Name: Pratik Sen

Roll No. ____________

Indian Institute of Technology Kanpur
Department of Chemistry
CHM102A (Quiz 1) 2014-15-II
FM: 30; Answer all questions; **Time: 30 mins**

SECTION

Information:
1 amu = 1.67×10^{-27} kg; $m_e = 9.1 \times 10^{-31}$ kg; $c = 3 \times 10^8$ ms^{-1}; $h = 6.626 \times 10^{-34}$ Js

1. (a) (**Marks: 4**) 200 nm light ejects electrons from sodium surface with kinetic energy of 5.36×10^{-19} J. Calculate the kinetic energy of the ejected electron when 350 nm light falls on sodium surface.

$$(1)\left[\frac{hc}{200\times10^{-9}} = \phi + 5.36\times10^{-19}\,J;\quad \frac{hc}{350\times10^{-9}} = \phi + KE\right.$$

$$\therefore KE = 5.36\times10^{-19} - 6.626\times10^{-34}\times3\times10^{8}\left(\frac{1}{200\times10^{-9}} - \frac{1}{350\times10^{-9}}\right)J\Big](1)$$

$$= 1.1\times10^{-19}\,J\Big](1)$$

(b) (**Marks: 3**) The wavelength of F^- ion accelerated through a potential of 100 volts is 'x' nm. Find the wavelength when the F^- ion being accelerated through a potential of 900 volts.

$$(1)\left[\frac{1}{2}mv^2 = Ve;\quad p = mv = \sqrt{2mVe}\right.$$

$$(1)\therefore\left[\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mVe}} = C\frac{1}{\sqrt{V}}\right.$$

$$\lambda_{V=100} = c\frac{1}{\sqrt{100}} = x$$

$$\lambda_{V=900} = c\frac{1}{\sqrt{900}} = \frac{x}{3}\Big](1)$$

(c) (**Marks: 3**) Find if the following functions are eigenfunctions of the linear momentum (p_x). If so also find the eigenvalue. (i) $\sin kx + \cos kx$ (ii) e^{ikx} where k is a constant.

$$\hat{p}_x = -i\hbar\frac{d}{dx}\Big](1)$$

(i) $-i\hbar\frac{d}{dx}(\sin kx + \cos kx) = i\hbar k(\cos kx - \sin kx)$

$\therefore$ Not an eigenfunction] (1)

(ii) $-i\hbar\frac{d}{dx}e^{-ikx} = k\hbar\, e^{-ikx}$

$\therefore$ An eigenfunction, eigenvalue is $k\hbar$] (1)

2. Consider a particle of mass m moving in a two dimensional rectangular box of lengths a (along x) and $a/2$ (along y). The potential energy is zero inside the box and infinite otherwise.

(a) (**Marks: 3**) Write the expressions of the energy and wavefunction of the ground state of the particle.

$$E_{11} = \frac{h^2}{8ma^2} + \frac{h^2}{8m(a/2)^2} = \frac{5h^2}{8ma^2} \;] \; (1)$$

$$\psi_{11}(x,y) = \sqrt{\frac{2}{a}}\sqrt{\frac{4}{a}} \sin\frac{\pi x}{a} \sin\frac{2\pi y}{a} \;] \; (2) \text{ or } (1)$$

(b) (**Marks: 3**) If the energy of an excited state of the particle is 4 times that of the ground state, identify the excited state in terms of its quantum numbers.

$$\frac{n_x^2 h^2}{8ma^2} + \frac{4n_y^2 h^2}{8ma^2} = \frac{20h^2}{8ma^2} \;] \; (1)$$

$$\therefore n_x^2 + 4n_y^2 = 20 \Rightarrow n_x = 4,\ n_y = 1 \;] \; (2)$$

another possibility

$$n_x = 2,\ n_y = 2$$

(c) (**Marks: 1**) What is the degeneracy of the excited state in 2(b)?

degeneracy = 2] (1) or (0)

(d) (**Marks: 3**) If the edge lengths of the box become 3 times that of stated earlier, by what factor the kinetic energy of the 3rd excited state will change?

$$E_{n_x n_y} = \frac{n_x^2 h^2}{8ma^2} + \frac{4n_y^2 h^2}{8ma^2}$$

$$= \frac{h^2}{8ma^2}\left(n_x^2 + 4n_y^2\right)$$

$a \rightarrow 3a$.

$$\therefore E'_{n_x n_y} = \frac{n_x^2 h^2}{8m(3a)^2} + \frac{n_y^2 h^2}{8m(\frac{3}{2}a)^2}$$

$$= \frac{1}{9}\left(\frac{n_x^2 h^2}{8ma^2} + \frac{4n_y^2 h^2}{8ma^2}\right)$$

$$= \frac{1}{9} E_{n_x n_y}.$$

$\therefore \frac{1}{9}$ times] (3) or (0)

3. (a) (**Marks: 3**) Write the hamiltonian operator for the vibration of a diatomic molecule within harmonic oscillator approximation. The bond is along the x-axis, its force constant is k and the masses of the two atoms are m_1 and m_2.

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 \Big] (2) ; \quad \mu = \frac{m_1 m_2}{m_1 + m_2}\Big] (1)$$

x = displacement from equilibrium.

(b) (**Marks: 3**) Write the expression of the first excited state energy level of the system stated in 3(a) in terms of force constant and mass.

$$E_1 = \frac{3}{2}h\nu \Big] (1) ; \quad \nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$$

$$= \frac{3h}{4\pi}\sqrt{\frac{k}{\mu}} \Big] (2) \sim (0)$$

(c) (**Marks: 4**) The vibration of $^1H^{35}Cl$ molecule can be considered as simple harmonic oscillation. The zero point energy of this molecule is E_0. What is the value of zero point energy of $^{35}Cl^{35}Cl$ if its force constant is half that of $^1H^{35}Cl$.

$$\nu_{HCl} = \frac{1}{2\pi}\sqrt{\frac{k_{HCl}}{\mu_{HCl}}} \quad ; \quad \nu_{ClCl} = \frac{1}{2\pi}\sqrt{\frac{k_{ClCl}}{\mu_{ClCl}}}$$

$$\therefore \frac{\nu_{HCl}}{\nu_{ClCl}} = \frac{\frac{1}{2}h\nu_{HCl}}{\frac{1}{2}h\nu_{ClCl}} = \sqrt{\frac{k_{HCl}}{k_{ClCl}} \cdot \frac{\mu_{ClCl}}{\mu_{HCl}}}$$

$$= \sqrt{\underset{(1)}{\boxed{2}} \cdot \frac{35\times 35}{35+35} \cdot \frac{(1+35)}{35}}$$

$$= 6$$

$$\therefore \frac{1}{2}h\nu_{ClCl}\Big]_{(1)} = \frac{\frac{1}{2}h\nu_{HCl}}{6} = \frac{E_0}{6}\Big] (2) \sim (0)$$