

Department of Physics, IIT Madras

Bohr&Wilson Sommerfeld theory, Laplace Runge Lenz Vector, Schrodinger equation for H atom

PCD_STiAP_P01

The first three problems are based on some background material students may have been exposed to prior to registering for the STiAP course. These are meant to revise/recapitulate some principles of 'old' quantum theory.

1. (a) State the (i) Bohr and (ii) Wilson - Sommerfeld quantization condition.

(b) Obtain the quantum energies of a ball bouncing up and down over a hard sphere:

$$V = \begin{cases} mgz, & \text{for } z > 0, \\ \infty, & \text{for } z < 0. \end{cases}$$

(c) Obtain the energy spectrum of a particle in a one dimensional box confined between $0 \leq x \leq a$ using the quantization of the phase integral.

2. (a) Obtain the (i) classical (ii) Wilson - Sommerfeld quantized energy of a rigid body which is constrained to rotate about a fixed axis.

(b) Obtain the Wilson - Sommerfeld quantized energy levels for a one - dimensional harmonic oscillator.

(c) Using the Wilson - Sommerfeld quantization determine the degeneracy of the n^{th} energy level of the three dimensional isotropic oscillator for $n = 3$.

3. (a) Apply the Wilson - Sommerfeld quantization to the Bohr - Kepler trajectory described by $r = \frac{p_\phi^2 / me^2}{1 - \epsilon \cos \phi}$. Apply the quantization condition explicitly to phase integrals $J_\phi = \oint p_\phi d\phi$ and $J_r = \oint p_r dr$.

(b) Show that energy of the system is quantized and is given by $E_n = -\frac{me^4}{2n^2\hbar^2}$, where n is the Principle quantum number which is the sum of the quantum numbers n_r and n_ϕ which are integers in the relations $J_r = n_r h$ and $J_\phi = n_\phi h$.

(c) Prove that the ratio of the semi - minor axis to semi - major axis of an ellipse is $\frac{b}{a} = \frac{n_\phi}{n}$.

(d) Sketch (to scale) the orbits for $n = 3$ for all possible values of ' n_r ' and ' n_ϕ '.

(e) If the major axis of the ellipse is equal to the radius of the circle, what would be the relation of the energies of the corresponding two orbits (circle and ellipse).

4. (a) In quantum mechanics if one were to define quantum mechanical Laplace - Runge - Lenz vector, would it be alright to simply use the classical expression for \vec{A} and replace the classical dynamical variables therein by corresponding quantum mechanical operators? If yes, explain why, and if not, give reasons.

(b) Give the expression for the quantum mechanical Laplace-Runge-Lenz vector \vec{A} .

(c) Prove that

c. i) $[\vec{A}, H]_- = 0.$

c. ii) $\vec{L}\vec{A} = \vec{A}\vec{L} = 0.$

c. iii) $\vec{A}^2 = \frac{2H}{\mu}(L^2 + \hbar^2) + \kappa^2.$

c. iv) $[A_i, L_j]_- = i\hbar\epsilon_{ijk}A_k.$

5. (a) Show that $[A_i, A_j] = -2i\frac{\hbar}{\mu}H\epsilon_{ijk}L_k$

(b) If we define $\vec{A}' = \sqrt{\frac{-\mu}{2E}}\vec{A}$ in the subspace of hydrogen atom's bound state part of the spectrum with energy $E(\leq 0)$, prove that $[A'_i, A'_j] = i\hbar\epsilon_{ijk}L_k.$

(c) Prove that the operators $\vec{I} = \frac{1}{2}(\vec{L} + \vec{A}')$ and $\vec{K} = \frac{1}{2}(\vec{L} - \vec{A}')$ obey $[I_x, I_y]_- = i\hbar I_z$

(d) Prove that $[K_x, K_y]_- = i\hbar K_z$

(e) Prove that $[I, K]_- = 0$

(f) Prove that $[I, H]_- = 0 = [K, H]_-$

6. Obtain the identity $I^2 + K^2 = \frac{-1}{2} - \frac{1}{4E}$ and deduce from it the Rydberg- Balmer - Bohr formula for the energy levels of the hydrogen atom.

7. (a) State the definition of the orbital angular momentum operator.

(b) Prove that $[L_x, y] = i\hbar z.$

(c) Prove that $[L_x, p_y] = i\hbar p_z.$

(d) Prove that $[L_x, x] = 0.$

(e) Prove that $[L_x, p_x] = 0.$

(f) Prove that $[L^2, L_z] = 0$.

(g) Prove that $\vec{L}^2 = r^2 p^2 - (\vec{r} \cdot \vec{p})^2$.

8. Prove that $\vec{L}^2 = r^2 \vec{p}^2 - r(r \cdot \vec{p}) \cdot \vec{p} + 2i\hbar(\vec{r} \cdot \vec{p})$ where $r(r \cdot \vec{p}) \cdot \vec{p} = \sum_{i=1}^3 \sum_{k=1}^3 r_i r_k p_k p_i$ (1,2,3 represent the coordinates of the vector).

9. Prove that (a) $\vec{L}^2 = r^2 \vec{p}^2 + \frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$ and (b) Prove that $T = \frac{\vec{L}^2}{2mr^2} - \frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$.

10. (a) Sketch the normalized associated Legendre functions $P_{l,m}$ for $l=1,2,3$ as a function of θ for $m=0$ in each case.

(b) Sketch the normalized associated Legendre functions $P_{l,m}$ for $l=1,2,3$ as a function of θ for $m=0$ in each case.

(c) Sketch the normalized associated Legendre functions $P_{l,m}$ for $l=1,2,3$ as a function of θ for $m=0$ in each case.

(d) Prove that $Y_{lm}(\pi - \theta, \pi + \theta) = (-1)^l Y_{lm}(\theta, \varphi)$

11. For the spherical harmonics, prove that:

(a) $Y_l^m = (-1)^m Y_l^{-m*}$

(b) $L_z Y_l^m = m\hbar Y_l^m$

(c) $L^2 Y_l^m = l(l+1)\hbar^2 Y_l^m$

(d) $\int_0^{2\pi} \int_0^\pi Y_l^{m*}(\theta, \varphi) Y_l^{m'}(\theta, \varphi) \sin \theta d\theta d\varphi = \delta_{l,l'} \delta_{m,m'}$

12. Consider the Schrodinger Equation for the Hydrogen Atom $H\psi = E\psi$ where

$$H = \frac{1}{2m} \left(p_r^2 + \hbar^2 \frac{L^2}{r^2} \right) + U(r)$$

(a) What is the explicit form of the radial component p_r of the momentum operator?

(b) Determine whether or not it is Hermitian.

(c) Does it correspond to an observable?

(d) Sketch the effective one dimensional potential

$$U_l(r) = U(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$$

13. (a) Prove that the radial solutions $R_l(r \rightarrow 0) \approx \text{constant} \times r^l$
 (b) Demonstrate that for the approximation of the above expression to be valid, the potential $U(r)$ must be such that

$$\lim_{r \rightarrow 0} U(r) r^2 = 0$$

14. (a) Show that if the potential $U(r)$ of question 12 is zero in the entire space, then the solution to the Schrodinger equation is given by

$$e^{ik \cdot \hat{r}} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta)$$

- (b) Show that the above expression is completely equivalent to

$$e^{ik \cdot \hat{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y_{lm}^*(\hat{k}) Y_{lm}(\hat{r})$$

15. Use the analytical forms of the H atom wavefunctions that you can find in any book on QM for this question:
 (a) Construct linear combination of $2p_{\pm 1}$ to get 'real' solutions for $n=2, l=1$.
 (b) Determine the zeroes of the radial function for 3s and 3p explicitly.
 (c) List the functions which have no radial nodes amongst the function with $n = 1, 2, 3, 4$ & 5.

Useful References.

1. Powell & Craseman: QM
2. Sakurai: Modern QM
3. Grenier, W. and Muller, B.; Quantum Mechanics Symmetries; Springer- Verlag Berlin, 2nd edition (1989).
4. Bohm, Arno; Quantum Mechnics; Springer – Verlag New York Inc (1979).
5. Condon, E. U. and Odabasi, H.; Atomic Structure, McGraw – Hill (1954).
6. Goldstein, H.; Classical Mechanics; Narosa Publishing House (1985).