ELEC 4700 - Assignment 1

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Due: Feburary 4th 2018

Question 1

A) Velocity

Calculation of Velocity

$$v_i = \sqrt{\frac{KT}{m_n}}$$

$$v_{th} = \sqrt{v_x^2 + v_y^2} = \sqrt{\frac{2KT}{m_n}}$$

where m_n is the effective mass of electrons $m_n = 0.26m_o$ T is the temperature in Kelvin (300K), and K is the Boltzmann Constant

```
T = 300;
Kbolt = 1.38064852E-23;
mo = 9.11e-31;
mn = mo * 0.26;
vx = (Kbolt*T/mn)^.5;
vy = (Kbolt*T/mn)^.5;
vth = (vx^2 + vy^2)^.5;
```

v_{th} is then equal to 187 000 m/s

B) Mean Free Path

The mean free path can be determined from the velocity multiplied by the time between collisions

$$l = v_{th}\tau_{mn}$$

where l is the mean free path, τ_{mn} is the time between collisions and v_{th} is the velocity.

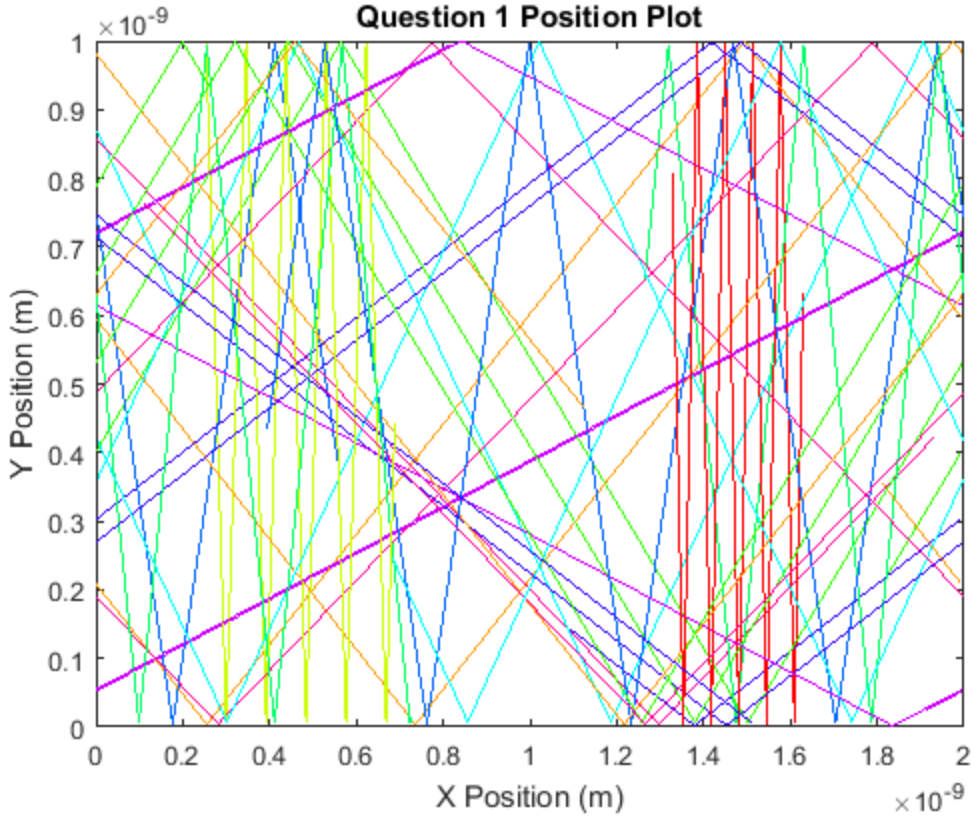
```
tmn = 0.2e-12; % in seconds
MeanFreePath = tmn*vth; % in meters
```

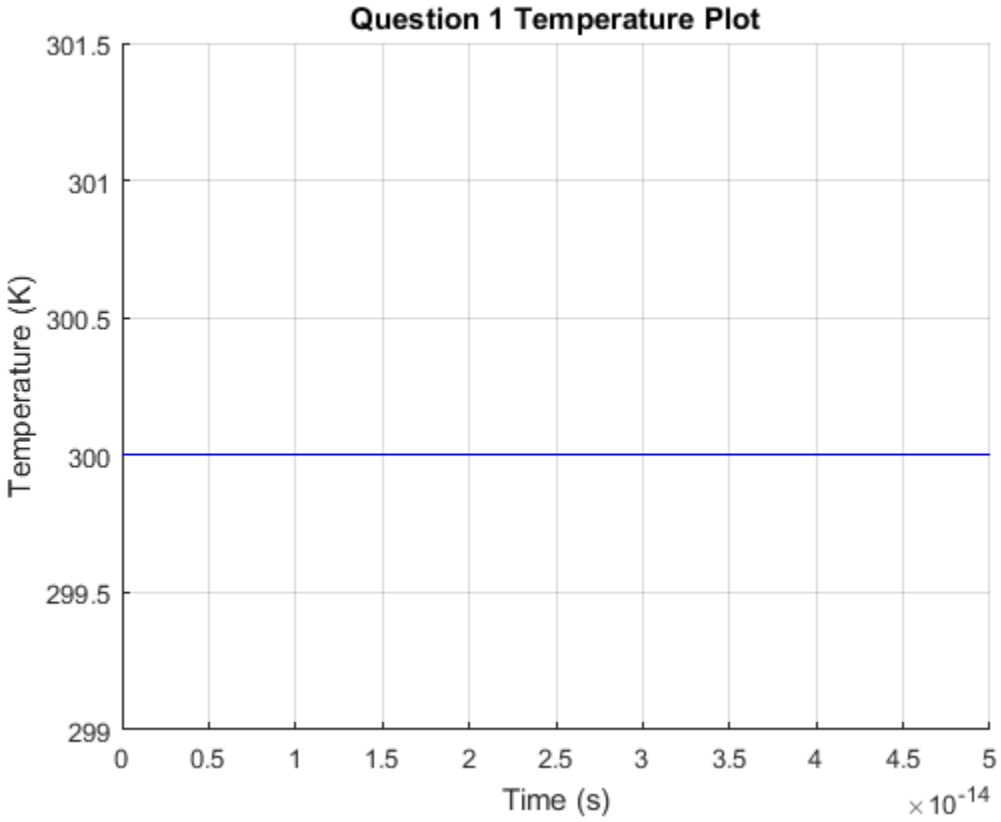
The Mean Free Path (l) is then calculated to be 37.4 nm.

C) Program

```
%Boundary Conditions
xlimits = [0, 2e-9];
ylimits = [0, 1e-9];
PlotHowMany = 10;
Timestep = 5e-17;
endtime = Timestep*1000;
NumParticles = 1000;

%%SETUP INITIAL PARAMETERS
mycolors = hsv(PlotHowMany);
xprev = zeros(1, NumParticles);
yprev = zeros(1, NumParticles);
x = zeros(3,NumParticles);
y = zeros(2,NumParticles);
temp = zeros(2, NumParticles);

%Start the random distribution in x position
x(1,:) =  rand(1,NumParticles);
y(1,:) =  rand(1,NumParticles);
x(1,:) =  xlimits(1) + x(1,:).*(xlimits(2) - xlimits(1));
y(1,:) =  ylimits(1) + y(1,:).*(ylimits(2) - ylimits(1));

%Assign the velocity in x and y direction
x(3,:) = rand(1, NumParticles)*2*pi;
x(2,:) = vth.*cos(x(3,:));
y(2,:) = vth.*sin(x(3,:));

%%Create the Time loop
figure(1);
xlim([xlimits(1), xlimits(2)]);
ylim([ylimits(1), ylimits(2)]);
Temperature = zeros(floor(endtime/Timestep)+ 1,1);
for i = 0:Timestep:endtime
    xprev(1,:) = x(1,:);
    yprev(1,:) = y(1,:);

    %Loop Through Each Particle
    for kt = 1:NumParticles
```

```
        %Check for the Limits
       if x(1,kt) +  x(2,kt)*Timestep < xlimits(1)
          x(1,kt) = xlimits(2);
          xprev(1,kt) = xlimits(2);
       elseif x(1,kt) +  x(2,kt)*Timestep > xlimits(2)
           x(1,kt) = xlimits(1);
           xprev(1,kt) = xlimits(1);
       end
       if y(1,kt) +  y(2,kt)*Timestep < ylimits(1) || y(1,kt) +
 y(2,kt)*Timestep > ylimits(2)
           y(2,kt) = -y(2,kt);
       end
       %Update Positions
        x(1,kt) = x(1,kt) + x(2,kt).*Timestep;
        y(1,kt) = y(1,kt) + y(2,kt).*Timestep;
   %Plot the new positions
   if kt <= PlotHowMany
         plot([xprev(1,kt), x(1,kt)], [yprev(1,kt), y(1,kt)],'color',
 mycolors(kt,:) );
         hold on;
   end

   end
   VelSquared = mean((x(2,:).^2 + y(2,:).^2));
   CalcTemp = VelSquared*mn/2/Kbolt;
   title(['Average Temperature: ' num2str(CalcTemp)]);
   Temperature(round(i/Timestep) + 1,1) = CalcTemp;
end

figure(1);
title('Question 1 Position Plot');
xlabel('X Position (m)');
ylabel('Y Position (m)');
hold off;
figure(3);
hold on;
title('Question 1 Temperature Plot');
plot(0:Timestep:endtime, Temperature(:, 1), 'b');
xlabel('Time (s)');
ylabel('Temperature (K)');
grid on;
hold off;
```


Question 1 Position Plot
×10^-9
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Y Position (m)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
X Position (m)
×10^-9


Question 1 Temperature Plot
301.5
301
300.5
300
299.5
299
Temperature (K)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
Time (s)
×10^-14

We can see that the temperature remains constant for the electrons as it should and that the movement of the electrons is elastic collisions on the y and flows freely on the x-axis.

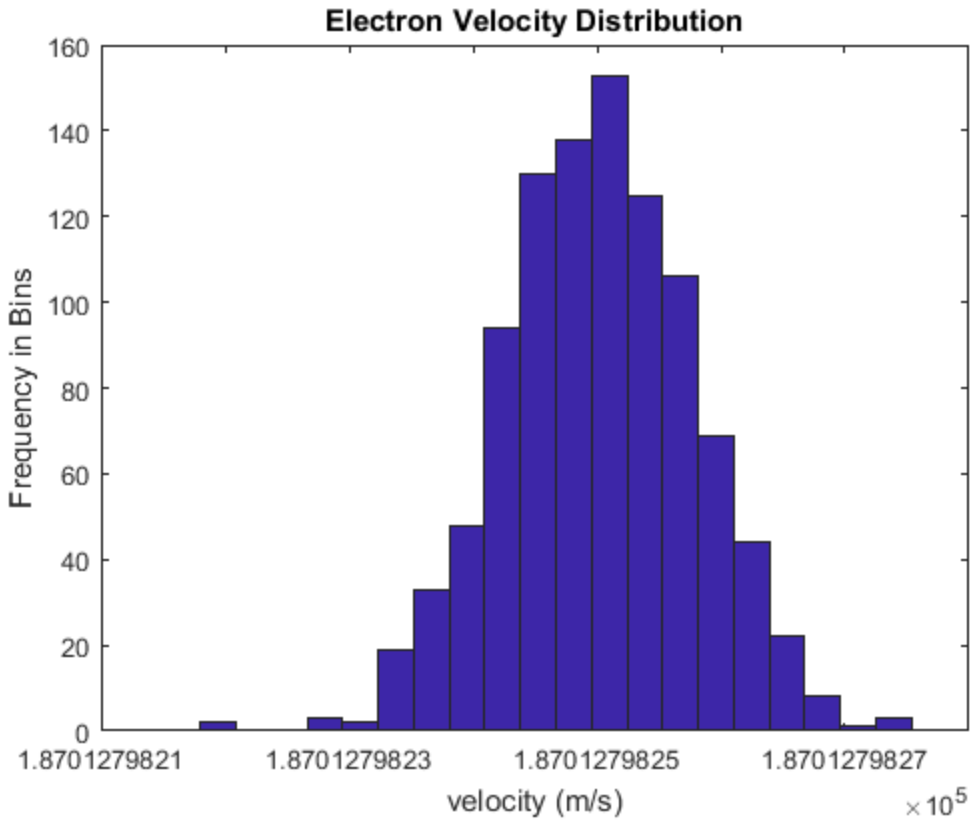
Question 2

```
%Initlialize some parameters
xprev = zeros(1, NumParticles);
yprev = zeros(1, NumParticles);
x = zeros(3,NumParticles);
y = zeros(2,NumParticles);
temp = zeros(2, NumParticles);
scatTime = zeros(1,NumParticles);
endtime = Timestep*50000;
graphfor = Timestep*1000;

%Start the random distribution in x position
x(1,:) =  rand(1,NumParticles);
y(1,:) =  rand(1,NumParticles);
x(1,:) =  xlimits(1) + x(1,:).*(xlimits(2) - xlimits(1));
y(1,:) =  ylimits(1) + y(1,:).*(ylimits(2) - ylimits(1));
```

A) Maxwell Boltzmann Distributed Velocity

The Maxwell Boltzmann Distribution can be taken as a Gaussian Distribution with a standard deviation of $\sqrt{\frac{m_n}{KT}}$

```
%Assign the random velocity and random angle
temp(1,:) = (normrnd(vx, sqrt(mn/(Kbolt*T)), 1, NumParticles).^2 +
 normrnd(vx, sqrt(mn/(Kbolt*T)), 1, NumParticles).^2).^.5;
x(3,:) = rand(1, NumParticles)*2*pi;
x(2,:) = temp(1,:).*cos(x(3,:));
y(2,:) = temp(1,:).*sin(x(3,:));
figure(2);
hist(sqrt(x(2,:).^2 + y(2,:).^2),20);
title('Electron Velocity Distribution');
xlabel('velocity (m/s)');
ylabel('Frequency in Bins');
```



B) Probability of Scattering

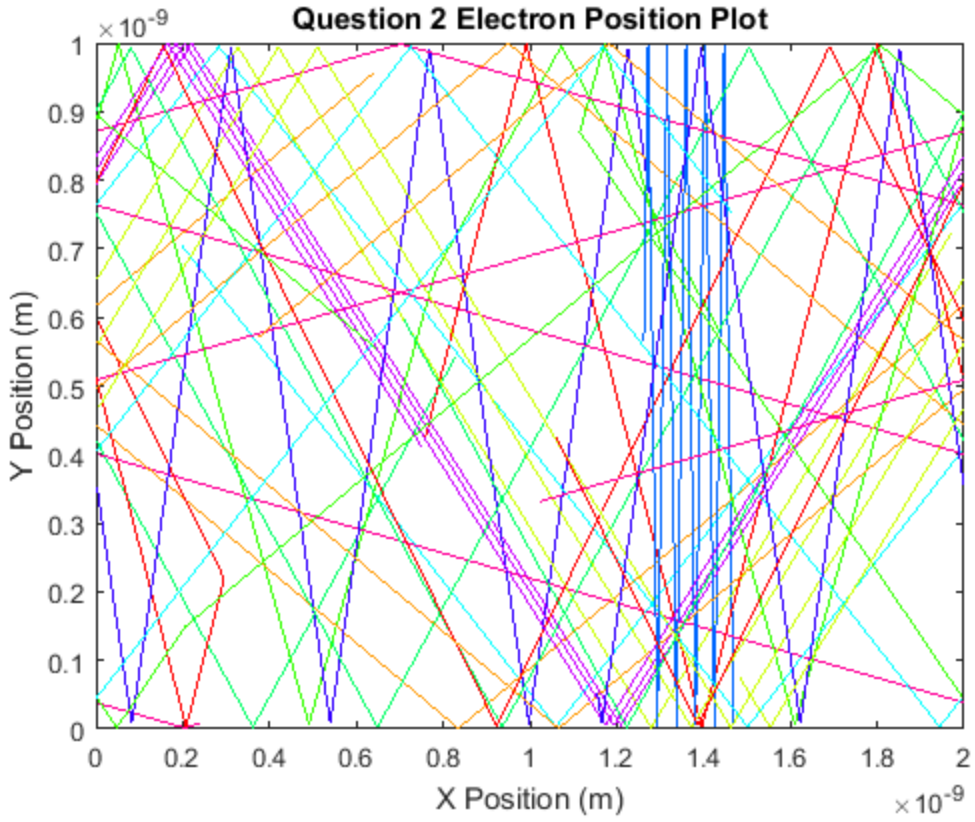
The probability of having a scattering event is $1 - e^{-\frac{dt}{\tau_{mn}}}$

```
Pscat = 1-exp(-Timestep/tmn);
```

In this specfic case with a time step of $9x10^{-17}s$ and a mean time between collisions τ_{mn} of 0.2ps the Probabiliyt of Scattering is $4.4990x10^{-4}$

```
figure(4);
%Update the Position
ScatterTime = zeros(floor(endtime/Timestep)+ 1,1);
Temperature = zeros(floor(endtime/Timestep)+ 1,1);
MFP = zeros(floor(endtime/Timestep)+ 1,1);
for i = 0:Timestep:endtime
   % pause(.1);
    xprev(1,:) = x(1,:);
    yprev(1,:) = y(1,:);
    for kt = 1:NumParticles
       if x(1,kt) +  x(2,kt)*Timestep < xlimits(1)
           x(1,kt) = xlimits(2);
           xprev(1,kt) = xlimits(2);
       elseif x(1,kt) +  x(2,kt)*Timestep > xlimits(2)
           x(1,kt) = xlimits(1);
           xprev(1,kt) = xlimits(1);
```

```
        end
        if y(1,kt) +  y(2,kt)*Timestep < ylimits(1) || y(1,kt) +
 y(2,kt)*Timestep > ylimits(2)
            y(2,kt) = -y(2,kt);
        end
    x(1,kt) = x(1,kt) + x(2,kt).*Timestep;
    y(1,kt) = y(1,kt) + y(2,kt).*Timestep;
    if kt <= PlotHowMany && i < graphfor
        plot([xprev(1,kt), x(1,kt)], [yprev(1,kt), y(1,kt)],'color',
 mycolors(kt,:) );
        hold on;
    end
    %Scattering Check
    if Pscat>rand()
        temp = (normrnd(vx, sqrt(mn/(2*pi*Kbolt*T)))^2 + normrnd(vy,
 sqrt(mn/(2*pi*Kbolt*T)))^2)^.5;
        x(3,kt) = rand*2*pi;
        x(2,kt) = temp*cos(x(3,kt));
        y(2,kt) = temp*sin(x(3,kt));
        scatTime(1,kt) = 0;
    end
    end
    hold on;
    AvgScat = mean(scatTime(1,:));
    scatTime(1,:) = scatTime(1,:) + Timestep;
    VelSquared = mean((x(2,:).^2 + y(2,:).^2));
    CalcTemp = VelSquared*mn/2/Kbolt;
    %title(['Average Temperature: ' num2str(CalcTemp) ' Average
 Scatter Time: ' num2str(AvgScat)]);
    xlim([xlimits(1), xlimits(2)]);
    ylim([ylimits(1), ylimits(2)]);
    ScatterTime(round(i/Timestep) + 1,1) = AvgScat;
    MFP(round(i/Timestep) + 1,1) = VelSquared^.5*AvgScat;
    figure(4);
    Temperature(round(i/Timestep) + 1,1) = CalcTemp;
end
title('Question 2 Electron Position Plot');
xlabel('X Position (m)');
ylabel('Y Position (m)');
hold off;
```

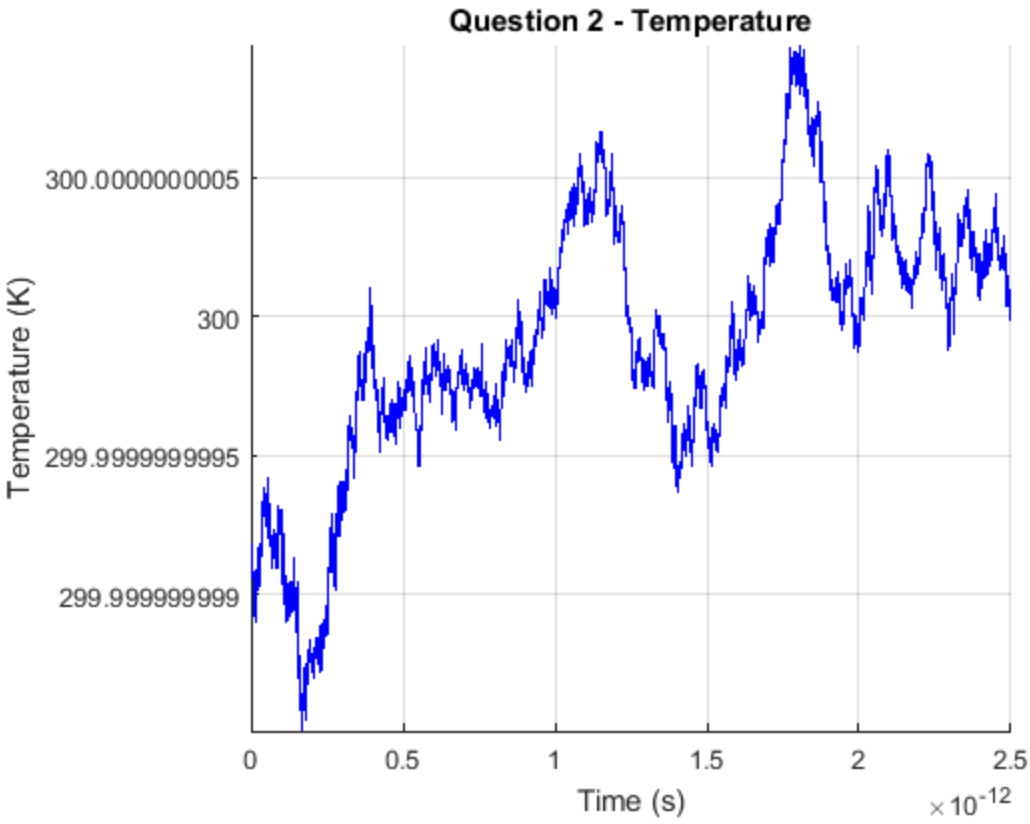


We can see the scattering occuring with the Electron Position Graph above.

C) Average Temperature Over Time

The graph shows now fluctuation in the temperature which is expected due to the scattering.

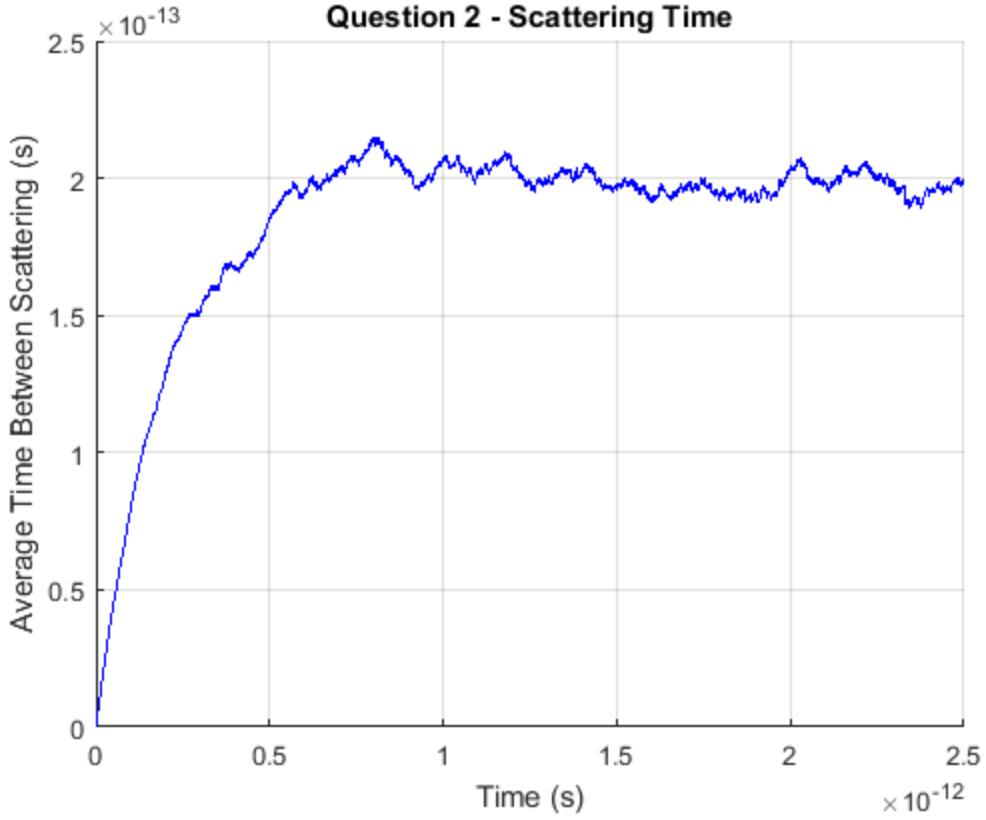
```
figure(5);
hold on;
plot(0:Timestep:endtime, Temperature(:, 1), 'b');
title('Question 2 - Temperature');
xlabel('Time (s)');
ylabel('Temperature (K)');
grid on;
hold off;
```

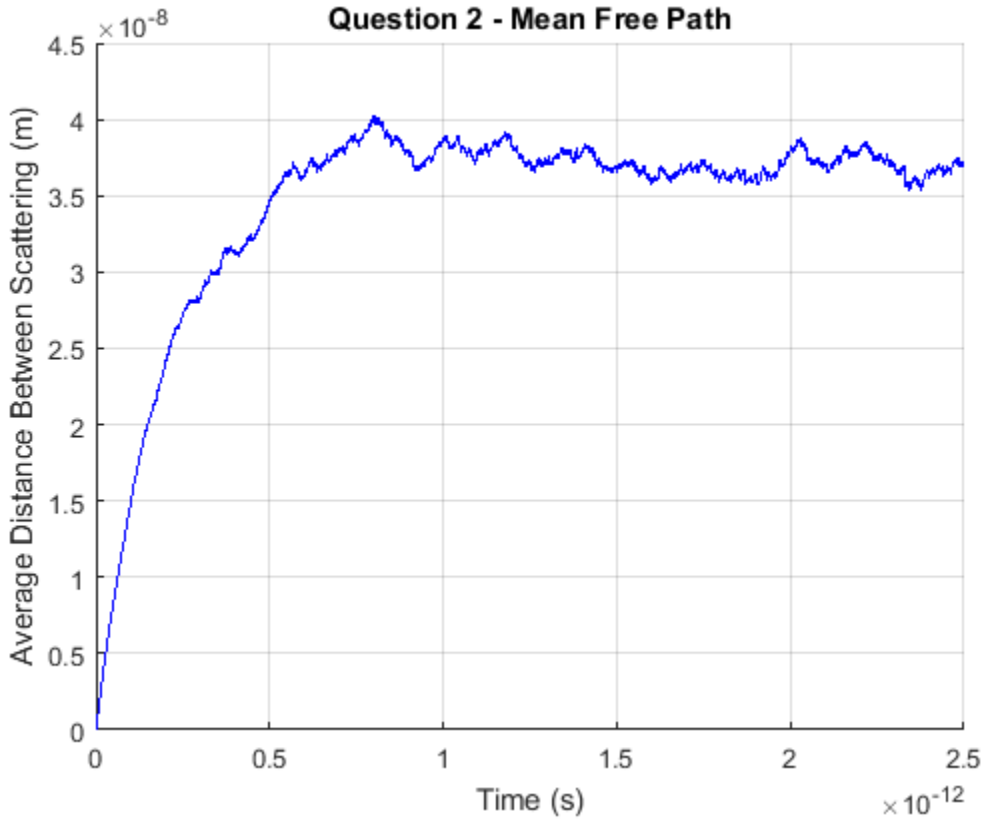


The temperature has some uncertainty but remains on average around 300K based upon the Gaussian Distribution in which we continue to reassign values from this distribution.

D) Mean Free Path and Mean Time Between Collisions

```
figure(6);
hold on;
plot(0:Timestep:endtime, ScatterTime(:, 1), 'b');
title('Question 2 - Scattering Time');
xlabel('Time (s)');
ylabel('Average Time Between Scattering (s)');
grid on;
hold off;

figure(7);
hold on;
plot(0:Timestep:endtime, MFP(:, 1), 'b');
title('Question 2 - Mean Free Path');
xlabel('Time (s)');
ylabel('Average Distance Between Scattering (m)');
grid on;
hold off;
```


Question 2 - Scattering Time
×10^-13
2.5
2
1.5
1
0.5
0
Average Time Between Scattering (s)
0
0.5
1
1.5
2
2.5
Time (s)
×10^-12


Question 2 - Mean Free Path
×10^-8
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
Average Distance Between Scattering (m)
0
0.5
1
1.5
2
2.5
Time (s)
×10^-12

The graph shows the mean free path stabilizing around 36 to 38 nm and with a calculated mean free path of 37.4 nm the simulation and calculated agree. The scattering time approaches 0.2 ps and stabilizies around the given time between collisions of 0.2 ps. Both these plots become asymptotic at the given and calculated values for mean free path and time between collisions.

Question 3

A) Adding A Bottle Neck

The Graph Below shows the Electron Position with time and the rectangular bottle neck that occurs with it.

```
%Assign the Box Height and Width as Percentages of the Limits
xboxLim = [.4*(xlimits(2)-xlimits(1)), .6*(xlimits(2)-xlimits(1))];
yboxLim1 = [ylimits(1), .4*(ylimits(2)-ylimits(1))];
yboxLim2 = [.6*(ylimits(2)-ylimits(1)), ylimits(2)];
xbox = xboxLim([1 1 2 2 1]);
ybox1 = yboxLim1([1 2 2 1 1]);
ybox2 = yboxLim2([1 2 2 1 1]);
endtime = Timestep*2000;
xprev = zeros(1, NumParticles);
yprev = zeros(1, NumParticles);
x = zeros(3,NumParticles);
y = zeros(2,NumParticles);
temp = zeros(2, NumParticles);
scatTime = zeros(1,NumParticles);

%Start the random distribution in x position
x(1,:) =  rand(1,NumParticles);
y(1,:) =  rand(1,NumParticles);
x(1,:) =  xlimits(1) + x(1,:).*(xlimits(2) - xlimits(1));
y(1,:) =  ylimits(1) + y(1,:).*(ylimits(2) - ylimits(1));

%Get the Particle Indexes that are out of bounds
IDX = uint32(1:NumParticles);
ind = IDX((y(1,:) >= yboxLim2(1) | y(1,:) <= yboxLim1(2))& x(1,:) >=
 xboxLim(1) & x(1,:) <= xboxLim(2));

%Reassign Positions
counter = 1;
%size(ind, 2)
while counter <= size(ind,2)
    x(1,ind(counter)) = xlimits(1) + rand*(xlimits(2) - xlimits(1));
    y(1,ind(counter)) = ylimits(1) + rand*(ylimits(2) - ylimits(1));
    if ~((y(1,ind(counter)) >= yboxLim2(1) || y(1,ind(counter)) <=
 yboxLim1(2))&& x(1,ind(counter)) >= xboxLim(1) && x(1,ind(counter))
 <= xboxLim(2))
        counter = counter + 1;
    end
end

%Assign the random velocity and random angle
temp(1,:) = (normrnd(vx, sqrt(mn/(Kbolt*T)), 1, NumParticles).^2 +
 normrnd(vx, sqrt(mn/(Kbolt*T)), 1, NumParticles).^2).^.5;
```

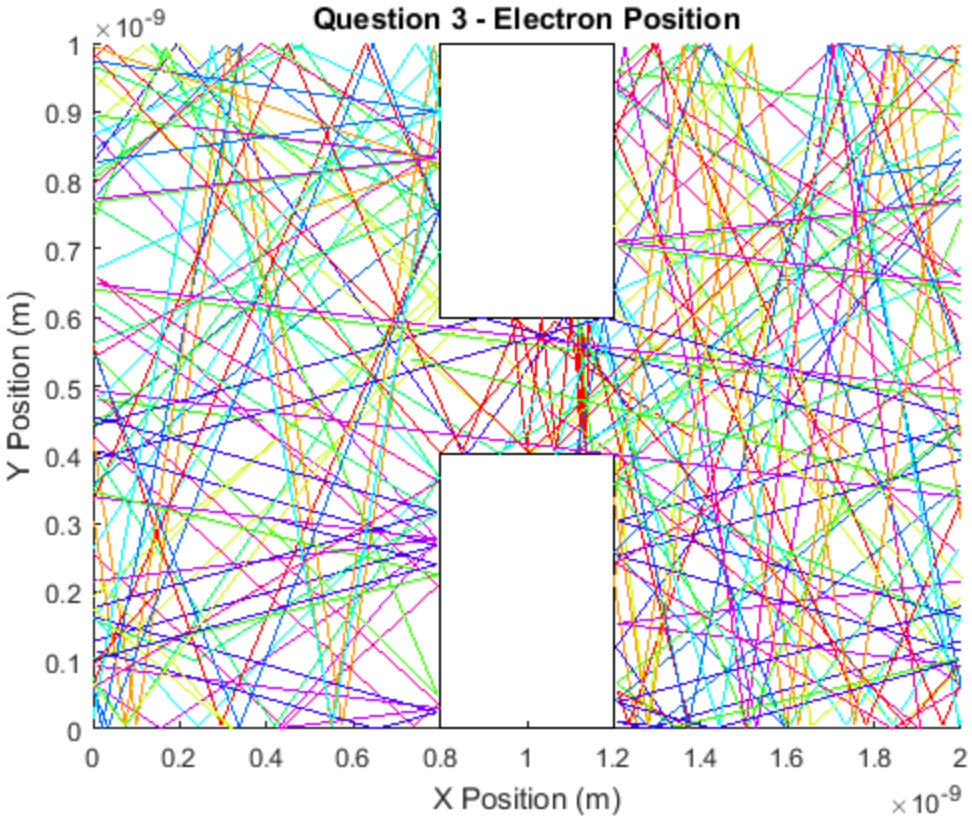
```
x(3,:) = rand(1, NumParticles)*2*pi;
x(2,:) = temp(1,:).*cos(x(3,:));
y(2,:) = temp(1,:).*sin(x(3,:));
```

B) Boundaries Specular or Diffusive

```
DiffusionBarrierProbability = 0.2;

figure(9);
title('Question 3 - Electron Position');
xlabel('X Position (m)');
ylabel('Y Position (m)');
xlim([xlimits(1), xlimits(2)]);
ylim([ylimits(1), ylimits(2)]);
hold on;
rectangle('Position', [xboxLim(1), yboxLim1(1), xboxLim(2)-xboxLim(1),
 yboxLim1(2)]);
rectangle('Position', [xboxLim(1), yboxLim2(1), xboxLim(2)-xboxLim(1),
 yboxLim2(2) - yboxLim2(1)]);

counter = 1;
for i = 0:Timestep:endtime
   % pause(.1);
    xprev(1,:) = x(1,:);
    yprev(1,:) = y(1,:);
    for kt = 1:NumParticles

       %PARTICLE'S HITTING TOP and
        if x(1,kt) +  x(2,kt)*Timestep < xlimits(1)
           x(1,kt) = xlimits(2);
           xprev(1,kt) = xlimits(2);
       elseif x(1,kt) +  x(2,kt)*Timestep > xlimits(2)
           x(1,kt) = xlimits(1);
           xprev(1,kt) = xlimits(1);
       end
       if y(1,kt) +  y(2,kt)*Timestep < ylimits(1) || y(1,kt) +
 y(2,kt)*Timestep > ylimits(2)
           if rand > DiffusionBarrierProbability
           y(2,kt) = -y(2,kt);
           else
               if y(1,kt) +  y(2,kt)*Timestep < ylimits(1)
                   x(3,kt) = rand*pi;
               elseif y(1,kt) +  y(2,kt)*Timestep > ylimits(2)
                   x(3,kt) = -rand*pi;
                end
        temp = (normrnd(vx, sqrt(mn/(2*pi*Kbolt*T)))^2 + normrnd(vy,
 sqrt(mn/(2*pi*Kbolt*T)))^2)^.5;
       x(2,kt) = temp*cos(x(3,kt));
       y(2,kt) = temp*sin(x(3,kt));
           end
       end

       %PARTICLE'S HITTING BOX
```

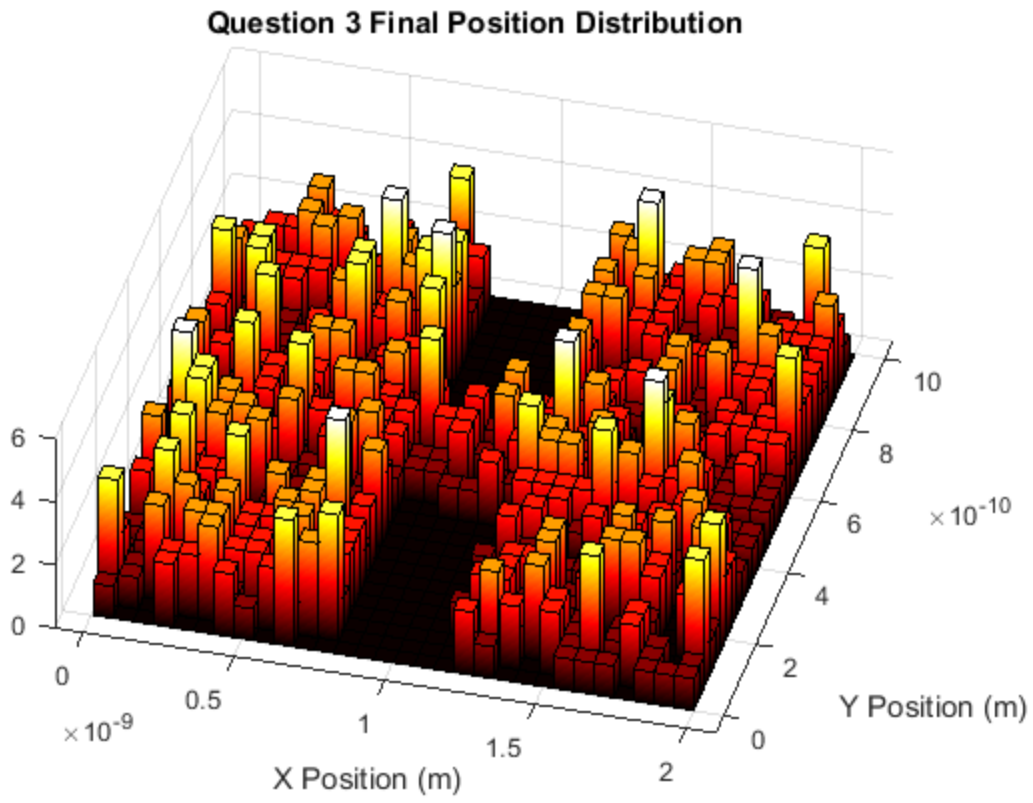
```
        if (y(1,kt) +  y(2,kt)*Timestep >= yboxLim2(1) && x(1,kt)
+  x(2,kt)*Timestep >= xboxLim(1) && x(1,kt) +  x(2,kt)*Timestep <=
xboxLim(2))
          [xinter1, xinter2, yinter1, yinter2]  =
BoxIntercept( x(1,kt), y(1,kt), x(1,kt) +  x(2,kt)*Timestep, y(1,kt)
+  y(2,kt)*Timestep, xboxLim(1), xboxLim(2),yboxLim2(1), ylimits(2));
          if rand > DiffusionBarrierProbability
           if xinter2 || xinter1
                x(2,kt) = - x(2,kt);
            end
            if yinter2 || yinter1
                y(2,kt) = - y(2,kt);
            end
          else
              if xinter1
                  x(3,kt) = pi/2 + rand*pi;
              elseif xinter2
                  x(3,kt) = pi/2 - rand*pi;
              elseif yinter2
                  x(3,kt) = rand*pi;
              elseif yinter1
                  x(3,kt) = -rand*pi;
              end
                     temp = (normrnd(vx, sqrt(mn/(2*pi*Kbolt*T)))^2 +
normrnd(vy, sqrt(mn/(2*pi*Kbolt*T)))^2)^.5;
       x(2,kt) = temp*cos(x(3,kt));
       y(2,kt) = temp*sin(x(3,kt));
          end
         elseif y(1,kt) +  y(2,kt)*Timestep <= yboxLim1(2) && x(1,kt)
+  x(2,kt)*Timestep >= xboxLim(1) && x(1,kt) +  x(2,kt)*Timestep <=
xboxLim(2)
          [xinter1, xinter2, yinter1, yinter2]  =
BoxIntercept( x(1,kt), y(1,kt), x(1,kt) +  x(2,kt)*Timestep,
y(1,kt) +  y(2,kt)*Timestep, xboxLim(1), xboxLim(2), ylimits(1),
yboxLim1(2));
          if rand > DiffusionBarrierProbability
          if xinter1 || xinter2
               x(2,kt) = - x(2,kt);
           end
           if yinter1 || yinter2
               y(2,kt) = - y(2,kt);
           end
          else
              if xinter1
                  x(3,kt) = pi/2 + rand*pi;
              elseif xinter2
                  x(3,kt) = pi/2 - rand*pi;
              elseif yinter2
                  x(3,kt) = rand*pi;
              elseif yinter1
                  x(3,kt) = -rand*pi;
              end
       temp = (normrnd(vx, sqrt(mn/(2*pi*Kbolt*T)))^2 + normrnd(vy,
sqrt(mn/(2*pi*Kbolt*T)))^2)^.5;
```

```
            x(2,kt) = temp*cos(x(3,kt));
            y(2,kt) = temp*sin(x(3,kt));
               end
             end

        %UPDATE POSITION
        x(1,kt) = x(1,kt) + x(2,kt).*Timestep;
        y(1,kt) = y(1,kt) + y(2,kt).*Timestep;
        %PLOT
        if kt <= PlotHowMany
            plot([xprev(1,kt), x(1,kt)], [yprev(1,kt), y(1,kt)],'color',
 mycolors(kt,:) );
            hold on;
        end
        %Scattering Check
        if Pscat>rand()
            x(3,kt) = rand*2*pi;
            temp = (normrnd(vx, sqrt(mn/(2*pi*Kbolt*T)))^2 + normrnd(vy,
 sqrt(mn/(2*pi*Kbolt*T)))^2)^.5;
            x(2,kt) = temp*cos(x(3,kt));
            y(2,kt) = temp*sin(x(3,kt));
            scatTime(1,kt) = 0;
        end
        end
        hold on;
        AvgScat = mean(scatTime(1,:));
        scatTime(1,:) = scatTime(1,:) + Timestep;
        averagevel = mean((x(2,:).^2 + y(2,:).^2).^.5);
        %title(['Average Temperature: ' num2str(averagevel) ' Average
 Scatter Time: ' num2str(AvgScat)]);
        figure(9);
    end
```



C) Electron Density Map

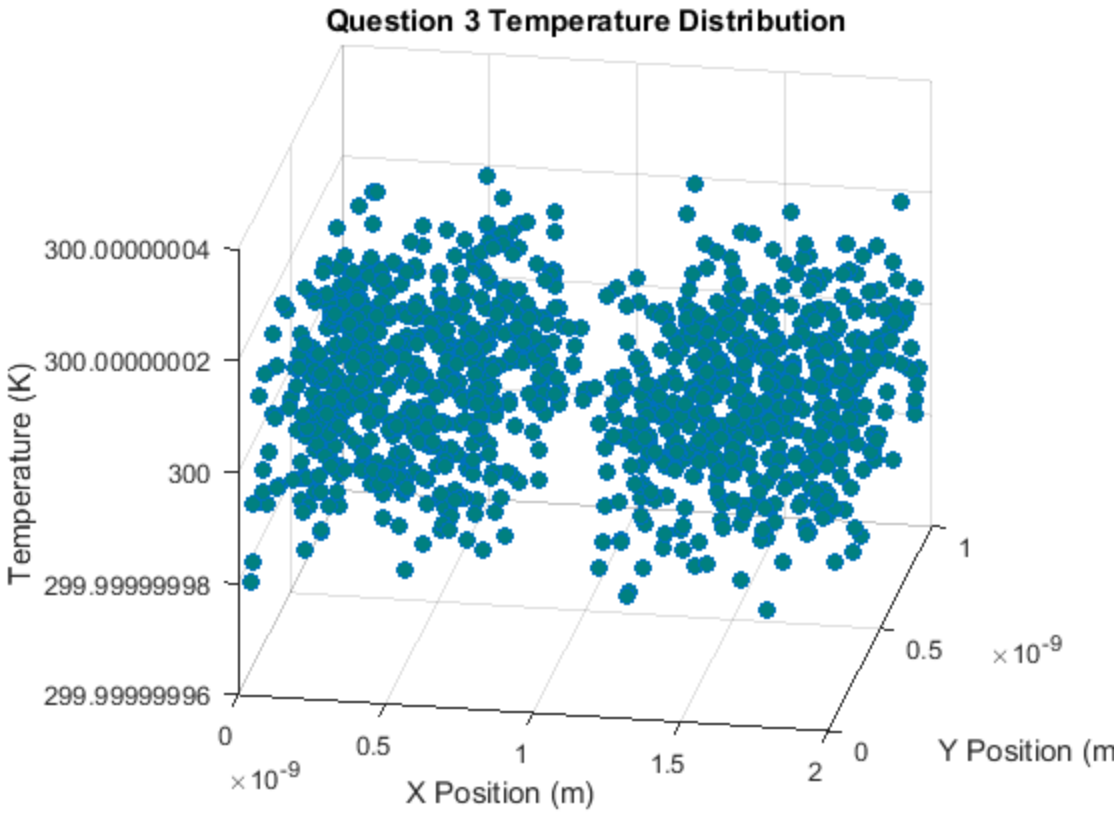
```
figure(10);

Z = [transpose(x(1,:)), transpose(y(1,:))];
hist3(Z, [30,30]);
hold on;
set(get(gca,'child'),'FaceColor','interp','CDataMode','auto');
colormap(hot);
view(15, 65);% heat map
grid on;
title('Question 3 Final Position Distribution');
xlabel('X Position (m)');
ylabel('Y Position (m)');
hold off;
```



From the figure above we can see that no electrons are present in the rectangular boxes.

D) Temperature Map

```
figure(11);
VelSquared = (x(2,:).^2 + y(2,:).^2);
CalcTemp = VelSquared.*mn./2./Kbolt;
h = scatter3(x(1,:), y(1,:), CalcTemp(1,:));
h.MarkerFaceColor = [0 0.5 0.5];
grid on;
xlabel('X Position (m)');
ylabel('Y Position (m)');
xlim([xlimits(1), xlimits(2)]);
ylim([ylimits(1), ylimits(2)]);
zlabel('Temperature (K)');
title('Question 3 Temperature Distribution');
view(10,25);
hold off;
```



Again from the figure above we can see that no electrons are present in the rectangular boxes.

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