Problem 5

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Find the ground state energy (in eV) of an electron entrapped in a 1D rectangular well of width = 2nm, and depth =1eV in the presence of an external bias = 0.1 V. The electron effective mass is equal to 0.067 m_0 inside the well, and m_0 outside it.

Answer: [12 pts] E_{grd} =

This problem is very similar to Chapter 8 - Problem 5. However, now we have an effective mass within the biased potential. Beware of this when building your transfer matrix!

Avocado and Mochi

Constants

In[999]:=

```
Clear["Global`*"]
h = 6.62607004 * 10^-34;
mfe = 9.10938 * 10^-31; (* Mass of a free electron*)
e = 1.60217 * 10^-19;
ℏ = h/(2 * Pi);
nano = 10^-9;
voltsPerNano = 1/nano;

α = Sqrt[(2 * mfe * e)/ℏ^2];
Vext = 0.1;
Uext = -0.1;
```

Given information and wave numbers

We will split this problem into three regions:

Region 1 - The region to the left of the well (free space)

Region 2 - The region inside the well with an external bias

Region 3 - The region to the right of the well

```
In[1009]:= mwell = 0.067 * mfe; (* Effective mass of the electron inside the well *)
L = 2 * nano;
F = Vext/L;
k1 = α * Sqrt[en] ;
k3 = α * Sqrt[en - Uext] ;
Vo = -1;
```

```
In[1015]:= zp[z_] = ((2 * mwell)/ℏ^2)^(1/3) * (((Vo - en) * e)/(e * F)^(2/3) - (e * F)^(1/3) * z);
z0 = zp[0];
zL = zp[L];
zprime = D[zp[z], z];
```

From Region 1 to Region 2

From free space to biased potential

Wave equation in free space is $e^{ikz} + e^{-ikz}$

Wave equation in the biased potential is Ai(zp(z)) + Bi(zp(z))

The second equation was given in Professor Manassah's Notes.

The boundary conditions states that at z = 0, the wave equations and their derivatives must be equal.

To build the following matrices, we just evaluate these wave equations and their derivatives at 0.

```
In[1019]:= region1 = {{1, 1}, 1/mfe * {I * k1, -I * k1}};
region20 = {{AiryAi[z0], AiryBi[z0]},
    1/mwell * {zprime * AiryAiPrime[z0], zprime * AiryBiPrime[z0]}};
transfer12 = Inverse[region1].region20;
```

From Region 2 to Region 3

Now the boundary conditions state that at L, the wave equations must be equal again.

The wave equation in Region 3 is almost the same as the one in Region 1, however we have to use a different wave number.

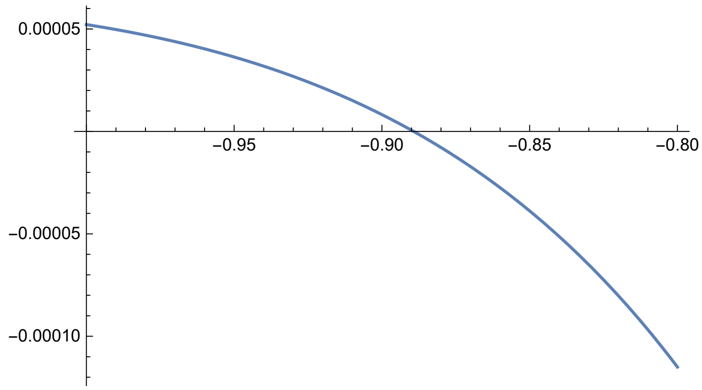
```
In[1022]:= region2L = {{AiryAi[zL], AiryBi[zL]},
    1/mwell * {zprime * AiryAiPrime[zL], zprime * AiryBiPrime[zL]}};
region3 = {{Exp[I * k3 * L], Exp[-I * k3 * L]},
    1/mfe * {I * k3 * Exp[I * k3 * L], -I * k3 * Exp[-I * k3 * L]}};
transfer23 = Inverse[region2L].region3 ;
```

The Full transfer matrix of the electron

In[1025]:=
```
fullTransferMatrix = transfer12.transfer23;
```

In[1029]:=
```
Plot[fullTransferMatrix[[1, 1]], {en, -1, -0.8}]
```

Out[1029]=



In[1030]:=
```
FindRoot[fullTransferMatrix[[1, 1]] == 0, {en, -0.89}]
```

Out[1030]=
```
{en → -0.889253 + 0. i}
```