Assignment 2a

PHYS4000 Advanced Computational Quantum Mechanics

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May 2023

1 Question 1

Equation 2.17 is written as:

$$\frac{d^2u_l(r)}{dr^2} + 2(E + \frac{Z}{r})u_l(r) = l(l+1)\frac{u_l(r)}{r^2} \tag{1}$$

First we need to make ρ the subject of the function which is done through the substitution of $\rho = kr$.

$$k^2\frac{d^2u_l(\rho)}{d\rho^2} + 2(-\frac{k^2}{8} + \frac{Z}{\rho k})u_l(\rho) = l(l+1)\frac{u_l(\rho)k^2}{\rho^2} \tag{2}$$

Where we have substituted for E by rearranging the definition of $k = 2\sqrt{-2E}$. We further simplify the differential Equation to the following by cancelling rho and multiplying the bracket:

$$\frac{d^2u_l(\rho)}{d\rho^2} - (\frac{1}{4} - \frac{2Z}{\rho k})u_l(\rho) = l(l+1)\frac{u_l(\rho)}{\rho^2} \tag{3}$$

In finding the solutions to the differential equation we rearrange it into the form...

$$\frac{d^2u_l(\rho)}{d\rho^2} - (\frac{1}{4} - \frac{2Z}{\rho k})u_l(\rho) - l(l+1)\frac{u_l(\rho)}{\rho^2} = 0 \tag{4}$$

The question presents the substitution $u_l(\rho) = \rho^{l+1}\exp\{-\rho/2\}\omega(\rho)$, which forms...

$$\frac{d^2}{d\rho^2}[\rho^{l+1}\exp\{-\rho/2\}\omega(\rho)] - (\frac{1}{4} - \frac{2Z}{\rho k})(\rho^{l+1}\exp\{-\rho/2\}\omega(\rho)) - l(l+1)\rho^{l-1}\exp\{-\rho/2\}\omega(\rho) = 0 \tag{5}$$

$$(l+1)[(l\rho^{l-1}\exp\{-\rho/2\} - \frac{1}{2}\rho^{l+1}\exp\{-\rho/2\})\omega(\rho) + \rho^l\exp\{-\rho/2\}\frac{d\omega(\rho)}{d\rho}]$$

$$-\frac{1}{2}\{[(l+1)\rho^l\exp\{-\rho/2\} - \frac{1}{2}\rho^{l+1}\exp\{-\rho/2\}]\omega(\rho) + \frac{d\omega(\rho)}{d\rho^2}\rho^{l+1}\exp\{-\rho/2\}\}$$

$$+[(l+1)\rho^l\exp\{-\rho/2\} - \frac{1}{2}\rho^{l+1}\exp\{-\rho/2\}]\frac{d\omega(\rho)}{d\rho} + \frac{d^2\omega(\rho)}{d\rho^2}\rho^{l+1}\exp\{-\rho/2\}$$

$$-(\frac{1}{4} - \frac{2Z}{k\rho})\rho^{l+1}\exp\{-\rho/2\}\omega(\rho) - l(l+1)\rho^{l-1}\exp\{-\rho/2\}\omega(\rho) = 0$$

and simplifies to

$$\frac{d^2\omega(\rho)}{d\rho^2}\rho^{l+1} + \frac{d\omega(\rho)}{d\rho}[2(l+1)\rho^l - \rho^{l+1}] - \omega(\rho)[(l+1)\rho^l - \frac{2Z}{k}\rho^l] = 0 \tag{6}$$

We now eliminate ρ^l on all terms to get:

$$\frac{d^2\omega(\rho)}{d\rho^2}\rho + [2(l+1) - \rho]\frac{d\omega(\rho)}{d\rho} - [(l+1) - \frac{2Z}{k}]\omega(\rho) = 0 \tag{7}$$

This differential equation has the form:

$$z\frac{d^2w}{dz^2} + (b-z)\frac{dw}{dz} - aw = 0 \tag{8}$$

Which has solutions in the confluent hypergeometric function;

$$F(a,b;\rho) = 1 + \frac{a}{b}\frac{\rho}{1!} + \frac{a}{b}\frac{(a+1)}{(b+1)}\frac{\rho^2}{2!} + \dots \tag{9}$$

In this case, the function will truncate so long as $a = 1 - n$ for $n = 1, 2, 3$, in this way, after the $n + 1$ term of the series and all subsequent terms must simplify to zero.

In this case then by comparing the equation we have with the general form, we can see that

$$a = l + 1 - \frac{2Z}{k} \tag{10}$$

$$b = 2(l + 1) \tag{11}$$

And knowing that the differential equation is has the general solution and that the series terminates, we know that this set of equations satisfies the conditions for a solution of $\omega(\rho)$.

2 Question 2

The equation:

$$F(a, b; \rho) = 1 + \frac{a}{b}\frac{\rho}{1!} + \frac{a}{b}\frac{(a+1)}{(b+1)}\frac{\rho^2}{2!} + \dots \tag{12}$$

Terminates for $a = 1 - n$, for $n \in \{1, 2, 3, \dots\}$. This prevents the series from growing exponentially in ρ.

In our case, we have $a = 1 + l - \frac{2Z}{k}$, which can be rewritten as $a = 1 - (\frac{2Z}{k} - l)$.
This makes our $n = \frac{2Z}{k} - l$ and subsequently $n + l = \frac{2Z}{k}$.
We then write $n = \frac{2Z}{k}$, $\forall\, n \in \{1 + l, 2 + l, 3 + l, \dots\}$.

3 Question 3

2.28 states:

$$\int_E^{yee} \tag{13}$$