Chapter 9 - Problem 4

9.4 Compare the values of the lowest energy bound states of an electron respectively entrapped in a metallized surface sphere and in a metalized surface cube, when the sphere radius and the cube edge are respectively equal.

So the cube is from Quantum mechanics and Degeneracy. So we know that the energy in relation to the radius is given by the following equation:

$$E_{n_x,n_y,n_z} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

https : // chem.libretexts.org/Bookshelves/Physical_and _Theoretical _Chemistry _Textbook _Maps/Supplemental_Modules _ (Physical_and _Theoretical _Chemistry)/Quantum_Mechanics/05.5 %3 A_Particle _in _Boxes/Particle_in _a _ 3 - Dimensional_box

That's the link if you need a quick refresher. The ground state energy would then be given by:

$$E_{1,1,1} = \frac{3h^2}{8mL^2}$$

Note: the numerator is h, not hbar. Where L is the radius. Now the proportion in terms of the radius is:

In[137]:=

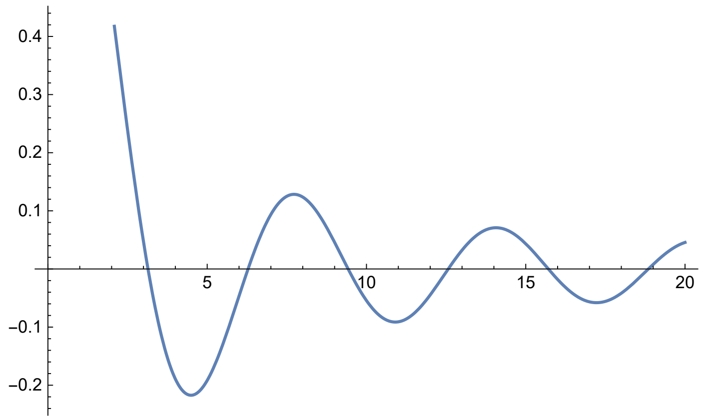
```
ClearAll["Global`*"]
h = 6.62607004 * 10^-34; (* Plankton's Constant *)
m = 9.10938 * 10^-31; (* Resting mass of an electron *)
ℏ = h/(2 * π);
nano = 1 * 10^-9;
e = 1.60217 * 10^-19;
EnCube = (3/8) (h^2/(m * e * r^2))
```

Out[141]= $\frac{1.1281\times10^{-18}}{r^2}$

In[142]:=

```
Plot[SphericalBesselJ[0, x], {x, 0, 20}]
besselzeros = roots /. FindRoot[SphericalBesselJ[0, roots], {roots, 3}]
```

Out[142]=



Out[143]= 3.14159

In[146]:=

$$\texttt{EnSphere} = \frac{h^2}{8 * m * \pi^2 * e} * \left(\left(\frac{\texttt{besselzeros}}{r}\right)^2\right)$$

In[148]:=

$$\frac{3.7603185993153736\grave{}*\hat{}-19}{r^2}$$

Out[148]=

$$\frac{3.76032 \times 10^{-19}}{r^2}$$

The above equation is from Question 9.3. The relationship between the ground state energies in a cube vs a sphere is:

In[147]:=

```
Print["Ground State energies(in terms of r):\n\t Cube:",
 EnCube , " eV \n\t Sphere:", EnSphere, " eV" ]
```

Ground State energies(in terms of r):

Cube: $\frac{1.1281 \times 10^{-18}}{r^2}$ eV

Sphere: $\frac{3.76032 \times 10^{-19}}{r^2}$ eV