Problem 4

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The transverse potential energy profile for a circularly symmetric quantum wire embedded in a cladding is approximated for $r < r_0$ (r_0 is the radius of the wire) by a flat potential V_0, and for $r > r_0$ by a zero potential. Compute the lowest three energy levels of this electron in this wire (in eV), corresponding to a cylindrically symmetric wave-functions, if the radius of the wire is 2nm, $V_0 = -0.5\ eV$, and the effective mass of the electron in the cladding to be the free electron mass, while inside the wire to be 0.5 m_0(Let $k_z = 0$).

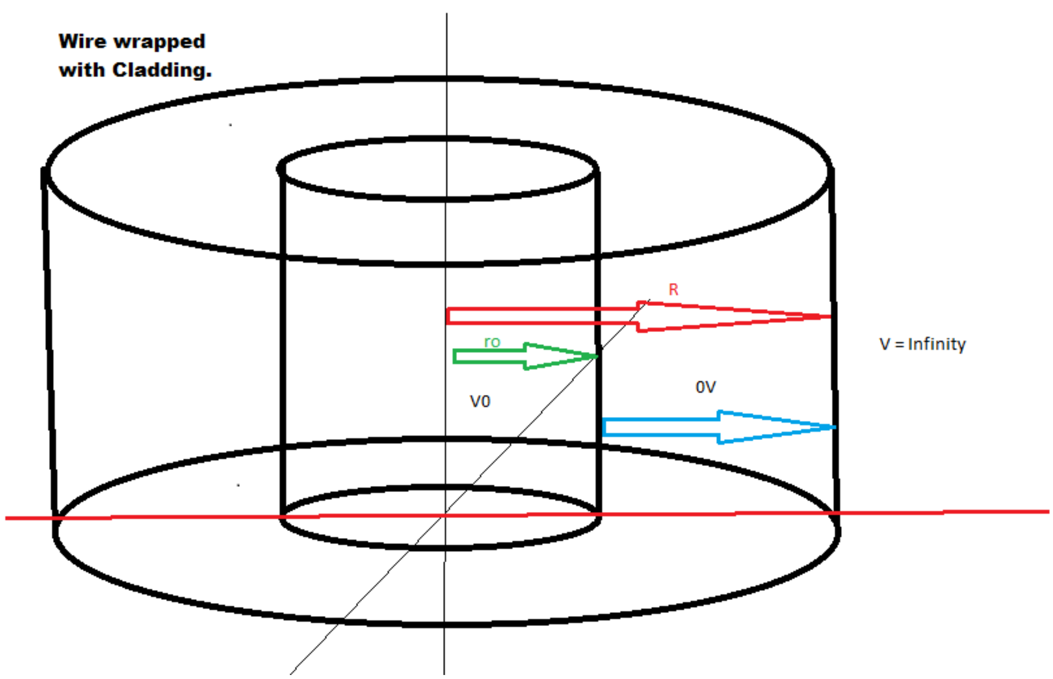
Answers: [4 pts] a) $E_{grd} =$

[4 pts] b) $E_{1-exc.} =$

[4 pts] c) $E_{2-exc.} =$

Mochi and Avocado

Diagram of what’s going on



Please ignore the V = Infinity.

Constants

In[969]:=
```
Clear["Global`*"]
h = 6.62607004 * 10^-34;
mfp = 9.10938 * 10^-31; (* Free particle mass *)
mwire = 0.5 * mfp; (* Mass of the electron inside the wire *)
e = 1.60217 * 10^-19;
ℏ = h / (2 * Pi);
nano = 10^-9;
```

Given Information & Wave numbers

In[976]:=
```
ro = 2 * nano; (* The radius of the wire *)
vwire = -0.5; (* the potential in the wire *)
vc = 0; (* The potential in the cladding *)
kwire = Sqrt[(2 * mwire * e)/ℏ^2 * (en - vwire)];
kclad = Sqrt[(2 * mfp * e)/ℏ^2 * en];
```

The wave equation and boundary conditions

The wave equations in the cladding and wire are given by

$$\phi_{wire}(r) = J_0(k_{wire} r)$$

$$\phi_{cladding}(r) = H_o^{(1)}(k_{cladding} r)$$

Where J_0 is the BesselJ function of the first kind and H_0 is the Hankel Function of the first kind.

As such the boundary conditions are still the same as they have been since Chapter 3.

Boundary conditions:

$$\phi_{wire}(r_0) = \phi_{cladding}(r_0)$$

$$\frac{1}{m_{effective}} \frac{d\phi_{wire(r0)}}{dr} = \frac{1}{m_{free\ electron}} \frac{d\phi_{cladding}(r_0)}{dr}$$

(Ctrl)

To find the energy, we simply have to find the determinant of this, then find the roots of the determinant.

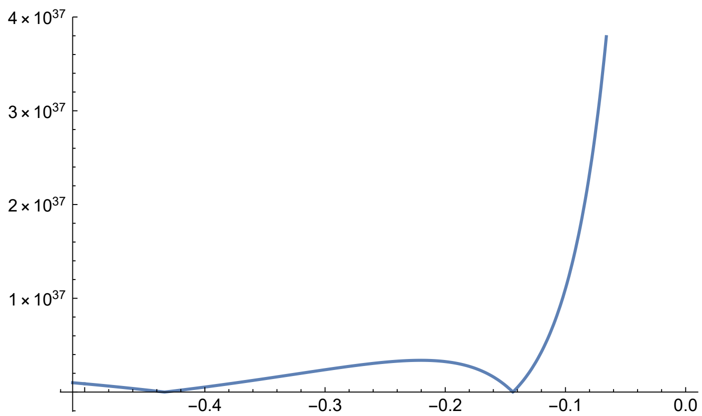
```
In[987]:= ϕwire [r_] = BesselJ[0, kwire * r];
          dϕwire[r_] = 1/mwire * D[ϕwire [r], r];

In[989]:= ϕcladding[r_] = HankelH1[0, kclad * r];
          dϕcladding[r_] = 1/mfp * D[ϕcladding[r], r];

In[991]:= determinant = (ϕwire [ro] * dϕcladding[ro]) - (ϕcladding[ro] * dϕwire[ro]);

In[992]:= Plot[Abs[determinant], { en, -0.51, -0.0001}]
```

Out[992]=




```
In[994]:= groundstate = FindRoot[Abs[determinant] == 0, {en, -0.42}]
```

FindRoot: The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances.

```
Out[994]= {en → -0.433542}

In[995]:= firstexcited = FindRoot[Abs[determinant] == 0, {en, -0.15}]
```

FindRoot: The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances.

```
Out[995]= {en → -0.14372}
```

Final solution

E_{ground} = -0.433542 eV

$E_{1-\text{exc}}$ = -0.14372 eV

$E_{2-\text{exc}}$ = Does not exist.