Quantum Tutorial 3 (CML100)-Rotational Motion and Hydrogen Atom

1. Show that the spherical harmonics are eigenfunctions of the operator $L_x^2 + L_y^2$. (The proof is short.) What are the eigenvalues?

2. Show by direct operation that the functions $\sin\theta \exp(i\phi)$, $\sin\theta \exp(-i\phi)$, and $\cos\theta$ are eigenfunctions of $\hat{L}_z$. What are the eigenvalues?

3. Confirm that the spherical harmonic Y_{10} is an eigenfunction of the Legendrian?

4. Compute the value of $\hat{L}^2 Y(\theta,\phi)$ for the following functions: (a) $1/(4\pi)^{1/2}$ (b) $(3/4\pi)^{1/2}\cos\theta$ (c) $(3/8\pi)^{1/2}\sin\theta\exp(i\phi)$.]

5. 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 $H^{79}Br$. [*3.35* x 10^{-47} *kgm²; 142 pm*]

6. 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 Å. Calculate the positions of the first three rotational transitions for $H^{35}Cl$, $H^{37}Cl$, and $D^{35}Cl$.

7. The J=0 to J=1 transition for Carbon Monoxide (CO) occurs at 1.153 x 10^5 MHz. Calculate the value of the bond length for CO. [*113 pm*]

8. This problem deals with angular momentum operators and spherical harmonics. You are given two operators $\hat{L}_+$ and $\hat{L}_-$ that can be written as $\hat{L}_+ = \hat{L}_x + i\hat{L}_y$ and $\hat{L}_- = \hat{L}_x - i\hat{L}_y$ with $\hat{L}_x$ and $\hat{L}_y$ being the angular momentum operators in the *x* and *y* directions respectively.
   (a) Express '$\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+$' in terms of $\hat{L}^2$ and $\hat{L}_z^2$ with L and L_z having their usual meaning. You may use any of the known commutation relations discussed in the class.
   (b) Are spherical harmonics eigenfunctions to $[\hat{L}_+, \hat{L}_-]$? If no, why not? If yes, what are the eigenvalues?
   (c) If a system is in the state described by the wavefunction $Y_{l,m_l}(\theta,\varphi)$, find $\langle L_x \rangle$. Use the following relations: $\hat{L}_+ Y_{l,m_l}(\theta,\varphi) = c_+ Y_{lm_l+1}(\theta,\varphi)$ and $\hat{L}_- Y_{l,m_l}(\theta,\varphi) = c_- Y_{l,m_l-1}(\theta,\varphi)$ where c_+ and c_- are constants.

9. The following functions are examples of spherical harmonics: $Y_1(\theta,\varphi) = N_1\sin^2\theta\cos\theta\exp(\pm 2i\phi)$ and $Y_2(\theta,\phi) = N_2(5\cos^3\theta - 3\cos\theta)$. Deduce the quantum numbers which characterize these spherical harmonics.

10. 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 $2\hbar$?

11. 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 for the 1s and 2p levels of this atom?

12. Show explicitly that $H\psi = -\dfrac{m_e e^4}{8\varepsilon_0^2 h^2}\psi$ for the ground state of a hydrogen atom.

13. For a hydrogen atom in the ground state find the classically forbidden region and calculate the probability of finding the electron in this region.

14. Calculate the probability that an electron described by a hydrogen 1s wavefunction will be found within one Bohr radius of the nucleus. Use the integral: $\int x^2 e^{bx} dx = e^{bx}\left(\frac{x^2}{b} - \frac{2x}{b^2} + \frac{2}{b^3}\right)$ [*0.323*]

15. Calculate the most probable distance (i.e., radius) at which the 1s electron of H-like atom with atomic number Z is to be found. Show that as Z increases, this most probable distance decreases. $\psi_{1s} = (Z^3/\pi a_0^3)^{1/2} e^{-Zr/a0}$.

16. Find the average distance of 1s electron from the nucleus in hydrogen atom for which, $\psi_{1s} = 1/(\pi a_0^3)^{1/2} e^{-r/a0}$.

17. We have seen before that any linear combination of eigenfunctions of a degenerate energy level is an eigenfunction of the Hamiltonian with the same eigenvalue. In this regard, the $2p_x$ angular orbital can be defined as: $\psi_{2p_x} = -\frac{Y_{1,1}(\theta,\phi) - Y_{1,-1}(\theta,\phi)}{\sqrt{2}}$. (a) Show that ψ_{2p_x} is normalized. (b) Is ψ_{2p_x} an eigenfunction of L^2? If so, what is the corresponding eigenvalue? (c) Is ψ_{2p_x} an eigenfunction of L_z? If so, what is the corresponding eigenvalue?

18. Show that the hydrogenlike atomic ψ_{210} is normalized and orthogonal to ψ_{200}.

19. Prove that $\langle V \rangle = 2\langle E \rangle$ for a 2s electron.

20. If we 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.

21. Show where the two maxima in the plot of $r^2\psi_{2s}^2(r)$ against r occur?

22. Consider the following total wavefunctions of the following hydrogen-like orbitals. Identify the n, l and m_l values and hence the respective orbital:

(i) $$\Psi_{nlm_l}(r,\theta,\phi) = \sqrt{\frac{5}{16\pi}\frac{1}{96\sqrt{5}}\left(\frac{Z}{a_0}\right)^{3/2}} e^{-\rho/2}(6-\rho)\rho^2(3\cos^2\theta - 1)$$

(ii) $$\Psi_{nlm_l}(r,\theta,\phi) = \sqrt{\frac{5}{32\pi}\frac{1}{96\sqrt{5}}\left(\frac{Z}{a_0}\right)^{3/2}} e^{-\rho/2}(6-\rho)\rho^2\sin^2\theta e^{2i\phi}$$

(iii) $$\Psi_{nlm_l}(r,\theta,\phi) = \sqrt{\frac{5}{8\pi}\frac{1}{9\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2}} e^{-\rho/2}\rho^2\sin\theta\cos\theta e^{-i\phi}$$

(iv) $$\Psi_{nlm_l}(r,\theta,\phi) = \sqrt{\frac{1}{4\pi}\frac{1}{9\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2}} e^{-\rho/2}(6-6\rho+\rho^2)$$

23. Make sure that you know how to draw schematically the wavefunctions of the radial wave functions and the radial probability distribution functions, taking care of the number of radial nodes

24. For an isolated hydrogen atom, why must the angular momentum vector L lie on a cone that is symmetric about the z-axis. Can the angular momentum vector evr point exactly along the z-axis? Why? (*Hint*: *Recall our discussion on space quantization*).

25. Prove that the average value of r in the 1s and 2s states of a hydrogenic atom is $\frac{3a_0}{2Z}$ and $\frac{6a_0}{Z}$ respectively.

26. The average values of $1/r$, $1/r^2$ and $1/r^3$ for a hydrogen-like atom can be evaluated in general and are given by:

$$\left\langle \frac{1}{r} \right\rangle = \frac{Z}{a_0 n^2}$$

$$\left\langle \frac{1}{r^2} \right\rangle_{nl} = \frac{Z^2}{a_0^2 n^3 \left(l + \frac{1}{2} \right)}$$

$$\left\langle \frac{1}{r^3} \right\rangle_{nl} = \frac{Z^3}{a_0^2 n^3 \left(l + \frac{1}{2} \right)(l+1)}$$

Verify these expressions explicitly for the ψ_{210} orbital.

27.

Some useful integrals you might need are provided below:

(i) $\int_0^\infty r \exp(-br)dr = \frac{1}{b^2}$ (ii) $\int_0^\infty r^2 \exp(-br)dr = \frac{1}{b^3}$ (iii) $\int_0^\infty r^3 \exp(-br)dr = \frac{6}{b^4}$ (iv) $\int_0^\infty x^n \exp(-ax)dx = \frac{n!}{a^{n+1}}$