

Chapter 9 - Problem 3

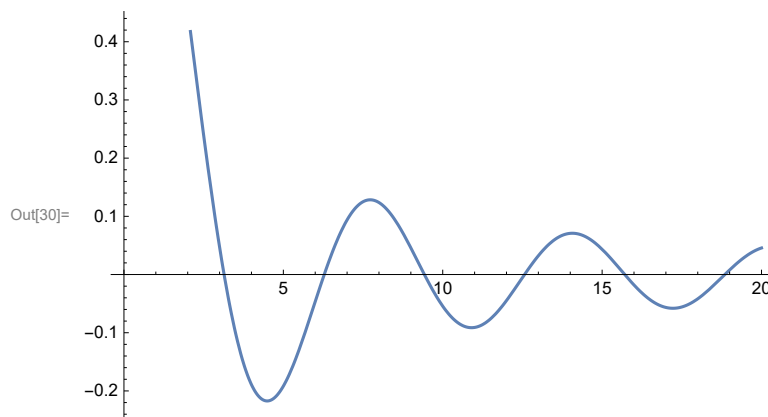


9.3 Find the lowest five eigenvalues corresponding to spherically symmetric states of an electron entrapped in a metalized surface sphere of radius R , where $R = 3$ nm.

For this problem, Spherical coordinates and Spherical Bessel Functions :(. In the Pillbox.pdf, it is covered from page 88 to 91. First let's find the zeros of the spherical bessel function.

Part I. Spherical Bessel Roots

```
In[28]:= ClearAll["Global`*"];
n = 0;
Plot[SphericalBesselJ[n, x], {x, 0, 20}]
x = {3, 6, 9, 12, 15, 19};
besselzeros = roots /. FindRoot[SphericalBesselJ[n, roots], {roots, x}]
```



Out[32]= {3.14159, 6.28319, 9.42478, 12.5664, 15.708, 18.8496}

```
In[ ]:= (* Alternative way of finding the bessel roots*)
(*Clear[besselzeros];
nRoots=5;
nBessel=3;
statenumber = 0;
SphBesselRoot[l_,k_] := N[BesselJZero[l+1/2,k]];
n = Table[SphBesselRoot[l,i],{l,0,nBessel},{i,1,nRoots}];
besselzeros = n[[1]]*)
```

Part II. Solving the god damn problem

Now that we have the roots, we can apply the same method as in Chapter 9 Problem 1.

```

In[33]:= h = 6.62607004 * 10^-34; (* Plankton's Constant *)
mo = 9.10938 * 10^-31; (* Effective mass of an electron *)
ħ =  $\frac{h}{2 * \pi}$ ;
nano = 1 * 10^-9;
e = 1.60217 * 10^-19;
r = 3 * nano; (* Radius of sphere *)
NumberOfEnergies = 5;

En = N[ $\frac{\hbar^2}{2 * mo} * \left( \left( \frac{\text{besselzeros}}{r} \right)^2 \right)$ ]; (* Energy values in Joules*)
EnEv = En / e; (* Energy values in electron volts *)

For[i = 1, i <= NumberOfEnergies, i++,
  Print[i, " lowest Energy Level is : \n\t", EnEv[[i]], " eV \t ", En[[i]], "J"]]
1 lowest Energy Level is :
  0.0417813 eV      6.69408×10^-21J
2 lowest Energy Level is :
  0.167125 eV      2.67763×10^-20J
3 lowest Energy Level is :
  0.376032 eV      6.02467×10^-20J
4 lowest Energy Level is :
  0.668501 eV      1.07105×10^-19J
5 lowest Energy Level is :
  1.04453 eV      1.67352×10^-19J

```

Faster way:

Instead of finding the roots of the Bessel functions, we can actually see that for BesselJo, the zeros are $n\pi$...thus our formula can change and we can create a function to find the energy at ANY state (ground, first excited, second excited, etc...).

```

In[51]:= Clear[n];
n = 1; (* ground state *)

In[57]:= EnJ[n_] = N[ $\frac{\hbar^2}{2 * mo} * \left( \left( \frac{n * \pi}{r} \right)^2 \right)$ ]; (* energy in joules *)
Enev[n_] = N[ $\frac{\hbar^2}{2 * mo * e} * \left( \left( \frac{n * \pi}{r} \right)^2 \right)$ ]; (* energy in electron volts *)

Out[57]= 6.69408 × 10^-21
Out[58]= 0.0417813

```

The above is a demonstration that the formula works, this matches our ground state, so let's write our

for loop again.

```
In[59]:= Clear[n];
For[n = 1, n ≤ NumberOfEnergies, n++,
  Print[n, " lowest Energy Level is : \n\t", Enev[n], " eV \t ", EnJ[n], "J"]]

1 lowest Energy Level is :
  0.0417813 eV      6.69408×10-21J

2 lowest Energy Level is :
  0.0417813 eV      6.69408×10-21J

3 lowest Energy Level is :
  0.0417813 eV      6.69408×10-21J

4 lowest Energy Level is :
  0.0417813 eV      6.69408×10-21J

5 lowest Energy Level is :
  0.0417813 eV      6.69408×10-21J
```

Same answers as above, except this is only one line of code (after writing constants).