of strength ε is applied parallel to the z-axis ($\perp$ to x and y). The perturbation may be taken as

$$H' = \varepsilon e z$$

2,2,3

3 The radial part of the Hamiltonian of a hydrogen atom is

$$\hat{H} = -\frac{1}{2r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{1}{r}$$

in atomic units, and the normalized eigenfunctions are $\frac{1}{\sqrt{\pi}}e^{-r}$

(a) Prove the following

$$<V> = -2<T>$$

average

where $<V>$ is the average potential energy and $<T>$ is the kinetic energy

(b) Show that the average distance of the electron in the ground state of the hydrogen atom is 1.5 times the most probable distance

3,4

4 (a) The Hamiltonian of an oscillator is given by $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}$ where $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$. Use the operators $\hat{b}^+$ and $\hat{b}$

$$\hat{b}^+ = \frac{1}{\sqrt{2m\hbar\omega}}[\hat{p} + i\omega m\hat{x}]$$

$$\hat{b} = \frac{1}{\sqrt{2m\hbar\omega}}[\hat{p} - i\omega m\hat{x}]$$

to estimate $<p^2>$ and $<x^2>$ for the n^{th} state (ψ_n)

(b) Give reasons why the following wavefunctions cannot be satisfactory for the harmonic oscillator

i $(2 - \xi - 3\xi^2)\exp(-\xi^2/2)$

ii $2\xi\exp(\xi^2/2)$

5,2

5 (a) Write down the Hamiltonian for the helium atom in atomic units

(b) Calculate the expectation value of the energy in the ground state assuming the ground state wavefunction to be a product of the two hydrogen wavefunctions Suggest an improvement in the choice of the wavefunction

[Given $\iint \varphi_{1s_1}^{(0)} \varphi_{1s_2}^{(0)} \frac{1}{r_{12}} \varphi_{1s_1}^{(0)} \varphi_{1s_2}^{(0)} d\tau = \frac{5}{8} Z$]

2,5

6 (a) (i) From the classical relation $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ for the angular momentum, $\mathbf{L}$, obtain expressions for the three components L_x, L_y and L_z in terms of the components of $\mathbf{r}$ and $\mathbf{p}$

(ii) Write down the quantum mechanical operators for the three components of the angular momentum in Cartesian coordinates

(b) The rigid rotator wavefunction depends on the variables θ and φ Show that the φ equation $\frac{1}{\Phi(\varphi)} \frac{d^2\Phi(\varphi)}{d\varphi^2} + \lambda = 0$ yields the solution $\Phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$ where $m = \sqrt{\lambda} = 0, \pm 1, \pm 2, \pm 3,$

3,4

Some useful integrals

$$\int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

$$\int_0^{\infty} e^{-\alpha x^2} dx = \frac{1}{2}\left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}}$$

$$\int_0^{\infty} x^{2n} e^{-\alpha x^2} dx = \frac{1 \cdot 3 \cdots (2n-1)}{2^{n+1}} \sqrt{\frac{\pi}{\alpha^{2n+1}}}$$

$$\int_0^{\infty} x^{2n+1} e^{-ax^2} dx = \frac{n!}{2a^{n+1}}$$