

CYL110 2010-2011 Quantum Tutorial 4

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1. The maximum potential energy that a diatomic molecule can store is $\frac{1}{2}kx^2$, where x is the amplitude of the vibration. If the force constant is $1.86 \times 10^3 \text{ N m}^{-1}$, calculate the maximum amplitude of vibration for the CO molecule in the ground vibrational state.
2. It can be proved generally that for a harmonic oscillator

$$\langle x^2 \rangle = \left(n + \frac{1}{2}\right) \frac{\hbar}{\sqrt{\mu k}}$$

and that

$$\langle x^4 \rangle = (n^2 + 2n + 1) \frac{3\hbar^2}{4\mu k}.$$

Verify these formulas for the first two states of the harmonic oscillator.

3. An analytic expression that is a good approximation to the potential energy curve of a diatomic molecule is $V(x) = D(1 - \exp(-\beta x))^2$ where D and β are parameters that depend on the molecule. Derive a relation between the force constant and the parameters D and β . Now show that

$$\beta = 2\pi c\tilde{\nu} \left(\sqrt{\frac{\mu}{2D}} \right),$$

where $\tilde{\nu}$ is the vibrational frequency expressed in cm^{-1} .

4. Verify the recursion relation

$$H_{n+1}(z) - 2zH_n(z) + 2nH_{n-1}(z) = 0$$

using the first few Hermite polynomials.

5. 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 .
6. In the vibrational motion of HI, the iodine atom remains stationary because of its large mass. Assume that the hydrogen atom undergoes harmonic motion and that the force constant is 317 N m^{-1} , what is the vibrational frequency ν_0 ? What is the zero point energy if H is replaced by D? Assume that there is no change in the force constant.
7. Calculate the moment of inertia of H^{35}Cl , H^{37}Cl , and D^{35}Cl all of which have an equilibrium bond length of 1.275 \AA . Determine the energies of the first three rotational states for H^{35}Cl . Use this information to predict these values for D^{35}Cl .
8. Show by direct operation that the functions $\sin \theta \exp(i\phi)$, $\sin \theta \exp(-i\phi)$, and $\cos \theta$ are eigen functions of \hat{L}_z . What are the eigen values?
9. Use the operator for \hat{L}^2 in polar coordinates to show that the function $(3 \cos^2 \theta - 1)$ is an eigen function of this operator. What is the eigen value? What is the quantum number l for this function?
10. The normalization of $Y_l^m(\theta, \phi) = N P_l^m(\cos \theta) \exp(im\phi)$ is performed as follows:

$$N^2 \int_{\theta=0}^{\pi} (P_l^m)^* P_l^m \sin \theta d\theta \int_{\phi=0}^{2\pi} \exp(-im\phi) \exp(im\phi) d\phi = 1,$$

while its orthogonality to $Y_l^{m'}$ implies that

$$\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} Y_l^m (Y_l^{m'})^* \sin \theta d\theta d\phi = 0.$$

- (a) Show that $Y_1^{-1}(\theta, \phi)$ is normalized and it is orthogonal to $Y_2^1(\theta, \phi)$.

- (b) Determine the normalization constant for the function given in problem 2.
11. For angular momentum with quantum number $l = 3$, how many m -values are there? What is the semi-angle of the cone subtended by the angular momentum vector if its z -projection is $2\hbar$?
 12. From the definition of angular momentum, $\vec{L} = \vec{r} \times \vec{p}$, and following the procedure outlined in the class obtain the Cartesian form of the y -component of the angular momentum operator.
 13. Show that $[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$. (Hint: Use the information from the previous problem.)
 14. Show that $[\hat{L}_x, y] = i\hbar z$.
 15. Determine the positions of the first three rotational transitions for H^{35}Cl and D^{35}Cl .
 16. In the far infrared spectrum of H^{79}Br , there is a series of lines separated by 16.72 cm^{-1} . Calculate the values of the moment of inertia and the internuclear separation in H^{79}Br .
 17. The $J = 0 \rightarrow J = 1$ line in the microwave absorption spectrum of $^{12}\text{C}^{16}\text{O}$ and of $^{13}\text{C}^{16}\text{O}$ was found to be at 3.84235 cm^{-1} and 3.67337 cm^{-1} . Calculate (a) the bond length of $^{12}\text{C}^{16}\text{O}$, (b) the relative atomic mass of ^{13}C .
 18. A hydrogen-like atom can be formed from a proton and a negative muon whose mass is approximately 206 times that of the electron. What are the energies and most probable radius for the $1s$ and $2p$ levels of this atom?
 19. Using the uncertainty principle argue that free electrons cannot exist in the nucleus. The diameter of a typical nucleus is 10^{-14} m .
 20. For a hydrogen atom in the ground state find the classically forbidden region and calculate the probability of finding the electron in this region.
 21. Compute the average value of r , the most probable value of r , and the root-mean-square value of r for the $1s$ and $2p$ levels of the hydrogen atom. Compare the three kinds of values and explain the origin of their differences.
 22. Show that the hydrogenlike atomic wave function ψ_{210} is normalized and that it is orthogonal to ψ_{200} .
 23. Calculate the probability that an electron described by a hydrogen $1s$ wave function will be found within one Bohr radius of the nucleus.
 24. Prove that $\langle V \rangle = 2 \langle E \rangle$ and, consequently, that $\langle K \rangle = - \langle E \rangle$, for a $2s$ electron.
 25. Compute $\langle r \rangle$ in the $2s$, $2p$ states of the hydrogen atom. Compare your result with the general formula

$$\langle r_{nl} \rangle = \frac{a_0}{2} [3n^2 - l(l+1)].$$
 26. Where do the maxima in $r^2\psi_{2s}^2(r)$ occur?
 27. What combinations of the d ($l = 2$) atomic orbitals will produce the Cartesian function $d_{xz} = xzR_{nl}(r)$ and $d_{xy} = xyR_{nl}(r)$.
 28. If we were to ignore the inter-electronic repulsion in helium, what would be its ground state energy and wave function? The experimental ground state energy of He is -79.0 eV .