PC2101

ONE HOUR THIRTY MINUTES

A list of constants is enclosed.

UNIVERSITY OF MANCHESTER

Fundamentals of Quantum Mechanics

20th January 2004, 2.00 p.m. - 3.30 p.m.

Answer **ALL** parts of question 1 and **TWO** other questions

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Electronic calculators may be used, provided that they cannot store text.

The numbers are given as a guide to the relative weights of the different parts of each question.

P.T.O.

1. (a) Calculate the kinetic energy of an electron which has a de Broglie wavelength of 1.5×10^{-10} m. [5 marks]

(b) A particle has a wavefunction given by $\Psi(x,t)$. What are the physical interpretations of $|\Psi|^2$ and $\int_{-\infty}^{\infty} \Psi^*(x,t) \left(-i\hbar\frac{\partial}{\partial x}\right) \Psi(x,t)dx$? [5 marks]

(c) Define the commutator $[\hat{A}, \hat{B}]$ of two quantum mechanical operators $\hat{A}$ and $\hat{B}$. What are the physical implications if $[\hat{A}, \hat{B}] = 0$? [5 marks]

(d) The mass of an oxygen atom is 2.7×10^{-26} kg, and the covalent bond between the two oxygen atoms in an O_2 molecule has a spring constant of 1200 N m^{-1}. What is the zero-point vibrational energy of an oxygen molecule? [5 marks]

(e) The wave function of a particle, in spherical polar coordinates, is

$$\psi(r,\theta,\phi) = \frac{N\mathrm{e}^{-\alpha r}}{r} \sin\theta\cos\theta\ \mathrm{e}^{i\phi},$$

where N and α are constants. Describe the orbital angular momentum properties of the particle. [5 marks]

2. Two possible wavefunctions for states of a particle, with definite energies E_1 and E_2, are:

$$\Psi_1(x,t) = \psi_1(x)\mathrm{e}^{-iE_1t/\hbar}$$

and

$$\Psi_2(x,t) = \psi_2(x)\mathrm{e}^{-iE_2t/\hbar}.$$

Explain why these are called stationary states. [3 marks]

Write down a wavefunction for a non-stationary state for which the expectation value of the energy is $\frac{1}{3}E_1 + \frac{2}{3}E_2$. [3 marks]

Show that the probability density for position for this state oscillates with time. [8 marks]

Calculate the frequency of the oscillations if $E_1 = 1.2$ eV and $E_2 = 0.3$ eV. [4 marks]

From a semi-classical perspective, what would be the consequences of such oscillations if the particle were electrically charged? [2 marks]

The expectation value of the energy-squared for this state is $\frac{1}{3}E_1^2 + \frac{2}{3}E_2^2$. Calculate the uncertainty in the energy. [5 marks]

3. A particle of mass m moves in a two-dimensional simple harmonic oscillator potential of the form

$$V(x, y) = \frac{1}{2}m\omega_o^2(x^2 + y^2),$$

where ω_o is a constant. Write down the two-dimensional version of the time-independent Schrödinger equation for this situation. [4 marks]

Consider a stationary-state solution of the time-dependent equation of the form

$$\Psi_{n_x,n_y} = \psi_{n_x,n_y}(x, y)\mathrm{e}^{-iE_{n_x,n_y}t/\hbar} = \phi_{n_x}(x)\phi_{n_y}(y)\mathrm{e}^{-iE_{n_x,n_y}t/\hbar},$$

where n_x and n_y are quantum numbers. What is the energy of this state, E_{n_x,n_y}, in terms of n_x, n_y and ω_o? [3 marks]

What is the degeneracy of the state with energy $5\hbar\omega_o$. [3 marks]

The first two functions ϕ_n take the form $\phi_0(x) \sim \mathrm{e}^{-x^2/2a^2}$ and $\phi_1(x) \sim x\mathrm{e}^{-x^2/2a^2}$. Ignoring normalisation constants, write $\psi_{1,0}(x, y)$ and $\psi_{0,1}(x, y)$ in both cartesian and plane-polar coordinates (r, ϕ), and show how two new orthogonal wavefunctions of the form $R(r)\mathrm{e}^{im\phi}$ can be constructed. [10 marks]

Describe the energy and angular momentum properties of the new wavefunctions. [5 marks]

4. The time-independent Schrödinger equation for the hydrogen atom can be written as

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{2mr^2}\hat{L}^2\psi-\frac{e^2}{4\pi\epsilon_0 r}\psi=E\psi,$$

which has solutions of the form

$$\psi(r,\theta,\phi)=R(r)Y(\theta,\phi).$$

Explain the significance of the separation of the wave function into radial and angular parts. [3 marks]

By writing $R(r)=u(r)/r$, obtain the equation satisfied by $u(r)$. [9 marks]

The following is one solution to the above equation:

$$\psi(r,\theta,\phi)=\sqrt{\frac{1}{64\pi a_0^3}}\left(\frac{r}{a_0}\right)\mathrm{e}^{-r/a_0}\sin\theta\;\mathrm{e}^{-i\phi}.$$

What results would be obtained for measurements of the square of the total angular momentum, L^2, and the z-component of the angular momentum, L_z, for this state? [3 marks]

For an electron with this wavefunction, calculate the *relative* probability of obtaining answers:

(a) a_0 and $2a_0$ in measurements of r,
(b) $0°$ and $45°$ in measurements of ϕ,
(c) $30°$ and $60°$ in measurements of θ. [10 marks]