

Engel 9.10

Problem. Show that the wave function given in Engel is a solution of the differential equation given there (assume $l = 1$) and provide an expression for the "eigenvalue" E , the total energy. Using this result, determine the value of the principal quantum number, n , for this function.

Answer. Comparison of the wave function with the functions listed on Engel p. 164 show that the function is the r -dependent portion of R_{21} , in other words, $n = 2$ and $l = 1$. You should also notice that the differential equation in problem 9.10 is nearly identical to the "radial" differential equation, Engel eq. 9.5, for the hydrogen atom. The only difference is that μ appears in problem 9.10 and m_e appears in eq. 9.5.

The simplest way to proceed is to break the left-hand side of the differential equation into three terms, evaluate each of them separately, and then combine them. The result should be the original function multiplied by a fixed constant.

First, define $R(r)$...

```
In[7]:= Clear[r, R, a0]
        R = ( r / a0 ) e^{-r/(2 a0)}
```

```
Out[8]=  $\frac{e^{-\frac{r}{2a_0}} r}{a_0}$ 
```

Evaluate the differential term ...

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In[19]:= Term1 =  $\partial_r R$ 
Term1 = Simplify[r2 Term1]
Term1 =  $\partial_r$  Term1
Term1 = Simplify[Term1]
Term1 = -  $\left( \frac{\hbar^2}{2 \mu r^2} \right)$  Term1
Term1 = Simplify[Term1]

```

$$\text{Out}[19]= \frac{e^{-\frac{r}{2a_0}}}{a_0} - \frac{e^{-\frac{r}{2a_0}} r}{2 a_0^2}$$

$$\text{Out}[20]= - \frac{e^{-\frac{r}{2a_0}} r^2 (-2 a_0 + r)}{2 a_0^2}$$

$$\text{Out}[21]= - \frac{e^{-\frac{r}{2a_0}} r^2}{2 a_0^2} - \frac{e^{-\frac{r}{2a_0}} r (-2 a_0 + r)}{a_0^2} + \frac{e^{-\frac{r}{2a_0}} r^2 (-2 a_0 + r)}{4 a_0^3}$$

$$\text{Out}[22]= \frac{e^{-\frac{r}{2a_0}} r (8 a_0^2 - 8 a_0 r + r^2)}{4 a_0^3}$$

$$\text{Out}[23]= - \frac{e^{-\frac{r}{2a_0}} \hbar^2 (8 a_0^2 - 8 a_0 r + r^2)}{8 a_0^3 r \mu}$$

$$\text{Out}[24]= - \frac{e^{-\frac{r}{2a_0}} \hbar^2 (8 a_0^2 - 8 a_0 r + r^2)}{8 a_0^3 r \mu}$$

Evaluate the l -dependent term (use $l = 1$)

```

In[25]:= l = 1
Term2 =  $\left( \frac{\hbar^2 l (l + 1)}{2 \mu r^2} \right) R$ 
Term2 = Simplify[Term2]

```

$$\text{Out}[25]= 1$$

$$\text{Out}[26]= \frac{e^{-\frac{r}{2a_0}} \hbar^2}{a_0 r \mu}$$

$$\text{Out}[27]= \frac{e^{-\frac{r}{2a_0}} \hbar^2}{a_0 r \mu}$$

Evaluate the Coulomb term. It is convenient to use the definition of a_0 given on Engel p. 163 to rewrite this term. $a_0 = \epsilon_0 \hbar^2 / \pi m_e e^2$. However, a problem arises because a_0 is defined using m_e and the differential equation is based on μ . Fortunately, the enormous disparity of the nuclear and electron masses makes the two quantities nearly identical, and the Coulomb term can be rewritten as $-\hbar^2 / \mu a_0 r$.

```
In[28]:= Term3 =  $\frac{-\hbar^2}{\mu a_0 r}$  R
          Term3 = Simplify[Term3]
```

```
Out[28]=  $-\frac{e^{-\frac{r}{2a_0}} \hbar^2}{a_0^2 \mu}$ 
```

```
Out[29]=  $-\frac{e^{-\frac{r}{2a_0}} \hbar^2}{a_0^2 \mu}$ 
```

```
In[30]:= LHS = Term1 + Term2 + Term3
          LHS = Simplify[LHS]
```

```
Out[30]=  $-\frac{e^{-\frac{r}{2a_0}} \hbar^2}{a_0^2 \mu} + \frac{e^{-\frac{r}{2a_0}} \hbar^2}{a_0 r \mu} - \frac{e^{-\frac{r}{2a_0}} \hbar^2 (8 a_0^2 - 8 a_0 r + r^2)}{8 a_0^3 r \mu}$ 
```

```
Out[31]=  $-\frac{e^{-\frac{r}{2a_0}} \hbar^2 r}{8 a_0^3 \mu}$ 
```

To obtain the eigenvalue (E) and show that $R(r)$ is a solution of the differential equation, we should divide the left-hand side by $R(r)$

```
In[32]:= Energy = LHS / R
```

```
Out[32]=  $-\frac{\hbar^2}{8 a_0^2 \mu}$ 
```

The result is a numerical constant, so we have successfully demonstrated that $R(r)$ is a solution of the equation. The result does not look like either of the energy formulas on p. 163, however, so a little additional work is required. Essentially, we need to rewrite the energy formula using the relationship $a_0 = \epsilon_0 \hbar^2 / \pi m_e e^2$

```
In[33]:= a0 =  $\frac{\epsilon_0 \hbar^2}{\pi \mu q e^2}$ 
          hbar =  $\frac{\hbar}{2 \pi}$ 
          Energy
```

```
Out[33]=  $\frac{\hbar^2 \epsilon_0}{\pi q e^2 \mu}$ 
```

```
Out[34]=  $\frac{\hbar}{2 \pi}$ 
```

```
Out[35]=  $-\frac{q e^4 \mu}{32 \hbar^2 \epsilon_0^2}$ 
```

This formula agrees with Engel 9.7 when $n = 2$ (which is exactly what we had noticed above).