

Assignment 2a

PHYS4000 Advanced Computational Quantum Mechanics

Ryan Craft

Unit Coordinated by
Dr. Igor Bray

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1 Question 1

Equation 2.17 is written as:

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

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

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

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 k^2 and multiplying the bracket:

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

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

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

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

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

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

and simplifies to

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

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

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

This differential equation has the form:

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

Which has solutions in the confluent hypergeometric function;

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

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

$$a = l + 1 - \frac{2Z}{k} \quad (10)$$

$$b = 2(l + 1) \quad (11)$$

And knowing that the differential equation 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:

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

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:

$$\int_0^\infty dr u_{n'l}(r) u_{nl}(r) = \delta_{n'n} \quad (13)$$

Which tell us that the eigenstates are orthogonal and normalised for $n = n'$, where the kronecker delta equals unity. This will allow us to calculate the normalisation coefficients for our wave-functions, $u_{21}(r)$ and $u_{31}(r)$.

For $\mathbf{u}_{21}(\mathbf{r})$;

First we establish what we are substituting for ρ , with $Z = 1$, $n = 2$, $l = 1$:

$$\begin{aligned} \rho = kr &= \frac{2Zr}{n} \\ \rho = kr &= \frac{2(1)r}{2} = r \\ \therefore k &= 1 \end{aligned} \quad (14)$$

With $l = 1 = Z = k = 1$ we have:

$$\begin{aligned} a &= l + 1 - \frac{2Z}{k} \\ a &= 1 + 1 - 2 = 0 \\ b &= 2(l + 1) \\ \hbar &\equiv \mathfrak{H}(2\hbar) \equiv 4 \end{aligned} \quad (15)$$

Calculating the $\omega(kr)$

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

$$F(0, 4; r) = 1 + \frac{0}{4} \frac{r}{1!} + \frac{0(0+1)}{4(4+1)} \frac{r^2}{2!} + \dots$$

$$F(0, 4; r) = \omega(r) = 1 \quad (16)$$

Substituting r for ρ to get back $u_{nl}(r)$ from $u_{nl}(\rho)$:

$$u_{nl}(r) = (kr)^{l+1} \exp\{-kr/2\} \omega(kr)$$

$$u_{21}(r) = r^{1+1} \exp\{-r/2\} (1)$$

$$u_{21}(r) = r^2 \exp\{-r/2\} \quad (17)$$

We need to add a constant of normalisation to this function in order for it to belong to the Hilbert space, and we will use (13) in order to normalise.

$$\int_0^\infty (Ar^2 \exp\{-r/2\})^2 dr = \delta_{n'n}$$

$$\int_0^\infty A^2 r^4 \exp\{-r\} dr = \delta_{2,2} = 1$$

Tabular integration will solve the integral

F(x)	G(x)
r^4	e^{-r}
$-4r^3$	$-e^{-r}$
$12r^2$	e^{-r}
$-24r$	$-e^{-r}$
24	e^{-r}
0	$-e^{-r}$
	e^{-r}

$$\int_0^\infty A^2 r^4 \exp\{-r\} dr$$

$$= A^2 [-r^4 \exp\{-r\} - 4r^3 \exp\{-r\} - 12r^2 \exp\{-r\} - 24r \exp\{-r\} - 24 \exp\{-r\}]_0^\infty$$

$$= A^2 [0 - (-24)]$$

$$= 24A^2 = 1$$

$$A = \frac{1}{2\sqrt{6}} \quad (18)$$

Which normalises the function to

$$u_{21}(r) = \frac{r^2}{2\sqrt{6}} \exp\{-r/2\} \quad (19)$$

as given in the problem statement.

For $\mathbf{u}_{31}(\mathbf{r})$:

We start in the same way, by defining the appropriate quantities starting with $Z = 1$, $n = 3$, $l = 1$. Subsequently computing parameters like k :

$$\begin{aligned} \rho &= kr = \frac{2Zr}{n} \\ \rho &= kr = \frac{2(1)r}{3} = r \\ \therefore k &= \frac{2}{3} \end{aligned} \quad (20)$$

a and $b \dots$

$$\begin{aligned} a &= l + 1 - \frac{2Z}{k} \\ a &= 1 + 1 - \frac{2(1)}{\frac{2}{3}} \\ a &= 1 + 1 - 3 = -1 \\ b &= 2(l + 1) \\ b &= 2(2) = 4 \\ a &= -1, \quad b = 4 \end{aligned} \quad (21)$$

Taking these