

Appendix E: Mathematica Derivation of Equations (3.18)–(3.21)

From our complementary Mathematica notebook, AppendixE.nb:

The reader may copy all Mathematica `In[#:]=` sections below into a new notebook and execute them one by one in order to repeat our calculations.

Introduce function $s(\theta) = \frac{1}{r}$ from (3.9):

$$\text{In}[1]:= \text{s}[\text{Theta}_] := (1 + \text{Epsilon} \text{Cos}[\text{Omega} \text{Theta}]) / (a (1 - \text{Epsilon}^2))$$

$$\begin{aligned} \text{In}[2]:= & \text{s}[\text{Theta}] \\ \text{Out}[2]= & \frac{1 + \epsilon \cos(\theta\omega)}{a(1 - \epsilon^2)} \end{aligned}$$

and evaluate its derivative:

$$\begin{aligned} \text{In}[3]:= & \text{D}[\text{s}[\text{Theta}], \text{Theta}] \\ \text{Out}[3]= & -\frac{\epsilon\omega \sin(\theta\omega)}{a(1 - \epsilon^2)} \end{aligned}$$

The r.h.s. of (3.4), evaluate:

$$\begin{aligned} \text{In}[4]:= & (\text{D}[\text{s}[\text{Theta}], \text{Theta}]^2 + (\text{s}[\text{Theta}])^2) \\ \text{Out}[4]= & \frac{(1 + \epsilon \cos(\theta\omega))^2 + \epsilon^2 \omega^2 \sin^2(\theta\omega)}{a^2(1 - \epsilon^2)^2} \end{aligned}$$

and substitute:

$$\begin{aligned} \text{In}[5]:= & \% /. \text{Sin}[\text{Theta} \text{Omega}]^2 \rightarrow 1 - (\text{Cos}[\text{Theta} \text{Omega}])^2 \\ \text{Out}[5]= & \frac{(1 + \epsilon \cos(\theta\omega))^2 + \epsilon^2 \omega^2 (1 - \cos^2(\theta\omega))}{a^2(1 - \epsilon^2)^2} \end{aligned}$$

Introduce S and eliminate cosine:

$$\begin{aligned} \text{In}[6]:= & \text{Solve}[S == (1 + \text{Epsilon} \text{Cos}[\text{Theta} \text{Omega}]) / (a (1 - \text{Epsilon}^2)), \text{Cos}[\text{Theta} \text{Omega}]] \\ \text{Out}[6]= & \left\{ \cos(\theta\omega) \rightarrow \frac{-1 + aS - aS\epsilon^2}{\epsilon} \right\} \end{aligned}$$

$$\begin{aligned} \text{In}[7]:= & \text{FullSimplify}[\% /. \text{Cos}[\text{Theta} \text{Omega}] \rightarrow (-1 + a S - a S \text{Epsilon}^2) / \text{Epsilon}] \\ \text{Out}[7]= & \frac{\omega^2 + aS (-2\omega^2 - aS(-1 + \epsilon^2)(-1 + \omega^2))}{a^2(1 - \epsilon^2)} \end{aligned}$$

As a result, in terms of S , the above expression becomes:

$$\begin{aligned} \text{In}[8]:= & \text{Collect}[\%, S] \\ \text{Out}[8]= & \frac{\omega^2}{a^2(1 - \epsilon^2)} - \frac{2S\omega^2}{a(1 - \epsilon^2)} - S^2(-1 + \omega^2) \end{aligned}$$

Equation (3.4), define the difference between r.h.s. and l.h.s.:

$$\begin{aligned} \text{In}[9]:= & P = (\text{En}/(m c^2) + (Z (e^2) S) / (m c^2))^2 - \\ & 1 - ((\text{HBar} \text{Subscript}[n, \text{Theta}]) / (m c))^2 * (\text{Omega}^2 / (a^2 (-1 + \text{Epsilon}^2)) - (2 S \text{Omega}^2) / (a (-1 + \text{Epsilon}^2)) - S^2 (-1 + \text{Omega}^2)) \\ \text{Out}[9]= & -1 + \left(\frac{En}{c^2 m} + \frac{e^2 SZ}{c^2 m} \right)^2 - \left(\frac{\omega^2}{a^2(1 - \epsilon^2)} - \frac{2S\omega^2}{a(1 - \epsilon^2)} - S^2(-1 + \omega^2) \right) \frac{\hbar^2 n_\theta^2}{c^2 m^2} \end{aligned}$$

and simplify:

$$\text{In}[10]:= \% /. e^2 \rightarrow \text{Alpha} * \text{HBar} * c ;$$

```
In[11]:= Collect[%, S]
Out[11]=
-1 +  $\frac{En^2}{c^4 m^2} - \frac{\omega^2 \hbar^2 n_\theta^2}{a^2 c^2 m^2 (1 - \epsilon^2)} + S \left( \frac{2EnZ\alpha\hbar}{c^3 m^2} + \frac{2\omega^2 \hbar^2 n_\theta^2}{ac^2 m^2 (1 - \epsilon^2)} \right) + S^2 \left( \frac{Z^2 \alpha^2 \hbar^2}{c^2 m^2} + \frac{(-1 + \omega^2) \hbar^2 n_\theta^2}{c^2 m^2} \right)$ 
```

To satisfy (3.4), all coefficients of this quadratic polynomials must be equal to zero:

```
In[12]:= {Subscript[C,
0] = (Z^2 \[Alpha]^2 \[HBar]^2)/(c^2 m^2) + ((-1 + \[Omega]^2) \[HBar]^2
\!\(\*\SubsuperscriptBox[\(n\), \(\[Theta]\), \(\(2\)\)\])/(c^2 m^2),
Subscript[C,
1] = (2 En Z \[Alpha] \[HBar])/(c^3 m^2) + (2 \[Omega]^2 \[HBar]^2
\!\(\*\SubsuperscriptBox[\(n\), \(\[Theta]\), \(\(2\)\)\])/(
a c^2 m^2 (-1 + \[Epsilon]^2)),
Subscript[C, 2] = -1 + En^2/(c^4 m^2) - (\[Omega]^2 \[HBar]^2
\!\(\*\SubsuperscriptBox[\(n\), \(\[Theta]\), \(\(2\)\)\])/(
a^2 c^2 m^2 (-1 + \[Epsilon]^2))}
Out[12]= {  $\frac{Z^2 \alpha^2 \hbar^2}{c^2 m^2} + \frac{(-1 + \omega^2) \hbar^2 n_\theta^2}{c^2 m^2}$ ,  $\frac{2EnZ\alpha\hbar}{c^3 m^2} + \frac{2\omega^2 \hbar^2 n_\theta^2}{ac^2 m^2 (1 - \epsilon^2)}$ ,  $-1 + \frac{En^2}{c^4 m^2} - \frac{\omega^2 \hbar^2 n_\theta^2}{a^2 c^2 m^2 (1 - \epsilon^2)}$  }
```

From the vanishing leading term, we choose the positive solution:

```
In[13]:= Solve[Subscript[C, 0] == 0, \[Omega]]
Out[13]= {  $\omega \rightarrow -\frac{\sqrt{-Z^2 \alpha^2 + n_\theta^2}}{n_\theta}$ ,  $\omega \rightarrow \frac{\sqrt{-Z^2 \alpha^2 + n_\theta^2}}{n_\theta}$  }
```

From the linear term, find the energy in terms of a as follows:

```
In[14]:= Solve[Subscript[C, 1] == 0, En]
Out[14]= {  $En \rightarrow -\frac{c \omega^2 \hbar n_\theta^2}{a Z \alpha (1 - \epsilon^2)}$  }
```

Alternatively, from (3.17):

```
In[15]:= Solve[(En Z \[Alpha])/\!\(\*\SubsuperscriptBox[\(n\), \(\[Theta]\), \(\(2\)\)]*c*\[HBar]*
*\SuperscriptBox[\(\[Omega]\), \(\(2\)\)] == 1/(a (1 - \[Epsilon]^2)), En]
Out[15]= {  $En \rightarrow -\frac{c \omega^2 \hbar n_\theta^2}{a Z \alpha (1 - \epsilon^2)}$  }
```

We verify that the linear term is vanished:

```
In[16]:= Subscript[C, 1] /. En -> -((c \[Omega]^2 \[HBar]
\!\(\*\SubsuperscriptBox[\(n\), \(\[Theta]\), \(\(2\)\)\])/(
a Z \[Alpha] (-1 + \[Epsilon]^2)))
Out[16]= 0
```

The constant term can be simplified in terms of (3.16):

```
In[17]:= Subscript[C, 2] /.
1/(-1 + \[Epsilon]^2) -> -((Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 +
\!\(\*\SubsuperscriptBox[\(n\), \(\[Theta]\), \(\(2\)\)\])^2/\(\[Omega]^2
\!\(\*\SubsuperscriptBox[\(n\), \(\[Theta]\), \(\(2\)\)\])^2))
Out[17]=  $-1 + \frac{En^2}{c^4 m^2} + \frac{\hbar^2 (n_r + \sqrt{-Z^2 \alpha^2 + n_\theta^2})^2}{a^2 c^2 m^2}$ 
```

The same for the linear term, in order to eliminate epsilon from the expression for energy:

```
In[18]:= Subscript[C, 1] /.
1/(-1 + \[Epsilon]^2) -> -((Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 +
\!\(\*\SubsuperscriptBox[\(n\), \(\[Theta]\), \(\(2\)\)\])^2/\(\[Omega]^2
\!\(\*\SubsuperscriptBox[\(n\), \(\[Theta]\), \(\(2\)\)\])^2))
Out[18]=  $\frac{2EnZ\alpha\hbar}{c^3 m^2} - \frac{2\hbar^2 (n_r + \sqrt{-Z^2 \alpha^2 + n_\theta^2})^2}{ac^2 m^2}$ 
```

```
In[19]:= Solve[% == 0, En]
Out[19]= {En -> \frac{c\hbar(n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})^2}{aZ\alpha}}
```

Exclude energy from the constant term:

```
In[20]:= -1 + En^2/(c^4 m^2) + (\hbar^2 (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^2)/(a^2 c^2 m^2) /.
En -> (c \hbar (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^2)/(a Z \[Alpha])
Out[20]= -1 + \frac{\hbar^2 (n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})^2}{a^2 c^2 m^2} + \frac{\hbar^2 (n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})^4}{a^2 c^2 m^2 Z^2 \alpha^2}
```

Now solve a modified equation for $A = a^2$:

```
In[21]:= Solve[(\hbar^2 (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^2)/(c^2 m^2) + (\hbar^2 (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^4)/(c^2 m^2 Z^2 \[Alpha]^2) == A, A]
Out[21]= {A -> \frac{\hbar^2 (n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})^2}{c^2 m^2} + \frac{\hbar^2 (n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})^4}{c^2 m^2 Z^2 \alpha^2}}
```

Transform the result as follows:

```
In[22]:= Factor[(\hbar^2 (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^2)/(c^2 m^2) + (\hbar^2 (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^4)/(c^2 m^2 Z^2 \[Alpha]^2)]
Out[22]= \frac{\hbar^2 (n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})^2 (n_r^2 + n_\theta^2 + 2n_r \sqrt{-Z^2\alpha^2 + n_\theta^2})}{c^2 m^2 Z^2 \alpha^2}
```

An equivalent expression:

```
In[23]:= (\hbar^2 (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^2 * ((Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^2 + Z^2 \[Alpha]^2)) / (c^2 m^2 Z^2 \[Alpha]^2)
Out[23]= \frac{\hbar^2 (n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})^2 \left( (n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})^2 + Z^2 \alpha^2 \right)}{c^2 m^2 Z^2 \alpha^2}
```

Verification:

```
In[24]:= Simplify[% - %]
Out[24]= 0
```

Finally, substitute the parameter a into the previously found expression for energy:

```
In[25]:= (c \hbar (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^2)/(a Z \[Alpha]) /.
a -> (\hbar (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2]) Sqrt[Z^2 \[Alpha]^2 + (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 + \[Alpha]^2 \[Theta]^2])^2])/(c m Z \[Alpha])
Out[25]= \frac{c^2 m (n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})}{\sqrt{Z^2\alpha^2 + (n_r + \sqrt{-Z^2\alpha^2 + n_\theta^2})^2}}
```

Compare the square of this result with the square of equation (3.18):

```

In[26]:= Simplify[(Z^2 \[Alpha]^2 + (Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 +
\!\(\*SubsuperscriptBox[\(n\), \(\[Theta]\), \((2\)\)]\)\)^2)/(Subscript[n, r] +
Sqrt[-Z^2 \[Alpha]^2 +
\!\(\*SubsuperscriptBox[\(n\), \(\[Theta]\), \((2\)\)]\)\)^2 - (1 + (
Z^2 \[Alpha]^2)/(Subscript[n, r] + Sqrt[-Z^2 \[Alpha]^2 +
\!\(\*SubsuperscriptBox[\(n\), \(\[Theta]\), \((2\)\)]\)\)^2)]
Out[26]= 0

```

Thus we derived equations (3.18)-(3.21) with the help of Mathematica computer algebra system

End of Mathematica session. (More details can be found in our complementary Mathematica notebook, AppendixE.nb.)

MORE MATHEMATICA SUPPORT: In addition to AppendixE.nb presented above, our complimentary Mathematica notebooks also include BohrAtomMathematica.nb and EllipsesAnimateAu.nb, both at introductory level. While EllipsesAnimateSofisticated.nb is designed to create advanced animations of the relativistic Keplerian motion of hydrogen-like ions in the periodic table of elements.