FAQs & their solutions for Module 6:
Hydrogen like atoms and other central potentials

Question1: In spectroscopy the energy levels are usually written in wave number units which are obtained by dividing E_n by *hc*:

$$T_n = \frac{E_n}{hc} = -\frac{Z^2}{n^2}R \tag{1}$$

Using the expression for E_n, show that the Rydberg constant R is given by

$$R = \frac{\mu c \alpha^2}{2h} \tag{2}$$

where

$$\alpha = \frac{q^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137.036} \tag{3}$$

represents the fine structure constant, $\hbar = \dfrac{h}{2\pi} = 1.05457266 \times 10^{-34}$ Js and

$c = 2.9979258 \times 10^8$ m/s represents the speed of light in free space.

Solution 1: The energy eigen-values for a hydrogen-like atom is given by:

$$E_n = -\frac{|E_1|}{n^2} \tag{4}$$

where

$$n = 1, 2, 3, \ldots$$

represents the total quantum number and

$$|E_1| = \frac{1}{2}\mu Z^2 \alpha^2 c^2 \tag{5}$$

represents the magnitude of the ground state energy. Thus we may write

$$T_n = \frac{E_n}{hc} = -\frac{Z^2}{n^2}R$$

where

$$R = \frac{\mu c \alpha^2}{2h} \qquad (6)$$

is known as the Rydberg's constant.

Question2: In continuation of the previous problem, calculate the values of the Rydberg constant for the hydrogen atom, the deuterium atom and the singly ionized Helium atom (which are all hydrogen like atoms).You may assume

$$m_e = 9.1093897 \times 10^{-31} \text{ kg }; \quad m_p = 1.6726231 \times 10^{-27} \text{ kg}; \quad m_n = 1.6749286 \times 10^{-27} \text{ kg};$$

$$m_d = 3.3435860 \times 10^{-27} \text{ kg} \quad \text{and} \quad m_\alpha = 6.644656209 \times 10^{-27} \text{ kg} \qquad (7)$$

where m_e, m_p, m_n, m_d and m_α represent the masses of the electron, proton, neutron, deuteron and the alpha particle respectively.

Solution2: The reduced mass is given by

$$\mu = \frac{m_e m_N}{m_e + m_N} \qquad (8)$$

Using $m_e = 9.1093897 \times 10^{-31}$ kg ; $m_p = 1.6726231 \times 10^{-27}$ kg; $m_n = 1.6749286 \times 10^{-27}$ kg ; $m_d = 3.3435860 \times 10^{-27}$ kg and $m_\alpha = 6.644656209 \times 10^{-27}$ kg we readily get

$R =$ 109677.58 cm^{-1} (for the hydrogen atom)
       109707.56 cm^{-1} (for the deuterium atom)
       109722.40 cm^{-1} (for the He^{+} - atom)

The slight difference in the values is because of the difference in the values of the reduced mass μ.

Question3: Show that (for a hydrogen like atom) for the $n = n_1 \rightarrow n = n_2$ transition, the wavelength of the emitted radiation is given by

$$\lambda = \frac{2h}{\mu Z^2 \alpha^2 c^2} \left[\frac{1}{n_2^2} - \frac{1}{n_1^2} \right]^{-1} \qquad (9)$$

When n_2 = 1, 2 and 3 we have what is known as Lyman series, the Balmer series and the Paschen series respectively.

Solution3: For the $n = n_1 \rightarrow n = n_2$ transition, the wavelength of the emitted radiation is given by

$$\lambda = \frac{hc}{E_{n_1} - E_{n_2}} \tag{10}$$

or

$$\lambda = \frac{2h}{\mu Z^2 \alpha^2 c^2} \left[\frac{1}{n_2^2} - \frac{1}{n_1^2} \right]^{-1} \tag{11}$$

Q uestion4: In continuation of the previous problem, calculate the wavelength of the emitted radiation for the $n = 3 \rightarrow n = 2$ and for the $n = 4 \rightarrow n = 2$ transitions in hydrogen and deuterium.

Solution4: For the $n = 3 \rightarrow n = 2$ transition, the wavelength of the emitted radiation is given by $\lambda = \frac{2h}{\mu Z^2 \alpha^2 c^2} \left[\frac{1}{4} - \frac{1}{9} \right]^{-1}$. Using the data given in Problem 6.2, we can calculate the reduced mass to obtain the following values of the wavelength of the emitted radiation: $6565.2 \overset{o}{A}$ and $6563.4 \overset{o}{A}$ in hydrogen and deuterium respectively. Similarly for the $n = 4 \rightarrow n = 2$ transition, the wavelength of the emitted radiation is given by $\lambda = \frac{2h}{\mu Z^2 \alpha^2 c^2} \left[\frac{1}{4} - \frac{1}{16} \right]^{-1}$ and using the data given in Problem 6.2, we can calculate the reduced mass to obtain the following values of the wavelength of the emitted radiation: $4863.1 \overset{o}{A}$ and $4861.7 \overset{o}{A}$ in hydrogen and deuterium respectively.

Question5: Write the radial part of the Schrodinger equation for the hydrogen-like atom problem for which

$$V(r) = -\frac{Zq^2}{4\pi \varepsilon_0 r} \tag{12}$$

where

$$Z = 1 \quad \text{for the H-atom problem,}$$

$$Z = 2 \quad \text{for the singly ionized He-atom problem (He}^+\text{)},$$

$$Z = 3 \quad \text{for the doubly ionized Li-atom problem (Li}^{++}\text{)}$$

Define a new radial function

$$u(r) \;=\; r\,R(r) \tag{13}$$

and also a new variable $\rho = \gamma r$ and study the solutions of the radial part of the Schrodinger equation as $\rho \to 0$ and as $\rho \to \infty$. Using these limiting behaviors, write the solution as

$$u(\rho) \;=\; \rho^{l+1}\, e^{-\rho/2}\, y(\rho) \tag{14}$$

and show that $y(\rho)$ satisfies the confluent hypergeometric equation. Show that if the confluent hypergeometric function is made into a polynomial, one obtains the energy eigenvalues of the problem.

Solution5: For the hydrogen-like atom problem, the radial part of the Schrödinger equation is given by

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2}\right]R(r) = 0 \tag{15}$$

If we define a new radial function

$$u(r) \;=\; r\,R(r) \tag{16}$$

we would get

$$r^2\frac{dR}{dr} = r^2\frac{d}{dr}\left[\frac{u(r)}{r}\right]$$

$$= r\frac{du}{dr} - u(r)$$

Thus

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = \frac{1}{r}\frac{d^2u}{dr^2} \tag{17}$$

and the radial part of the Schrödinger equation would become

$$\frac{d^2u(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E + \frac{Zq^2}{4\pi\varepsilon_0 r} - \frac{l(l+1)\hbar^2}{2\mu r^2}\right]u(r) = 0 \qquad (18)$$

We introduce the variable $\rho = \gamma r$ to obtain

$$\frac{d^2u}{d\rho^2} + \left[-\frac{1}{4} + \frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2}\right]u(\rho) = 0 \qquad (19)$$

where $\quad \gamma^2 = -\frac{8\mu E}{\hbar^2} \qquad (20)$

and $\qquad \lambda = \frac{2\mu Z}{\hbar^2\gamma}\left(\frac{q^2}{4\pi\varepsilon_0}\right) = Zc\alpha\sqrt{\frac{\mu}{2|E|}} \qquad (21)$

As $\rho \to 0$, Eq.(11) becomes $\frac{d^2u}{d\rho^2} - \frac{1}{4}u(\rho) = 0$ the well-behaved solution of which is

$u(\rho) = e^{-\rho/2}$. As $\rho \to \infty$, Eq.() becomes $\frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2}u(\rho) = 0$ the well-behaved solution of

which is $u(\rho) = \rho^{l+1}$. This suggests we try out the solution $u(\rho) = \rho^{l+1} e^{-\rho/2} y(\rho)$. Simple manipulations would give

$$\rho\frac{d^2y}{d\rho^2} + (c-\rho)\frac{dy}{d\rho} - a\, y(\rho) = 0 \qquad (22)$$

which is the confluent hypergeometric equation. In the above equation

$a = l+1-\lambda \quad$ and $\quad c = 2l+2 \qquad (23)$

The well behaved solution of the above equation is

$$y(\rho) = {}_1F_1(a,c,\rho) = 1 + \frac{a}{c}\rho + \frac{a(a+1)}{c(c+1)}\frac{\rho^2}{2!} + \cdots \qquad (24)$$

represents the confluent hypergeometric function. If the series is not terminated, then as $\rho \to \infty$, it will behave as e^ρ. Thus the series must be made into a polynomial and for that to happen we must have

$a = -n_r\,;\quad$ where $\quad n_r = 0,1,2..... \qquad (25)$

which is known as the radial quantum number. Thus $\lambda = l+1+n_r = n$ and we readily obtain

$$E_n = -\frac{\mu Z^2 \alpha^2 c^2}{2n^2} \quad (26)$$

Question6: For the hydrogen-like atom problem, the radial part of the wave function is given by:

$$R_{nl}(\rho) = N \; e^{-\rho/2} \; \rho^l \; {}_1F_1\left(l+1-n, 2l+2, \rho\right) \; ; \quad n = 1, 2, 3, \dots \quad (27)$$
$$l = 0, 1, 2, \dots n-1$$

where

$$\left.\begin{aligned} \rho &= \gamma r \; ; & \gamma &= \frac{2Z}{na_0} \\ a_0 &= \frac{\hbar^2}{\mu(q^2/4\pi\varepsilon_0)} \end{aligned}\right\} \quad (28)$$

is the Bohr radius. Further

$${}_1F_1(a, c, \rho) = 1 + \frac{a}{c}\rho + \frac{a(a+1)}{c(c+1)}\frac{\rho^2}{2!} + \cdots \quad (29)$$

represents the confluent hypergeometric function and N represents the normalization constant. Obtain the normalized functions $R_{20}(r), R_{21}(r), R_{30}(r), R_{31}(r)$ and $R_{32}(r)$.

Solution 6: The normalization condition is given by

$$\int_0^\infty \left| R_{nl}(r) \right|^2 \; r^2 \; dr = 1 \quad (30)$$

For $n = 2, l = 0$ we will have ${}_1F_1\left(-1, 2, \rho\right) = 1 - \frac{\rho}{2}$. Thus the normalization condition becomes

$$\frac{N^2}{\gamma^3} \int_0^\infty e^{-\rho}\left(1 - \frac{\rho}{2}\right)^2 \rho^2 \; d\rho = 1$$

$$\Rightarrow \frac{N^2}{\gamma^3} \int_0^\infty e^{-\rho}\left(\rho^2 - \rho^3 + \frac{\rho^4}{2}\right) d\rho = 1$$

Simple integrations will give

$$N = \gamma^{3/2}\left[\frac{2!}{4\times 1}\right]^{1/2} = \frac{1}{\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2} \quad (31)$$

Thus

$$R_{2\,0}(r) = \frac{1}{\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(1-\frac{1}{2}\xi\right)e^{-\xi/2} \qquad (32)$$

where $\xi = \dfrac{r}{a_0}$. Similarly, one can calculate other wave functions:

$$R_{1\,0}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-\xi} \qquad (33)$$

$$R_{2\,1}(r) = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} \xi\, e^{-\xi/2}$$

$$R_{3\,0}(r) = \frac{2}{3\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2}\left(1-\frac{2}{3}\xi+\frac{2}{27}\xi^2\right)e^{-\xi/3}$$

$$\qquad\qquad\qquad\qquad\qquad\qquad (34)$$

$$R_{3\,1}(r) = \frac{8}{27\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\xi-\frac{1}{6}\xi^2\right)e^{-\xi/3}$$

$$R_{3\,2}(r) = \frac{4}{81\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2} \xi^2\, e^{-\xi/3}$$

Question7: Write the radial part of the Schrodinger equation for the 3-dimensional oscillator problem for which

$$V(r) = \frac{1}{2}\mu\omega^2 r^2 \qquad\qquad (35)$$

Define a new variable

$$\xi = \gamma^2 r^2;\ \gamma = \sqrt{\frac{\mu\omega}{\hbar}} \qquad\qquad (36)$$

and study the solutions of the radial part of the Schrodinger equation as $\xi \to 0$ and as $\xi \to \infty$. Using these limiting behaviors, write the solution as

$$R(\xi) = \xi^{l/2}\, e^{-\xi/2}\, y(\rho) \qquad\qquad (37)$$

and show that $y(\rho)$ satisfies the confluent hypergeometric equation. Show that if the confluent hypergeometric function is made into a polynomial, one obtains the energy eigenvalues of the problem.

Solution7: For the 3-dimensional oscillator problem for which

$$V(r) = \frac{1}{2}\mu\omega^2 r^2 \text{ , the radial part of the Schrödinger equation is given by}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu}{\hbar^2}\left[E - \frac{1}{2}\mu\omega^2 r^2 - \frac{l(l+1)\hbar^2}{2\mu r^2}\right]R(r) = 0 \qquad (38)$$

We define a new variable

$$\xi = \gamma^2 r^2 ; \ \gamma = \sqrt{\frac{\mu\omega}{\hbar}} \qquad\qquad (39)$$

to obtain

$$\frac{d^2R}{d\xi^2} + \frac{3}{2\xi}\frac{dR}{d\xi} + \left[\frac{E}{2\hbar\omega\xi} - \frac{l(l+1)}{4\xi^2} - \frac{1}{4}\right]R(\xi) = 0 \qquad (40)$$

As $\xi \to 0$, the above equation becomes $\dfrac{d^2R}{d\xi^2} - \dfrac{1}{4}R(\xi) = 0$ the well-behaved solution of

which is $R(\xi) \ = e^{-\xi/2}$. As $\xi \to \infty$, the equation becomes

$$\frac{d^2R}{d\xi^2} + \frac{3}{2\xi}\frac{dR}{d\xi} - \frac{l(l+1)}{4\xi^2}R(\xi) = 0 \qquad (41)$$

the well-behaved solution of which is $R(\xi) \ = \xi^{l/2}$. This suggests we try out the

solution $R(\xi) \ = \xi^{l/2}\ e^{-\xi/2}\ y(\xi)$. Simple manipulations would give

$$\xi\frac{d^2y}{d\xi^2} + (c - \xi)\frac{dy}{d\xi} - a\ y(\xi) = 0 \qquad\qquad (42)$$

which is the confluent hypergeometric equation. In the above equation

$$a = \frac{l}{2} + \frac{3}{4} - \frac{E}{2\hbar\omega} \quad \text{and} \quad c = l + \frac{3}{2} \qquad\qquad (43)$$

Once again, the well behaved solution of the above equation is

$$y(\xi) = {}_1F_1(a,c,\xi) = 1 + \frac{a}{c}\xi + \frac{a(a+1)}{c(c+1)}\frac{\xi^2}{2!} + \cdots \qquad\qquad (44)$$

which represents the confluent hyper geometric function. If the series is not terminated, then as $\xi \to \infty$, it will behave as e^{ξ}. Thus the series must be made into a polynomial and for that to happen we must have

$$a = -n_r ; \quad \text{where} \quad n_r = 0,1,2..... \qquad (45)$$

Thus the eigen values of the problem are

$$E = \left(2n_r + l + \frac{3}{2}\right)\hbar\omega \qquad (46)$$