Quantum Tutorial 3 (CYL110)-Harmonic Oscillator (Vibrational Motion)

1. Show that the function $\exp(-\beta x^2)$ satisfies the Schrödinger equation for the quantum harmonic oscillator. What conditions does this place on β? What is E?

2. (a) Is $\psi_1(x) = \left(\frac{4\alpha^3}{\pi}\right)^{1/4} x \exp[-\frac{1}{2}\alpha x^2]$ is an eigenfunction of the kinetic energy operator where $\alpha = \sqrt{k\mu/\hbar^2}$.

   (b) What are the average values of kinetic and potential energies for a quantum mechanical oscillator in this state.

3. Consider the following wavefunctions for the $v = 0$ and $v = 1$ states of a harmonic oscillator: $\psi_0(y) = (1/\pi)^{1/4} \exp(-y^2/2)$ and $\psi_1(y) = (4/\pi)^{1/4}\, y\exp(-y^2/2)$ where $y = x/\alpha$.
   (a) Are the wavefunctions normalized?
   (b) Show that both wavefunctions satisfy the Schrödinger equation and find the corresponding energies.
   (c) Find the expectation value of the kinetic and potential energy for each of the states
   (d) Show that the wavefunctions satisfy the uncertainty principle.

4. Calculate $\langle x \rangle$, $\langle p_x \rangle$ and $\langle x^2 \rangle$ for a harmonic oscillator for the ground state n = 0?

5. A strong absorption band of infrared radiation is observed for $^{1}H^{35}Cl$ at 2991 cm^{-1}. (a) Calculate the force constant, *k*, for this molecule. (b) By what factor do you expect the frequency to shift if H is replaced by D? Assume the force constant to be unaffected by this substitution. [*516.3 Nm^{-1}; 0.717*]

6. The Hamiltonian of a 2-dimensional (2-D) isotropic harmonic oscillator has the form $H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}m\omega^2(x^2 + y^2)$. (a) Write an expression for the wave function for the of the 2-D oscillator. (b) What is the energy eigenvalue for this system. (c) Find the degeneracy of the energy levels.

7. Consider a particle confined to the right hand half of a harmonic oscillator potential with $V(x) = \infty$ if $x < 0$ and $V(x) = 0.5kx^2$ if $x \geq 0$. Compare the allowed wavefunctions for this system with those of a normal harmonic oscillator having the same values of *m* and *k*. what are the allowed energies of this half-oscillator.

8. Intensity of spectroscopic transitions between the vibrational states of a molecule are proportional to the square of the integral $\int \Psi_{v'}\, x\, \Psi_v\, dx$ over all space. Show that the only permitted transitions are those for which $v' = v \pm 1$ and evaluate the integral.

9. In the infrared spectrum of $H^{79}Br$, there is an intense line at 2559 cm^{-1}. Calculate the force constant of $H^{79}Br$ and the period of vibration of $H^{79}Br$.

10. Carbon Monoxide binds strongly to the Fe^{2+} ion of the haem group pf the protein myoglobin. Estimate the vibrational frequency of CO bound to myoglobin (force constant for CO is 1902 N m^{-1}). Assume that the protein is infinitely more heavy as compared to the C atom through which binding occurs and that the C atom that binds to the haem group is immobilized. Also binding of the CO to the protein does not alter the force constant of the CO bond.

11. Find the maxima and minima in the probability distribution for the $v = 3$ state of a harmonic oscillator described by the wavefunction $\psi_3 = N_3(8y^3 - 12y)\exp(-y^2/2)$.

12. It can be proved generally that $\langle x^2 \rangle = \frac{\hbar}{(\mu k)^{1/2}}(\upsilon + \frac{1}{2})$ and $\langle x^4 \rangle = \frac{3\hbar^2}{4\mu k}(2\upsilon^2 + 2\upsilon + 1)$ for a harmonic oscillator. Verify these for the first 2 states of a harmonic oscillator.

13. The maximum potential energy that a diatomic molecule can store is ½ kx^2, where x is the amplitude of the vibration. If the force constant is 1.86×10^3 N m^{-1}, calculate the maximum amplitude of vibration for the CO molecule in the ground vibrational state.

14. (a) Derive the expression for the standard deviation of the bond length of a diatomic molecule when it is in its ground state. (b) What percentage of the equilibrium bond length is this standard deviation for CO in its ground state? For CO, $\tilde{\nu} = 2170$ cm^{-1} and $R_e = 113$ pm. [*2.98 %*]