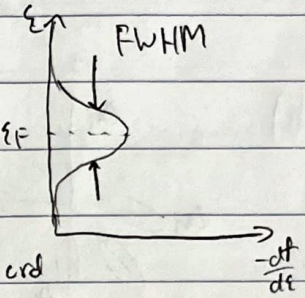
HW 3

1) a) FWHM ~ $7k_BT$

I'm going to call $\frac{\varepsilon-\varepsilon_F}{kT} = x$ to simplify solutions

$f = \frac{1}{e^x+1}$, $\frac{df}{d\varepsilon} = \frac{d}{d\varepsilon}(e^x+1)^{-1} \rightarrow -1(e^x+1)^{-2}\cdot(\varepsilon-\varepsilon_F)\times e^x$

$\frac{df}{d\varepsilon} = \frac{-e^x}{k_BT(e^x+1)^2} \rightarrow -\frac{df}{d\varepsilon} = \frac{e^x}{k_BT(e^x+1)^2}$



this plot from class shows $\max\left(\frac{-df}{d\varepsilon}\right)$ is at $\varepsilon = \varepsilon_F$. Then, we can find $\frac{1}{2}\max\left(\frac{-df}{d\varepsilon}\right)$, and get the ε values, and find the difference, $\Delta\varepsilon_{1/2\,max}$

$\frac{df}{d\varepsilon}(\varepsilon_F) = \frac{e^0}{k_BT(e^0+1)^2} = \frac{1}{4k_BT} \rightarrow \frac{1}{2}\max = \frac{1}{8k_BT}$

$\frac{1}{8k_BT} = \frac{e^x}{k_BT(e^x+1)^2} \rightarrow \frac{1}{8} = \frac{e^x}{(e^x+1)^2}$, $(e^x+1)^2 = 8e^x$

$(e^x)^2 + 2e^x + 1 = 8e^x \rightarrow (e^x)^2 - 6e^x + 1 = 0$ Quadratic

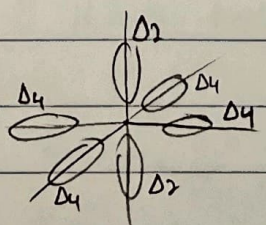
$\frac{6 \pm \sqrt{(6)^2 - 4(1)(1)}}{2} = \frac{3 \pm \sqrt{32}}{2} = 3 \pm 2\sqrt{2} = e^x$

$\ln(e^x) = \ln(3 \pm 2\sqrt{2}) \rightarrow x = 1.7627$ AND -1.7627, $\Delta x = 2(1.7627) = 3.525$

remember $x = \frac{\varepsilon-\varepsilon_F}{k_BT}$, $\Delta\frac{\varepsilon-\varepsilon_F}{k_BT} = 3.5 \rightarrow$ $\boxed{\varepsilon_c - \varepsilon_F = 3.5\,k_BT}$

b) The inequality must now focus on the valence band compared to the fermi-level. Since the fermi-level has higher energy than the valence band, we now have $\boxed{\varepsilon_F - \varepsilon_v > 3.5k_BT}$

2) a)

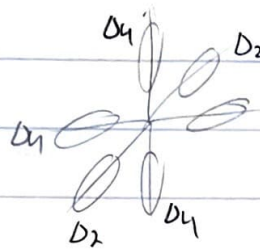


3)a) No confinement in x. So confinement in y, z.

$$E = E_c + \frac{\hbar^2}{2}\frac{q_x^2}{m_x} + \frac{\hbar^2}{2m_y}\left(\frac{n_y}{L_y}\right)^2 + \frac{\hbar^2}{2m_z}\left(\frac{n_z}{L_z}\right)^2$$

(confinement)

b)



y and z both have confinement, should have same degeneracy, Δ_4

x is the lone Δ_2

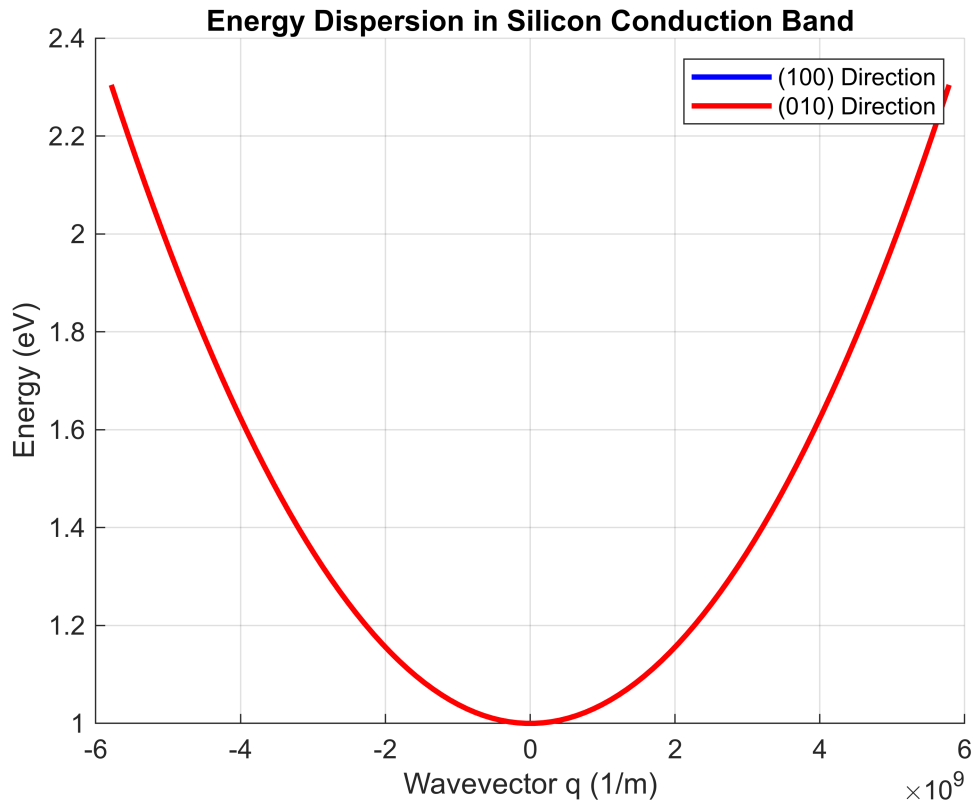
5) $n = \int g_{2D}(\varepsilon) f_0 \, d\varepsilon = g_{2D,well}(\varepsilon) \int \frac{1}{1+e^{(\varepsilon-\varepsilon_F)/kT}} d\varepsilon \rightarrow \ln\left(1+e^{(\varepsilon_F-\varepsilon)/kT}\right)$

$$n = \frac{m_{DOS}}{\pi\hbar^2} kT \ln\left(1+e^{(\varepsilon_F-\varepsilon)/kT}\right)$$

Problem 2

b)

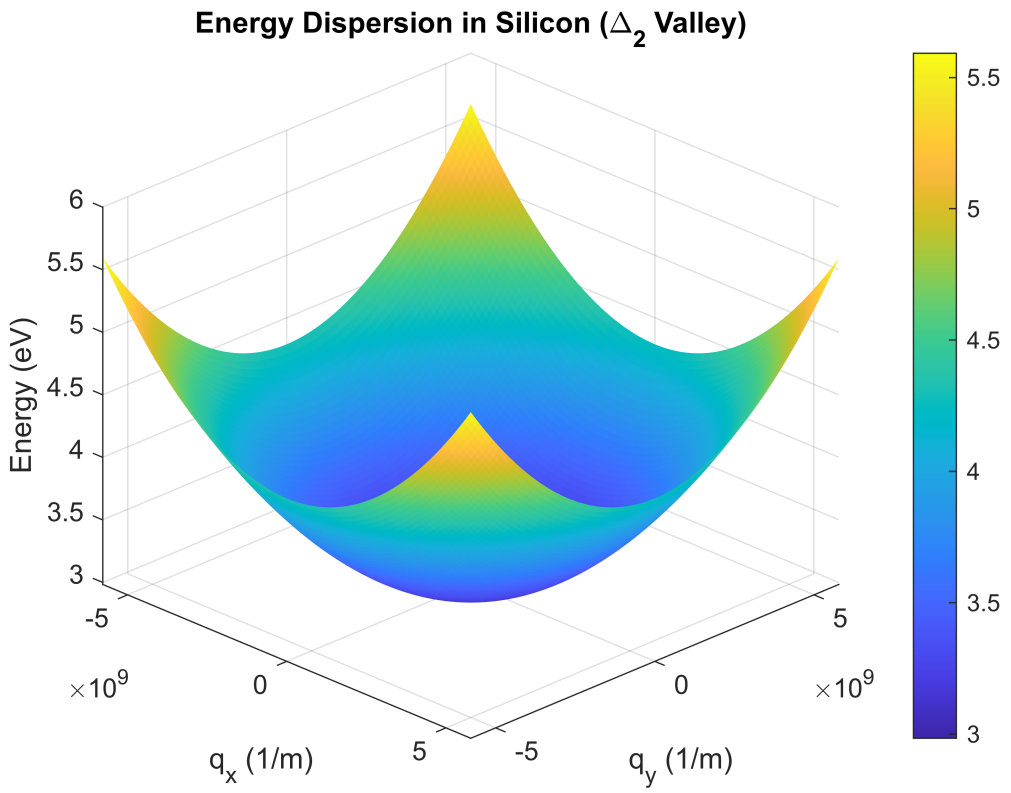
```
clc
clear
close all

a = 5.43e-10;           % Angstrom
L = 1e-9;               % 1 nm
e = 1.6e-19;            % C
n = 1;
e_c = e;                % 1 eV, for simplicity
h_bar = (6.626e-34) / (2 * pi);
m_o = 9.1e-31;          % mass of electron
m_l = 0.98 * m_o;
m_t = 0.19 * m_o;
m_z = m_l;              % z-direction effective mass
m_y = m_l;              % y-direction effective mass
m_x = m_l;              % x-direction effective mass

qx = linspace(-pi/a, pi/a, 100);  % x-space
qy = linspace(-pi/a, pi/a, 100);  % y-space

e_x = e_c + (h_bar^2 / 2) * (qx.^2 / m_x); % from (000) to (100)
e_y = e_c + (h_bar^2 / 2) * (qy.^2 / m_y); % from (000) to (010)

figure;
hold on;
plot(qx, e_x / e, 'b', 'LineWidth', 2);  % Energy along (100)
plot(qy, e_y / e, 'r', 'LineWidth', 2);  % Energy along (010)
xlabel('Wavevector q (1/m)');
ylabel('Energy (eV)');
title('Energy Dispersion in Silicon Conduction Band');
legend('(100) Direction', '(010) Direction');
grid on;
hold off;
```



These curves overlap each other, meaning they have the same energy

c) twofold degenerate (along z-direction)

```
m_z = m_t;              % z-direction effective mass
m_y = m_l;              % y-direction effective mass
m_x = m_l;              % x-direction effective mass

[QX, QY] = meshgrid(qx, qy);

e_twofold = e_c + (h_bar^2 / 2) * ((QX.^2 / m_x) + (QY.^2 / m_y)) + (h_bar^2 / (2 *
m_z)) * (n * pi / L)^2;
figure;
surf(QX, QY, e_twofold / e, 'EdgeColor', 'none');  % Smooth surface plot
xlabel('q_x (1/m)');
ylabel('q_y (1/m)');
zlabel('Energy (eV)');
title('Energy Dispersion in Silicon (\Delta_2 Valley)');
colorbar;
view(45, 30);  % Adjust view angle
grid on;
```



Since this is bounded in the z-direction, is is a 2D density of states (DOS), while the z-axis mass is m_l

$$m^*_{DOS} = \sqrt{m_1 m_2} = \sqrt{m_x m_y} = \sqrt{m_t m_t} = m_t$$

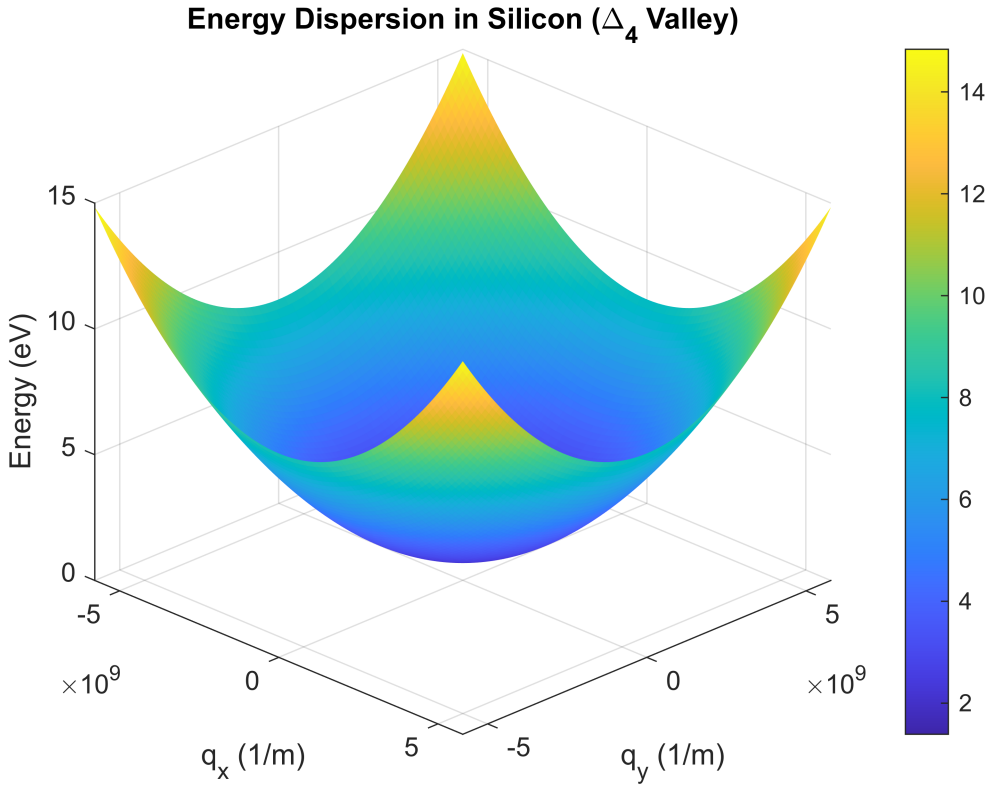
$$g_{2D} = \frac{m^*}{\pi \hbar^2} = \frac{m_t}{\pi \hbar^2}$$

```
g_2D_D2 = m_t / (pi * h_bar^2);
g_2D_D2 = g_2D_D2/ e;
```

d) fourfold degenerate (along x and y-direction)

```
m_z = m_l;              % z-direction effective mass
m_y = m_t;              % y-direction effective mass
m_x = m_t;              % x-direction effective mass
e_fourfold = e_c + (h_bar^2 / 2) * ((QX.^2 / m_x) + (QY.^2 / m_y)) + (h_bar^2 / (2
* m_z)) * (n * pi / L)^2;
figure;
surf(QX, QY, e_fourfold / e, 'EdgeColor', 'none');  % Smooth surface plot
xlabel('q_x (1/m)');
ylabel('q_y (1/m)');
zlabel('Energy (eV)');
title('Energy Dispersion in Silicon (\Delta_4 Valley)');
colorbar;
view(45, 30);  % Adjust view angle
```

```
grid on;
```



$$m^*_{DOS} = \sqrt{m_1 m_2} = \sqrt{m_x m_y} = \sqrt{m_t m_l}$$

for either x or y direction, that axes will be m_t, while the other will be m_l, so they will both have the same m^*_{DOS}

$$g_{2D} = \frac{m^*}{\pi \hbar^2} = \frac{\sqrt{m_l m_t}}{\pi \hbar^2}$$

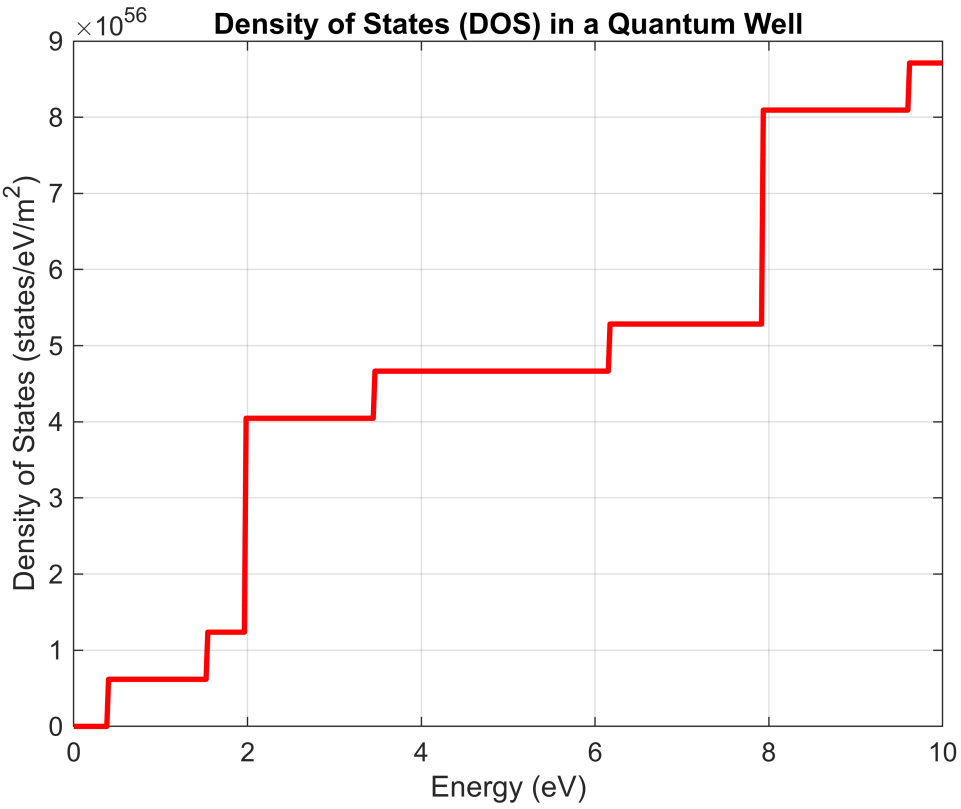
```
g_2D_D4 = sqrt(m_l * m_t) / (pi * h_bar^2);
g_2D_D4 = g_2D_D4 / e;
```

e)

For each subgroup, n, there should be two steps. One for the twofold degeneracy and one for the fourfold.

```
E_n_D2 = zeros(1, 5);
E_n_D4 = zeros(1, 5);

for n = 1:5         % calculating for the first 5 subbands
    E_n_D2(n) = (h_bar^2 / (2 * m_l)) * (n * pi / L)^2;
    E_n_D4(n) = (h_bar^2 / (2 * m_t)) * (n * pi / L)^2;
end

E = linspace(0, 10, 500) * e;  % Energy range from 0 to 0.5 eV
g_DOS_2D = zeros(size(E));
```

```
for n = 1:5
    for i = 1:length(E)
        if E(i) >= E_n_D2(n)
            g_DOS_2D(i) = g_DOS_2D(i) + 2 * g_2D_D2; % Add DOS for 2-fold valley
        end
        if E(i) >= E_n_D4(n)
            g_DOS_2D(i) = g_DOS_2D(i) + 4 * g_2D_D4; % Add DOS for 4-fold valley
        end
    end
end

% Plot the quasi-2D density of states
figure;
plot(E / e, g_DOS_2D, 'r', 'LineWidth', 2);
xlabel('Energy (eV)');
ylabel('Density of States (states/eV/m^2)');
title('Density of States (DOS) in a Quantum Well');
grid on;
```

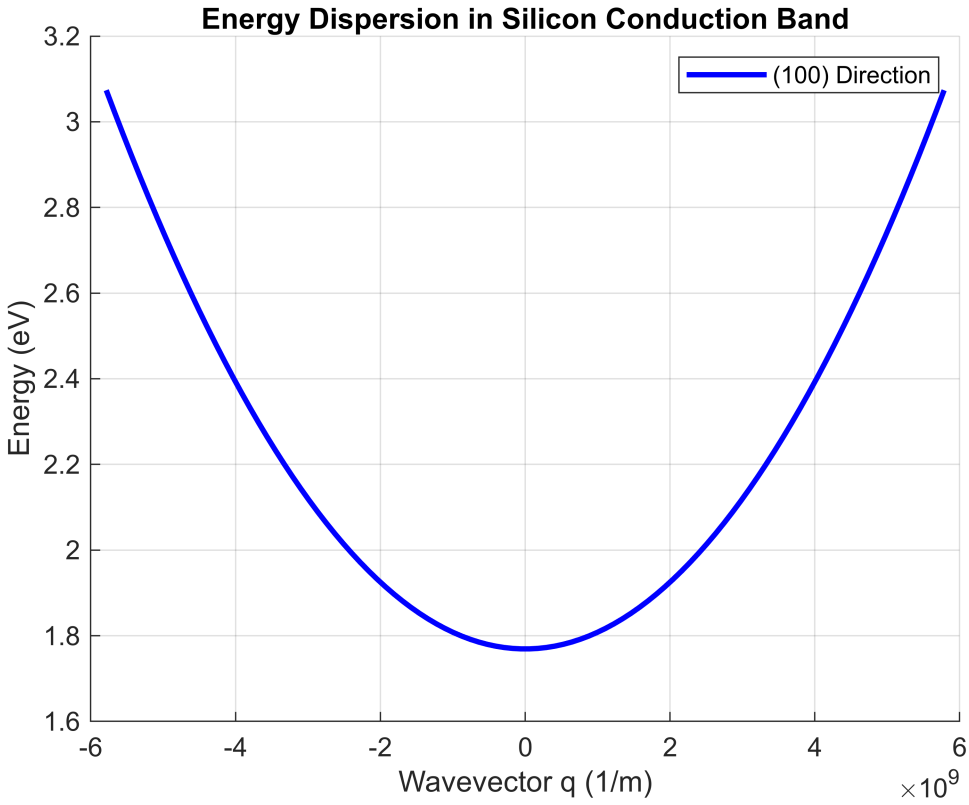


Problem 3

We are confined in both the y and z-direction, therefore, we can only calculate the energy dispersion relationship over momentum in the k-direction.

c)

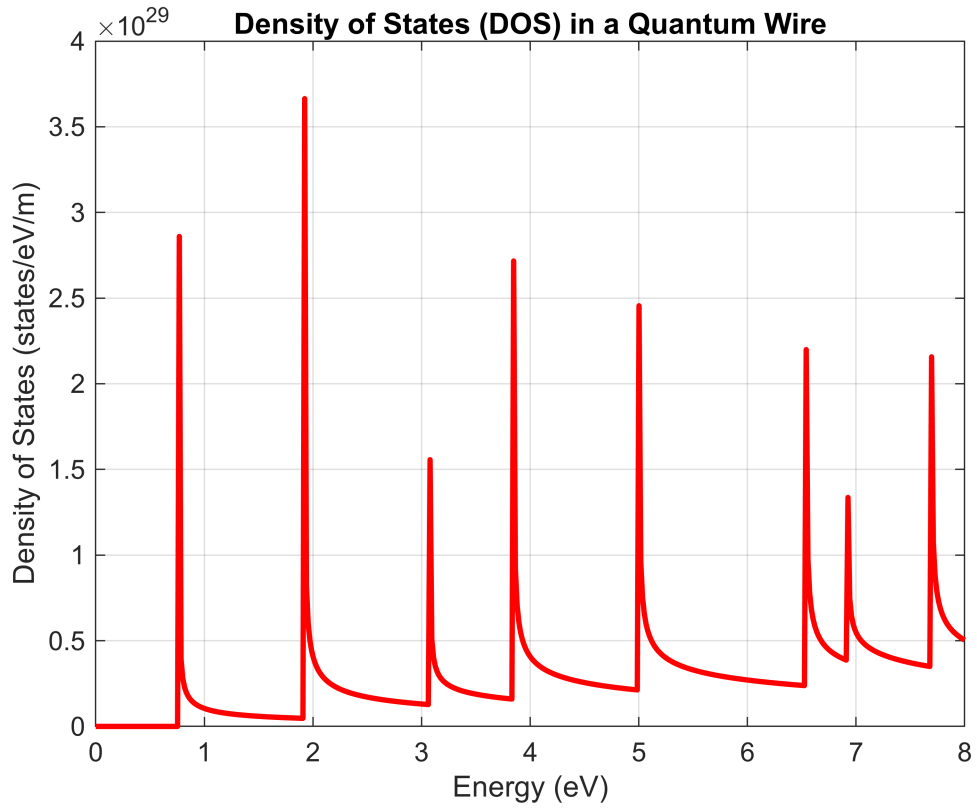
```
a = 5.43e-10;           % Angstrom
L_z = 1e-9;             % 1 nm
L_y = L_z;
e = 1.6e-19;            % C
n = 1;
e_c = e;                % 1 eV, for simplicity
h_bar = (6.626e-34) / (2 * pi);
m_o = 9.1e-31;          % mass of electron
m_l = 0.98 * m_o;
m_t = 0.19 * m_o;
m_z = m_l;              % z-direction effective mass
m_y = m_l;              % y-direction effective mass
m_x = m_l;              % x-direction effective mass
n_y = 1;
n_z = 1;

qx = linspace(-pi/a, pi/a, 100);  % x-space

e_x = e_c + (h_bar^2 / 2) * (qx.^2 / m_x) + (h_bar^2 / (2 * m_y)) * (n_y * pi /
L_y)^2 + ...
    (h_bar^2 / (2 * m_z)) * (n_z * pi / L_z)^2;

figure;
hold on;
plot(qx, e_x / e, 'b', 'LineWidth', 2);  % Energy along (100)
xlabel('Wavevector q (1/m)');
ylabel('Energy (eV)');
title('Energy Dispersion in Silicon Conduction Band');
legend('(100) Direction');
grid on;
hold off;
```



d)

```
E = linspace(0, 8, 500) * e;  % Energy range from 0 to 0.5 eV
En = zeros(5, 5);

for n_y = 1:5
    for n_z = 1:5
        En(n_y, n_z) = (h_bar^2 / (2 * m_y)) * (n_y * pi / L_y)^2 + ...
                       (h_bar^2 / (2 * m_z)) * (n_z * pi / L_z)^2;
    end
end

g_DOS = zeros(size(E));

for n_y = 1:5
    for n_z = 1:5
        E_nyz = En(n_y, n_z);
        for i = 1:length(E)
            if E(i) >= E_nyz
                g_DOS(i) = g_DOS(i) + (1 / (pi * h_bar)) * sqrt(m_x / (2 * (E(i) -
E_nyz)));
            end
        end
    end
end
```

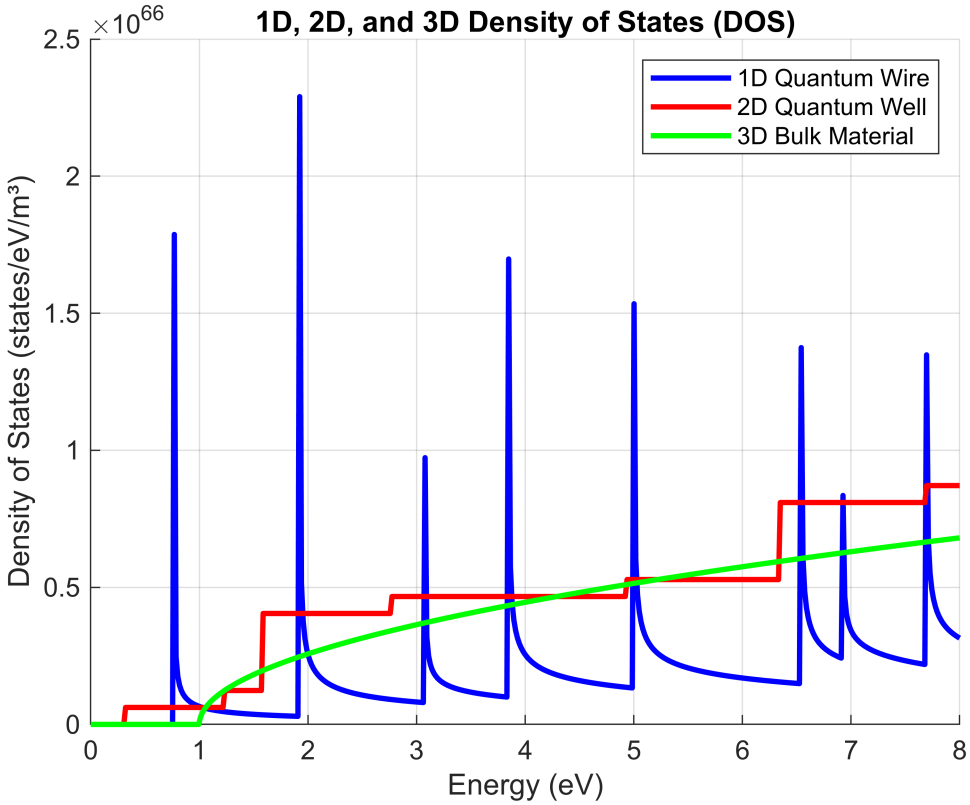
```
g_DOS_1D = g_DOS / e;

% Plot the 1D density of states
figure;
plot(E / e, g_DOS, 'r', 'LineWidth', 2);
xlabel('Energy (eV)');
ylabel('Density of States (states/eV/m)');
title('Density of States (DOS) in a Quantum Wire');
grid on;
```



Problem 4

```
g_DOS_2D = g_DOS_2D / L_z;
g_DOS_1D = g_DOS_1D / L_z^2;

g_DOS_3D = zeros(size(E));
m_DOS = (m_l^3)^(1/3);          % not needed but still did it to show
                                % how the effective mass is obtained

for i = 1:length(E)
    if E(i) > e_c
        g_DOS_3D(i) = (1 / (2 * pi^2)) * ((2 * m_DOS / h_bar^2)^(3/2)) * sqrt(E(i)
- e_c);
    end
end
```

```
g_DOS_3D = g_DOS_3D / e;

figure;
hold on;
plot(E / e, g_DOS_1D, 'b', 'LineWidth', 2); % 1D DOS (Quantum Wire)
plot(E / e, g_DOS_2D, 'r', 'LineWidth', 2); % 2D DOS (Quantum Well)
plot(E / e, g_DOS_3D, 'g', 'LineWidth', 2); % 3D DOS (Bulk Material)
xlabel('Energy (eV)');
ylabel('Density of States (states/eV/m³)');
title('1D, 2D, and 3D Density of States (DOS)');
legend('1D Quantum Wire', '2D Quantum Well', '3D Bulk Material');
grid on;
hold off;
```

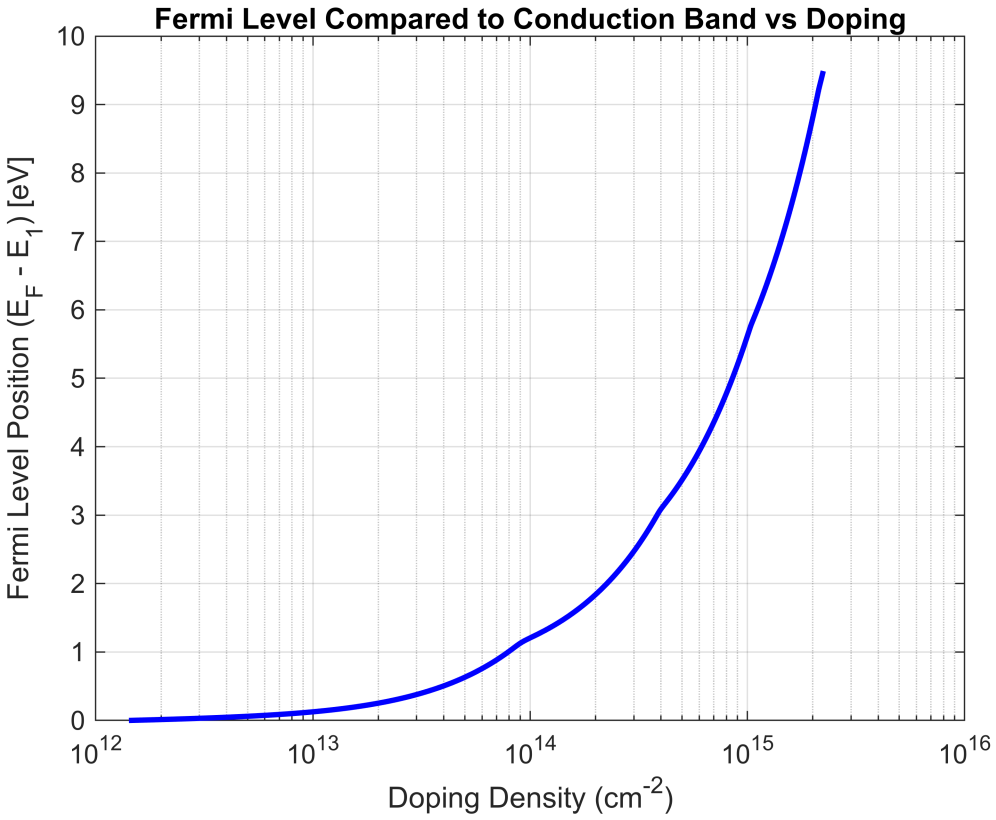


```
clc
close all
clear

L = 1e-9;                 % 1 nm
e = 1.6e-19;              % C
kT = 0.0259 * e;          % J
h_bar = (6.626e-34) / (2 * pi);
m_o = 9.1e-31;            % kg
m_t = 0.19 * m_o;         % in-plane effective mass
m_z = 0.98 * m_o;         % confinement direction

% 2D DOS per subband
g_2D = m_t / (pi * h_bar^2);

% Calculating for 5 subbband energies
En = zeros(1, 5);
for n = 1:5
    En(n) = (h_bar^2 * (n * pi / L)^2) / (2 * m_z);
end
E1 = En(1);
```

Since there are discrete subbands we must acount for them when calculating the Fermi-level energy. I originally tried using fsolve() for this, but I struggled and had problems obtaining a graph that looked like this.

```
% Sweep a range of Ef values (J)
Ef_range = linspace(E1, En(end) + 10*kT, 1000);
n_vals = zeros(size(Ef_range));

% Loop over Ef and compute total density
for i = 1:length(Ef_range)
    Ef = Ef_range(i);
    n_total = 0;
    for n = 1:5
        n_total = n_total + g_2D * kT * log(1 + exp((Ef - En(n)) / kT));
    end
    n_vals(i) = n_total;
end

n = n_vals / 1e4;

% Convert Ef to eV relative to the bulk conduction band
Ef_rel = (Ef_range - E1) / e;

% Plot
figure;
semilogx(n, Ef_rel, 'b', 'LineWidth', 2);
xlabel('Doping Density (cm^{-2})');
ylabel('Fermi Level Position (E_F - E_1) [eV]');
title('Fermi Level Compared to Conduction Band vs Doping');
```

```
grid on;
```



Now you can see that this follows the exponential what we might expect. It will gradually take us greater and greater doping to increase the fermi-level. The subbands of the well introduce steps within the plot that make it different than a typical 3D, unbounded, plot.

I'm having difficulty plotting any values for doping as high as 10^16 and above with the logarithms. This property of the graph still stays the same, with the steps being introduced from the subbands.