OBAFEMI AWOLOWO UNIVERSITY, ILE-IFE, NIGERIA
DEPARTMENT OF CHEMISTRY
B.Sc. Degree (Chemistry) Examination (Part III)
CHM 303: Quantum Chemistry
2023/2024 Mid-Semester Test (Part B)

Time Allowed: 45 Minutes **Attempt ALL Questions** **Date: 23rd January, 2025**

1. The classical energy of a harmonic oscillator of amplitude x_o was found to have a value equivalent to the energy spacing of its quantum mechanical treatment.

(a) Express the quantum vibrational frequency, ν of the oscillator in terms of k, x_o and h. Where k is the force constant and h is the Planck's constant.

(b) If the force constant is 200 Nm^{-1} and the quantum mechanical energy spacing is one-$h\nu$ unit, find the value of x_o.

2. The wave function for the 1st excited state of a harmonic oscillator is $\psi(x) = Axe^{-\alpha x^2}$, where A and α are constants.

(a) Show that the normalization constant, A is $\left(\frac{32\alpha^3}{\pi}\right)^{\frac{1}{4}}$ [Use: $\int_0^\infty x^2 e^{-\alpha x^2} dx = \frac{1}{4}\left(\frac{\pi}{\alpha^3}\right)^{\frac{1}{2}}$]

(b) Express the second derivative, $\frac{d^2}{dx^2}$ of ψ in terms of α, x and ψ.

(c) By comparing the equivalent terms in 2(b) above and those of the Schrodinger wave equation:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2 x^2\right)\psi = 0$$

Show that: $\alpha = \frac{m\omega}{2\hbar}$ and $E = \frac{3}{2}\hbar\omega$