IISER Mohali

[August 2024 Session]

PHY 403 (Atomic and molecular physics)

Exercises

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Review of one electron atoms/ions

1. In classical mechanics, for $\frac{1}{r}$ potential, apart from orbital angular momentum ($\vec{L}$), there exists another conserved quantity known as Laplace-Runge-Lunz vector,

$$\vec{N} = \frac{\vec{p} \times \vec{L}}{m} - \frac{c}{r}\vec{r} \tag{1}$$

where c is a dimensionful constant. Argue that the correct generalization of this quantity to quantum mechanics is given by the operator,

$$\vec{N} = \frac{1}{2m}(\vec{p} \times \vec{L} - \vec{L} \times \vec{p}) - \frac{c}{r}\vec{r} \tag{2}$$

Further, show that it commutes with the Hamiltonian for the H-atom. Take $c = \frac{e^2}{4\pi\epsilon_0}$.

2. Show that, for a general eigenstate $\psi_{n\ell m}$, the expectation values of kinetic energy T and potential energy V, satisfy

$$2\langle T \rangle = -\langle V \rangle . \tag{3}$$

3. Compare the expectation value of the radial coordinate and the most probable radial location of the electron in the ground state of the H-atom.

4. Estimate the binding energy of a pionic atom (a system of π^- and nucleus).

5. Show that the parity of the eigenstate $\psi_{n\ell m}$ is determined by $(-1)^\ell$.

6. Go through the Appendix 7 of B & J for the non-relativistic limit of the Dirac equation which leads to relativistic corrections, H_1', H_2' and H_3' discussed in the class. [**This exercise is optional. Any difficulty in following the derivation can be discussed outside the regular class schedule.**]

7. The fine structure formula for the Hydrogen atom obtained by solving Dirac equation exactly is given by,

$$E_{nj} = mc^2\left\{\left[1+\left(\frac{\alpha}{n-(j+\frac{1}{2})+\sqrt{(j+\frac{1}{2})^2-\alpha^2}}\right)^2\right]^{-1/2}-1\right\}. \tag{4}$$

Noting that $\alpha << 1$, show that the fine structure result obtained in perturbation theory agrees with above result at $\mathcal{O}(\alpha^4)$.

8. Show that for $\ell = 0$ states of the Hydrogen atom,

$$\langle\frac{3\mathbf{S}_e.\hat{r}\mathbf{S}_p.\hat{r}-\mathbf{S}_e.\mathbf{S}_p}{r^3}\rangle = 0 \tag{5}$$

9. Argue that for typical magnetic fields that can be produced in the laboratory, the quadratic term in $\mathbf{A}$ is negligible with respect to the linear term in the NR Hamiltonian for the Hydrogen atom in presence of constant magnetic field.

10. Prove the following identity,

$$(\mathbf{L}.\mathbf{S})\mathbf{S}\times\mathbf{J}-\mathbf{S}\times\mathbf{J}(\mathbf{L}.\mathbf{S}) = i\hbar(\mathbf{J}\ \mathbf{S}.\mathbf{J}-\mathbf{S}\ \mathbf{J^2}) \tag{6}$$

11. Argue that the unperturbed degenerate states,

$$|2\pm\rangle = \frac{1}{\sqrt{2}}(|200\rangle \pm |210\rangle) \tag{7}$$

qualify for *good* states in the study of linear Satrk effect in Hydrogen atom by showing that,

(a) $|2\pm\rangle$ are orthogonal.

(b) $\langle 2+|H'|2-\rangle = 0$.

(c) $E^{(1)}_{\pm} = \langle 2\pm|H'|2\pm\rangle$, a result from non-degenerate perturbation theory.

12. *Landau Levels*: Problem 5.2 B&J.

Two electron atoms/ions

1. Evaluate the following integral.

$$\int_0^\infty dr_2 \ \frac{r_2^2}{r_>} e^{-2Zr_2} \tag{8}$$

   where $r_> = r_1$ if $r_1 > r_2$ and $r_> = r_2$ if $r_2 > r_1$.

2. Show that if the ground state wave function has an uncertainty of $\mathcal{O}(\epsilon)$, then the uncertainty in the estimation of ground state energy using the Variational method is of $\mathcal{O}(\epsilon^2)$.

3. Show that for singly excited states of the helium atom,

$$\langle \phi_+^0 | \frac{1}{r_{12}} | \phi_-^0 \rangle = 0. \tag{9}$$

   Further, show that four integrals in $\langle \phi_+^0 | \frac{1}{r_{12}} | \phi_+^0 \rangle$ can be written in terms of two integrals J and K introduced in the class.

4. Problem 6.4 B&J.

5. Discuss the suitable choice of trial wave functions for He atom in 2^1S and 2^3S states. Estimate their energies using variation method.

Many electron atoms/ions

1. Determine the form of the normalized symmetric and antisymmetric total eigenfunction for a system of three particles, in which the interactions between the particles can be ignored.