

Aims and Objectives Quantum Physics I Session 18

THE QUANTUM HARMONIC OSCILLATOR, HIGHER ENERGY LEVELS AND VIBRATIONAL MODES OF MOLECULES

Aims (What I intend to do)

- 1) To use the time Independent Schrödinger equation to find the spacing between the energy levels of the quantum mechanical harmonic oscillator.
- 2) To examine the form of the wavefunctions associated with the simple harmonic oscillator.
- 3) To apply our simple harmonic oscillator model in trying to understand the vibrational modes of simple molecules.

Objectives (What you should be able to do after completing the lecture and worksheet)

- 1) To be able to work out the spacing between the lowest three energy levels of the quantum mechanical harmonic oscillator.
- 2) To be able to write down draw and describe the wavefunction and associated probability distribution for the lowest three energy levels of the quantum harmonic oscillator.
- 3) To be able to apply the quantum harmonic oscillator model to vibrational modes of simple molecules, and to use it to find the 'spring' constant of the associated molecular bond.

Quantum Physics 1 PHY2002 Worksheet 18

- Task 1.** Go over your lecture notes and consult section 2.6 of Rae.
- Task 2.** You might also like to look at section 4.8 of Rae for a more advanced way of dealing with the harmonic oscillator.
- Task 3.** In the previous class we found the energy of the lowest state ($n=0$), the zero point energy, $E_0 = \frac{1}{2}\hbar\omega_0$. Use the wavefunction we took for the next lowest energy state, $n=1$, i.e.

$$\Psi_1(x) = x \cdot \exp\left(\frac{-x^2}{2a^2}\right)$$

find, $\frac{d^2\Psi_1(x)}{dx^2}$ and hence find E_1 by substitution into the time dependent Schrödinger equation. You should get,

$$E_1 = \frac{3}{2}\sqrt{\frac{2\beta_2}{m}} = \frac{3}{2}\hbar\omega_0$$

- Task 4.** Carry out a similar calculation to that undertaken in class to find the spring constant of the CO molecule. The lowest order absorption peak is found to occur at 2146 cm^{-1} . You should find it to be approx. 950 N/m