INDIAN INSTITUTE OF TECHNOLOGY KANPUR

CHM102A Quiz-1

Saturday, January 27, 2018

Write the answers in the space provided. Answer all questions.
Time: 30 minutes
Maximum Marks: 20

Name: SOLUTIONS

Roll no.:

Section no.:

Information: $1 \text{ amu} = 1.67 \times 10^{-27}\text{ kg}$; $\hbar = 1.06 \times 10^{-34}\text{ Js}$; $c = 3 \times 10^{8}\text{ ms}^{-1}$.

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1. (4 marks) Calculate the de-Broglie wavelength for $^{12}C_{60}$ molecule moving with a velocity of 220 ms^{-1}.

Answer. Given momentum $p = m_{60} \times 220$

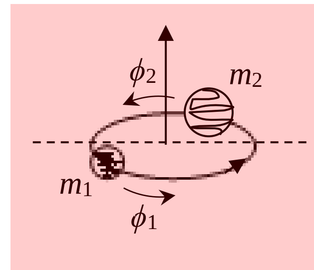
Now, $m_{60} = 12 \times 60 \times 1.67 \times 10^{-27}$ kg $= 1.2 \times 10^{-24}$ kg

Thus, de-Broglie wavelength,

$$\lambda = \frac{h}{p} = \frac{6.6 \times 10^{-34}\text{Js}}{1.2 \times 10^{-24} \times 220 \text{ kgm/s}} = 2.5 \times 10^{-12}\text{m} = 252 \text{ Å}$$

2. Consider the case of two non-identical and non-interacting quantum particles with masses m_1 and m_2 in a ring of radius R.
   a. (2 marks) Write the Hamiltonian operator for this problem in polar coordinates and define the variables used in your equation.

Moment of inertia of this system that is independently consisting on masses m_1 and m_2 in a ring of radius R is given by: $I_1 + I_2 = m_1 R^2 + m_2 R^2$ rotating at respective angles of ϕ_1 and ϕ_2.



So, the Hamiltonian operator is given by:

$$\hat{H} = \left(-\frac{\hbar^2}{2I_1}\frac{\partial^2}{\partial\phi_1^2}\right) + \left(-\frac{\hbar^2}{2I_2}\frac{\partial^2}{\partial\phi_2^2}\right) = -\frac{\hbar^2}{2m_1R^2}\frac{\partial^2}{\partial\phi_1^2} - \frac{\hbar^2}{2m_2R^2}\frac{\partial^2}{\partial\phi_2^2}$$

   b. (2 marks) Write the normalized wavefunction for this problem.
   (Note: derivation is not required).

$$\Psi(\phi_1,\phi_2) = \psi_1(\phi_1)\,\psi_2(\phi_2) = \left(\frac{1}{\sqrt{2\pi}}\exp(iN_1\phi_1)\right)\left(\frac{1}{\sqrt{2\pi}}\exp(iN_2\phi_2)\right)$$
$$= \frac{1}{2\pi}\big(\exp(iN_1\phi_1)\big)\big(\exp(iN_2\phi_2)\big)$$

where $N_1 = 0, \pm1, \pm2, \ldots$ and $N_2 = 0, \pm1, \pm2, \ldots$ are the quantum numbers.

   c. (4 marks) Determine the probability for finding the two particles at the same location.

We note the following:

$$|\psi_1^*(\phi_1)\,\psi_2^*(\phi_2)\psi_1(\phi_1)\,\psi_2(\phi_2)d\phi_1 d\phi_2|$$
$$= \left(\frac{1}{\sqrt{2\pi}}\exp(-iN_1\phi_1)\right)\left(\frac{1}{\sqrt{2\pi}}\exp(-iN_2\phi_2)\right)\left(\frac{1}{\sqrt{2\pi}}\exp(iN_1\phi_1)\right)\left(\frac{1}{\sqrt{2\pi}}\exp(iN_2\phi_2)\right)$$
$$= \frac{1}{4\pi^2}$$

For the location to be the same: $\phi_1 = \phi_2$. Let us set them both to be ϕ.
The probability density for the particle in the same location can be written as: $\frac{d\phi}{4\pi^2}$
The probability of finding the two particles at the same location is:

$$\int_0^{2\pi} \Psi^*(\phi)\Psi(\phi)d\phi = \int_0^{2\pi} \frac{1}{4\pi^2}d\phi = \frac{1}{2\pi}$$

3. Given below is the wavefunction of the 1D Simple Harmonic Oscillator in some specific state:

$$\sqrt{\frac{2\alpha^3}{\sqrt{\pi}}}\ x\ \exp\left(-\frac{1}{2}\alpha^2x^2\right)$$

where α is some constant.

a. (1 mark) Identify the location of the node(s) of this state.

$|\psi|^2 = constant^2 . \frac{2\alpha^3}{\sqrt{\pi}}\ x^2\ \exp(-\alpha^2x^2)$

For finding location of nodes, need to set: $\left(constant^2\ \frac{2\alpha^3}{\sqrt{\pi}}\ x^2\ \exp(-\alpha^2x^2)\right) = 0$

On inspection, $x = \pm\infty$ (not nodes: location of boundary)

and $x = 0$ (the only location of the Node)

b. (2 marks) Identify the quantum number of this state.

$$\psi = (Normalization\ constant)(Hermite\ Polynomial)(Gaussian)$$

$$= constant\sqrt{\frac{2\alpha^3}{\sqrt{\pi}}}\ x\ \exp\left(-\frac{1}{2}\alpha^2x^2\right)$$

$\because$ Hermite Polynomial of quantum number 1 $\propto x$,

$\therefore$ the Quantum number (n) of this state is 1.

c. (5 marks) Derive the locations of maximum probability (in terms of α) for this state.

$$\frac{d|\psi|^2}{dx} = \frac{d}{dx}\left(constant^2\ \frac{2\alpha^3}{\sqrt{\pi}}\ x^2\ \exp(-\alpha^2x^2)\right) = 0$$

$$i.e.,\ 2x\ \exp(-\alpha^2x^2) + x^2\ (-2\alpha^2x)\ \exp(-\alpha^2x^2) = 0$$

$$2x\ (1 - \alpha^2x)\ \exp(-\alpha^2x^2) = 0$$

This will give: $x = \pm\infty$ (location of boundary); $x = 0$ (location of node) and also the position of the maximum probability: $x = \pm\frac{1}{\alpha}$