

1. A harmonic oscillator specified by the Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m} \left(\frac{d^2}{dx^2} \right) + \frac{1}{2} kx^2$ is in its lowest energy state, for which $\Psi_0(x) = \left(\frac{\alpha}{\pi} \right)^{1/4} \exp(-\alpha x^2/2)$, with $\alpha = (mk)^{1/2}/\hbar$
 - a) Evaluate $\langle x \rangle$ in terms of α
 - b) Evaluate $\langle x^2 \rangle$ in terms of α
 - c) Evaluate $\langle p \rangle$ in terms of α
 - d) Evaluate $\langle p^2 \rangle$ in terms of α
 - e) Use the above results to calculate the uncertainty product $\Delta x \Delta p$. Verify that Heisenberg's uncertainty principle, $\Delta x \Delta p \geq \hbar/2$, is satisfied. Note that in this case the lowest possible value of the uncertainty product, $\Delta x \Delta p$, is obtained. For this reason the wavefunction $\Psi_0(x)$ is an example of what is called a minimum-uncertainty wavepacket. It represents the best we can do, given the fundamental limitations imposed by the uncertainty principle, to represent a particle localized at the position given by your calculated value of $\langle x \rangle$, moving with a momentum given by your calculated value of $\langle p \rangle$.
 - f) Use the result of a) and b) to verify that the average kinetic and potential energies of this system are equal, i.e. $\langle T \rangle = \langle V \rangle$.
2.
 - a) The force constant k of the H-H bond in H_2 is $5.754 \times 10^5 \text{ g}\cdot\text{s}^{-2}$. Assuming that the vibrational motion of H_2 is purely harmonic, and using the reduced mass $\mu = 0.50391252 \text{ amu}$, calculate the spacing between vibrational energy levels in this molecule in cm^{-1} . ($\text{amu} = 1.6605655 \times 10^{-24} \text{ g}$, remember that for the harmonic oscillator, the spacing between levels is given by $\hbar\omega$, where $\omega = \left(\frac{k}{\mu} \right)^{1/2}$).
 - b) Calculate the uncertainty in the inter-nuclear distance in this molecule, assuming it is in its ground vibrational level. For this you may use your result for Δx obtained from problem 1, where Δx was calculated in terms of α . Simply use the reduced mass, μ , in place of m and the force constant given above in place of k , and remember that $\alpha = (\mu k)^{1/2}/\hbar$.
 - c) Repeat calculation of ω and Δx for the HD and D_2 molecules, which have the same force constant, k , as H_2 , but larger reduced mass ($\mu = 0.67171124 \text{ amu}$ for HD and 1.00705089 amu for D_2 , respectively).
 - d) Under what circumstance (i.e. large or small values of k , large or small values of μ) is the uncertainty in inter-nuclear distance large? Think of any relationship between this observation and the

fact that at atmospheric pressure helium remains a liquid down to absolute zero [Hint: think about the size of uncertainty in position, Δx , as compared to the nearest neighbor distance in a crystal].

3. For the particle of mass μ confined to motion on a ring of radius of r , with $V(\phi) = 0$, the

Hamiltonian is given by $\hat{H} = -\frac{\hbar}{2\mu r^2} \frac{d^2}{d\phi^2}$,

the eigenfunctions of this system are then given by $\psi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$, with $m = 0, \pm 1, \pm 2, \dots$

and the corresponding energy eigenvalues are given by $E_m = \frac{m^2 \hbar^2}{2\mu r^2}$

Suppose that this system exists in a state given by

$$\psi = \frac{1}{2} \left(\frac{1}{\sqrt{2\pi}} e^{i\phi} \right) + \frac{i}{2} \left(\frac{1}{\sqrt{2\pi}} e^{-i\phi} \right) - \frac{1}{2} \left(\frac{1}{\sqrt{2\pi}} e^{3i\phi} \right) - \frac{i}{2} \left(\frac{1}{\sqrt{2\pi}} e^{-3i\phi} \right)$$

- What are the possible results of a measurement of the energy, E , and what are the probabilities of these results?
 - What is the expectation value of the Hamiltonian for this state of the system?
 - Is this state a stationary state of the system? Why?
4. In the infrared spectrum of H^{127}I , there is an intense line at 2309 cm^{-1} . Calculate the force constant of H^{127}I and period of vibration of H^{127}I .