PH 427 Homework 10 -- John Waczak

5. Calculate the probability that the electron is in the classically forbidden region for the n=2 states of hydrogen. Discuss the differences between the results for *l*=0 and *l*=1.

In order to define the classically forbidden region, we need to consider the quantum version of the Effective Potential. (I am using SI units)

In[332]:=

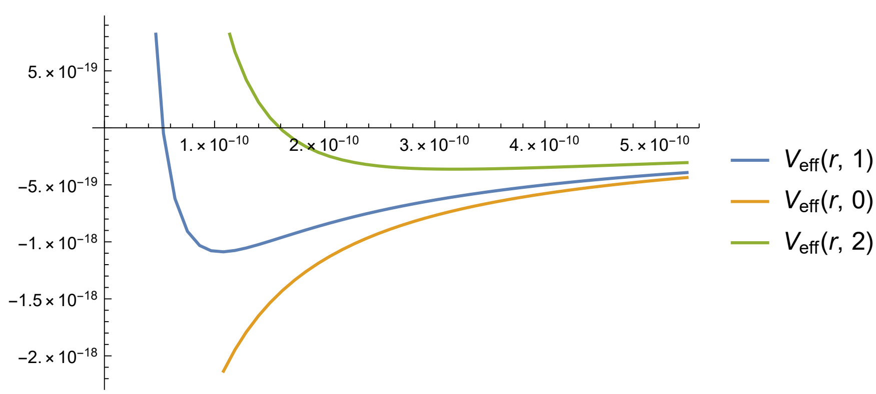
```
Z = 1
ϵ0 = 8.854 * 10^(-12)
V[r_] := -e^2 / (4 * π * ϵ0 * r)
m_e = 9.1 * 10^(-31)
m_p = 1.7 * 10^(-27)
μ = (m_e * m_p) / (m_e + m_p)
V_eff[r_, ℓ_] = ((ℏ^2 * ℓ * (ℓ + 1)) / (2 * μ * r^2) + V[r])
a0 = 5.29 * 10^-11
```

The following plot shows $V_{eff}(r)$ for l values 0,1, and 2

In[340]:=

```
Plot[{V_eff[r, 1], V_eff[r, 0], V_eff[r, 2]}, {r, 0, 10 * a0}, PlotLegends → "Expressions"]
```

Out[340]=

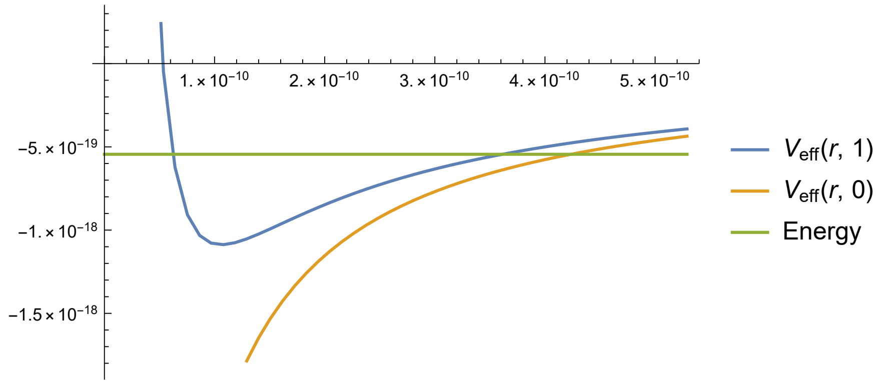


Now we know that for our states, n=2 which means that the total energy is $\frac{-13.6\ \text{eV}}{2^2}$ which we can use to solve for the bounds of the classically forbidden region. To do this we observe that -13.6/v eV = -5.44*10^-19 Joules

In[341]:=
```
Energy = (-13.6/4) * e
Plot[{Veff[r, 1], Veff[r, 0], Energy}, {r, 0, 10 * a0}, PlotLegends → "Expressions"]
```

Out[341]= -5.4468×10^{-19}

Out[342]=



In[343]:=
```
Solve[Veff[r, 0] == Energy, r]
```

Out[343]= $\{\{r \to 4.23481 \times 10^{-10}\}\}$

In[344]:=
```
Solve[Veff[r, 1] == Energy, r]
```

Out[344]= $\{\{r \to 6.21234 \times 10^{-11}\}, \{r \to 3.61358 \times 10^{-10}\}\}$

In[352]:=
```
r1 = 4.23481*^-10
r2 = 6.21234*^-11
r3 = 3.61358*^-10
```

Out[352]= 4.23481×10^{-10}

Out[353]= 6.21234×10^{-11}

Out[354]= 3.61358×10^{-10}

Now we have that the classical region for l=0 is [0,r1] and for l=1 is [r2, r3]. We can now use this information to evaluate the probability that a particular eigenstate |n,l,m⟩ is in the classical region. Then 1-P will give the probability that we can find the particle in the classically forbidden region. I have chosen to do this as I'd imagine integrating outside of those bounds will be more difficult as it will involve ∞. There are 4 possible states for n=2: |2,0,0⟩ which corresponds to l=0 and |2,1,-1⟩, |2,1,0⟩, |2,1,-1⟩ which correspond to l=1.

In[349]:=

$$\psi_{200}[r\_, \theta\_, \phi\_] := \frac{1}{\sqrt{\pi}} * \left(\frac{Z}{2 * a0}\right)^{\frac{3}{2}} * \left(1 - \frac{Z * r}{2 * a0}\right) * \mathrm{Exp}\left[\frac{-Z * r}{2 * a0}\right]$$

$$\psi_{210}[r\_, \theta\_, \phi\_] := \frac{1}{2 * \sqrt{\pi}} * \left(\frac{Z}{2 * a0}\right)^{\frac{3}{2}} * \frac{Z * r}{a0} * \mathrm{Exp}\left[\frac{-Z * r}{2 * a0}\right] * \mathrm{Cos}[\theta]$$

In[367]:=

$$\psi_{211}[r\_, \theta\_, \phi\_] := \frac{-1}{2 * \sqrt{2\pi}} * \left(\frac{Z}{2 * a0}\right)^{\frac{3}{2}} * \frac{Z * r}{a0} * \mathrm{Exp}\left[\frac{-Z * r}{2 * a0}\right] * \mathrm{Sin}[\theta] * \mathrm{Exp}[i * \phi]$$

$$\psi_{21-1}[r\_, \theta\_, \phi\_] := \frac{1}{2 * \sqrt{2\pi}} * \left(\frac{Z}{2 * a0}\right)^{\frac{3}{2}} * \frac{Z * r}{a0} * \mathrm{Exp}\left[\frac{-Z * r}{2 * a0}\right] * \mathrm{Sin}[\theta] * \mathrm{Exp}[-i * \phi]$$

We now find the probabilities for being within the classically allowed region

In[369]:=
```
Integrate[Conjugate[ψ200[r, θ, ϕ]] * ψ200[r, θ, ϕ] * r^2 * Sin[θ],
  {r, 0, r1}, {θ, 0, π}, {ϕ, 0, 2 * π}]
```
Out[369]= 0.815002

In[370]:=
```
Integrate[Conjugate[ψ210[r, θ, ϕ]] * ψ210[r, θ, ϕ] * r^2 * Sin[θ],
  {r, r2, r3}, {θ, 0, π}, {ϕ, 0, 2 * π}]
```
Out[370]= 0.803924

In[372]:=
```
Integrate[Conjugate[ψ21-1[r, θ, ϕ]] * ψ21-1[r, θ, ϕ] * r^2 * Sin[θ],
  {r, r2, r3}, {θ, 0, π}, {ϕ, 0, 2 * π}]
```
Out[372]= 0.803924

In[373]:=
```
Integrate[Conjugate[ψ211[r, θ, ϕ]] * ψ211[r, θ, ϕ] * r^2 * Sin[θ],
  {r, r2, r3}, {θ, 0, π}, {ϕ, 0, 2 * π}]
```
Out[373]= 0.803924

In[374]:=
```
P200 = 1 - 0.815002
P210 = 1 - 0.803924
P21-1 = 1 - 0.803924
P211 = 1 - 0.803924
```
Out[374]= 0.184998

Out[375]= 0.196076

Out[376]= 0.196076

Out[377]= 0.196076

As we can see from above, the probabilities are nearly the same for the *l* = 0 and *l* = 1 states.