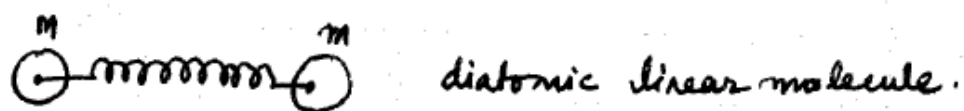


Homework is from Eisberg and Resnick (E&R) unless otherwise indicated. Please note that “questions” can be answered briefly; “problems” may be more involved. Each question usually counts 5 points; each problem counts 10 points.

1. E&R, chapter 6, **question** 30. (10 points)
2. E&R, chapter 6, problem 30.
3. E&R, chapter 6, problem 31.
4. E&R, chapter 6, problem 33.
5. E&R, chapter 6, problem 34.
6. E&R, Appendix I, problem 1.
7. E&R, Appendix I, problem 2.



The energy expression for the diatomic molecule is;

$$E = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2} C (x_1 - x_2)^2$$

Use centre of mass and relative co-ordinates to extract vibrational energy.

$$x = x_{\text{rel}} = x_1 - x_2$$

$$X = X_{\text{cm}} = \frac{x_1 + x_2}{2}$$

In this co-ord.

$$E = \frac{P^2}{2(2m)} + \frac{p^2}{2(\frac{m}{2})} + \frac{1}{2} C x^2$$

Total mass $M = 2m$, reduced mass is $\mu = \frac{m}{2}$

$$\frac{P^2}{2(2m)} = \frac{P^2}{4M} \text{ describes C.M. motion}$$

$$E = E_{\text{cm}} + E_{\text{vibrational}}$$

$$E_{\text{vib}} = \frac{p^2}{2\mu} + \frac{1}{2} C x^2$$

The energy levels of this system is

$$E_{\text{vib}} = \hbar \omega \left(n + \frac{1}{2} \right) \quad \text{where } \omega = \sqrt{\frac{C}{\mu}}$$

The zero point energy is

$$E_0 = \frac{\hbar \omega}{2} \quad \text{where } \omega = \sqrt{\frac{C}{\mu}}$$

$$\mu = \frac{m}{2} = \frac{M}{4} \rightarrow \text{Mass of molecule}$$

$$\omega = 2 \sqrt{\frac{C}{M}} = E_0 = \frac{\hbar \omega}{2}$$

$$\omega = 2 \sqrt{\frac{10^3}{4.1 \times 10^{-26}}} = 3.1 \times 10^{14} \text{ sec}^{-1}$$

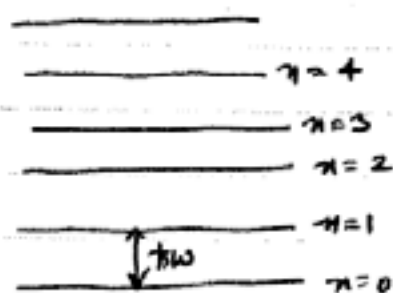
$$E_0 = \frac{1.055 \times 10^{-34} \times 3.1 \times 10^{14}}{2} = 1.6 \times 10^{-20} \text{ Joule}$$

$$E_0 = 1.6 \times 10^{-20} \text{ Joule} \times \frac{1 \text{ eV}}{1.6 \times 10^{-19} \text{ J}} = 1 \times 10^{-1} \text{ eV} = 0.1 \text{ eV}$$

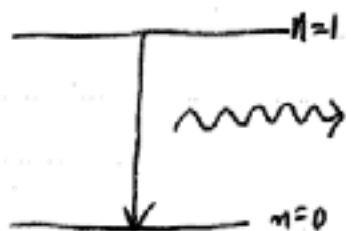
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a) $E_n = \hbar \omega \left(n + \frac{1}{2}\right)$ $\omega = 2\sqrt{\frac{C}{M}}$

$$E_2 - E_1 = \hbar \omega = 0.2 \text{ eV}$$



b)



The energy of emitted γ quantum is $E_1 - E_0 = \hbar \omega = 1.28 \text{ eV}$

$$\Psi(x, t) = N \left(\Psi_0(x) e^{-iE_0 t/\hbar} + \Psi_1(x) e^{-iE_1 t/\hbar} \right)$$

$$|\Psi(x, t)|^2 = |N|^2 \left(|\Psi_0(x)|^2 + |\Psi_1(x)|^2 + 2\Psi_0(x)\Psi_1(x) \cos \frac{E_1 - E_0}{\hbar} t \right)$$

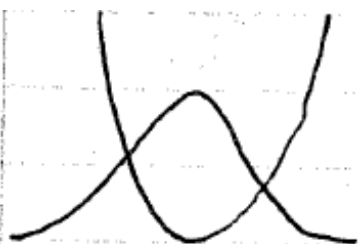
c) Frequency of the photon is $\nu = \frac{\omega}{2\pi} = \frac{(E_1 - E_0)}{\hbar 2\pi} = \frac{3.1 \times 10^{14} \text{ sec}^{-1}}{2\pi}$

$$\omega = 0.5 \times 10^{14} \text{ sec}^{-1}$$

Classical Oscillation frequency is $\nu = \frac{\omega}{2\pi} = 2\sqrt{\frac{C}{M}} = 5 \times 10^{15} \text{ sec}^{-1}$

d) $\lambda = \frac{3 \times 10^8}{0.5 \times 10^{14}} = 6 \times 10^{-6} \text{ m} = 6 \times 10^4 \text{ \AA}^\circ \text{ (Infrared)}$

(33)



$$V(x) = \frac{1}{2} k x^2 + \frac{1}{2} m \omega^2 x^2$$

Consider classically forbidden region

$$\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi(x) = 0 \quad ; \quad k^2(x) = -\frac{2m}{\hbar^2} (E - V(x))$$

$$\frac{d^2 \psi}{dx^2} - k^2(x) \psi(x) = 0 \quad V(x) > E \text{ in that region}$$

The solution behaves as $\psi(x) \sim e^{-k(x)x}$ in a region where $k(x)$ changes very little.

$$\psi(x) \sim e^{-k(x)x}$$

Since E is constant for any level.

$$k(x) = \sqrt{\frac{2m}{\hbar^2} (E - V(x))} \approx \sqrt{\frac{2m V(x)}{\hbar^2} \left(1 - O\left(\frac{E}{V}\right)^{1/2}\right)}$$

$$\approx \sqrt{\frac{2m V(x)}{\hbar^2}} = \sqrt{\frac{2m^2 \omega^2 x^2}{2\hbar^2}} = \frac{m\omega x}{\hbar}$$

$$\text{Hence } \psi(x) \sim e^{-\frac{m\omega}{\hbar} x \cdot x} = e^{-\frac{m\omega}{\hbar} x^2}$$

.) The recursion relation in Appendix I is;

$$a_{l+2} = \frac{-(\frac{\beta}{\alpha} - 1 - 2l)}{(l+1)(l+2)} a_l.$$

where the actual differential equation is;

$$\frac{d^2 \psi}{dx^2} + (\beta - \alpha^2 x^2) \psi = 0$$

& after assuming a solution of the form
 $\psi(u) = A e^{-u^2/2} H(u)$

$$\frac{d^2 H}{du^2} - 2u \frac{dH}{du} + \left(\frac{\beta}{\alpha} - 1\right) H = 0$$

The recursion relation is arrived at
where from this equation.

$$\psi_0(u) = A e^{-u^2/2} a_0$$

$$\psi_1(u) = A e^{-u^2/2} [a_0 + a_1 u]$$

$$\psi_2(u) = A e^{-u^2/2} \left[a_0 + a_1 u + \frac{a_2}{a_0} a_0 u^2 \right]$$

$$\psi_3(u) = A e^{-u^2/2} [a_0 + a_1 u + a_2 u^2 + a_3 u^3]$$

$$Y_4 = A e^{-u^2/2} \left[a_0 + a_1 u + a_2 u^2 + a_3 u^3 + a_4 u^4 \right]$$

$$Y_5 = A e^{-u^2/2} \left[a_0 + a_1 u + a_2 u^2 + a_3 u^3 + a_4 u^4 + a_5 u^5 \right]$$

a_1 & a_0 are arbitrary constants

$$a_2 = -\left(\frac{\beta}{\alpha} - 1\right) \frac{a_0}{2} \quad ; \quad a_4 = -\left(\frac{\beta}{\alpha} - 5\right) \frac{a_2}{12}$$

$$= \frac{\left(\frac{\beta}{\alpha} - 5\right) \left(\frac{\beta}{\alpha} - 1\right)}{2 \cdot 12} a_0$$

$$a_3 = -\left(\frac{\beta}{\alpha} - 3\right) \frac{a_1}{6} \quad ; \quad a_5 = -\left(\frac{\beta}{\alpha} - 7\right) \frac{a_3}{20}$$

$$= \frac{\left(\frac{\beta}{\alpha} - 7\right) \left(\frac{\beta}{\alpha} - 3\right)}{6 \cdot 20} a_1$$

substituting the values of the coefficients one gets
the solutions in terms of a_1 & a_0

$$\frac{d^2 Y}{du^2} + \left(\frac{\beta}{\alpha} - u^2\right) Y = 0$$

$$Y = \sum_{n=0}^{\infty} a_n u^n$$

$$Y'' = \sum_{n=2}^{\infty} a_n n(n-1) u^{n-2} \quad ; \quad Y' = \sum_{n=1}^{\infty} a_n (n-1) u^{n-1}$$

Substituting in the equation one has,

$$\sum_{n=2}^{\infty} a_n n(n-1) u^{n-2} + \left(\frac{\beta}{\alpha} - u^2\right) \sum_{n=0}^{\infty} a_n u^n$$

$$\sum_{n=2}^{\infty} a_n n(n-1) u^{n-2} + \frac{\beta}{\alpha} \sum_{n=0}^{\infty} a_n u^n - \sum_{n=0}^{\infty} a_n u^{n+2}$$

$n-2 = j$ one has,

$$\sum_{j=0}^{\infty} a_{j+2} (j+2)(j+1) u^j + \frac{\beta}{\alpha} \sum_{j=-2}^{\infty} a_j u^j - \sum_{j=-2}^{\infty} a_j u^{j+4}$$

$$a_j = 0 \text{ for } j < 0$$

$$\therefore \sum_{j=0}^{\infty} a_{j+2} (j+2)(j+1) u^j + \frac{\beta}{\alpha} \sum_{j=0}^{\infty} a_{j+2} u^{j+2} - \sum_{j=2}^{\infty} a_{j+2} u^{j+4}$$

if we now take the co-eff of u^j

$$\text{we have } a_{j+2} (j+2)(j+1) + \frac{\beta}{\alpha} a_{j+2} - a_{j-2}$$

$$\therefore a_{j+2} (j+2) (j+1) + \frac{\beta}{\alpha} a_j - a_{j-2} = 0.$$

The recursion relation is ~~to~~ ~~now~~ now has three terms unlike the two term recursion relations one normally has and it can be shown that solution for this does not work out in the ordinary way. This is an indication that the solution must be attempted by the asymptotic method.