HW 1

1) a) $\langle x|\hat{x}|x'\rangle = x\,\delta(x-x')$

$\langle k|\hat{x}|k'\rangle = i\hbar\,\partial/\partial p\,\delta(p-p')$

This is from Fourier transform of $p = -i\hbar\,\partial/\partial x$

b) $\langle x|\hat{k}|x'\rangle = -i\hbar\,\partial/\partial x\,\delta(x-x')$

$\langle k'|\hat{k}|k'\rangle = k\,\delta(k-k')$

c) $\langle x|\hat{E}_{kin}|x'\rangle = \langle x|\frac{k^2}{2m}|x'\rangle \rightarrow \frac{1}{2m}(-i\hbar\,\partial/\partial x)^2\,\delta(x-x')$

$\langle k|\hat{E}_{kin}|k'\rangle = \langle k|\frac{k^2}{2m}|k'\rangle \rightarrow \frac{p^2}{2m}\,\delta(k-k')$

d) $\langle x|\hat{V}|x'\rangle \rightarrow \langle x|\hat{V}(x)|x'\rangle \rightarrow \hat{V}(x)\,\delta(x-x')$

$\langle k|\hat{V}|k'\rangle \rightarrow \langle k|\hat{V}(x)|k'\rangle \rightarrow V(i\hbar\,\partial/\partial p)\,\delta(k-k')$

e) $L = \hat{x}\times\hat{k} \rightarrow \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ k_x & k_y & k_z \end{vmatrix}$

$L_x = yk_z - zk_y \qquad L_y = xk_z - zk_x \qquad L_z = xk_y - yk_x$

$\langle x|\hat{L}|x'\rangle \longrightarrow L_x = -i\hbar(y\,\partial/\partial z - z\,\partial/\partial y)\,\delta(x-x')$

$L_y = -i\hbar(x\,\partial/\partial z - z\,\partial/\partial x)\,\delta(x-x')$

$L_z = -i\hbar(x\,\partial/\partial y - y\,\partial/\partial x)\,\delta(x-x')$

$\langle k|\hat{L}|k'\rangle \longrightarrow L_x = i\hbar(k_z\,\partial/\partial k_y - k_y\,\partial/\partial k_z)\,\delta(k-k')$

$L_y = i\hbar(k_z\,\partial/\partial k_x - k_x\,\partial/\partial k_z)\,\delta(k-k')$

$L_z = i\hbar(k_y\,\partial/\partial k_x - k_x\,\partial/\partial k_y)\,\delta(k-k')$

Both delta function and partial derivative b/c function of both $\hat{x}/\hat{k}$

f) $\hat{v} = \frac{dx}{dt} \to \frac{i}{\hbar}[\hat{H}, \hat{x}] \to \frac{i}{\hbar}\left[\frac{\hat{k}^2}{2m} + \hat{V}(x), \hat{x}\right]$

$[\hat{V}(x), \hat{x}] = 0$

a general formula is $\frac{d\hat{A}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}]$ Heisenberg eqn of motion

$= \frac{i}{\hbar}\left[\frac{\hat{k}^2}{2m}, \hat{x}\right] = \frac{i}{\hbar}\frac{1}{2m}[\hat{k}^2, \hat{x}] \to [\hat{k}^2, \hat{x}] = \hat{k}[\hat{k}, \hat{x}] + [\hat{k}, \hat{x}]\hat{k}$

not sure if you're expecting me to show how this is true, I just looked up the properties for it

$[\hat{x}, \hat{k}] = i\hbar \to [\hat{k}, \hat{x}] = -i\hbar \qquad [\hat{k}^2, \hat{x}] = -\hat{k}i\hbar - \hat{k}i\hbar = -2i\hbar\hat{k}$

$= \cancel{\frac{i}{\hbar}} \frac{1}{\cancel{2}m}(\cancel{-2}\cancel{i}\cancel{\hbar}\hat{k}) \quad i^2 \to -1$

$\hat{V} = \frac{\hat{k}}{m}$, so it is momentum over mass I guess...

$\langle x | \hat{V} | x' \rangle \to \langle x | \frac{\hat{k}}{m} | x' \rangle = -i\hbar/m \, \partial/\partial x \, \delta(x-x')$

$\langle k | \hat{V} | k' \rangle \to \langle k | \frac{\hat{k}}{m} | k' \rangle = \frac{k}{m}\delta(k-k')$

2) a) 3D $\quad g_{dim}(\varepsilon) = \lim_{\Delta\varepsilon \to 0} \frac{\#\text{states within } [\varepsilon, \varepsilon+\Delta\varepsilon]}{\Delta\varepsilon \cdot V_{dim}} \quad \left[\frac{1}{eV \cdot m^{dim}}\right]$

Set numerator to integral/V

$\Delta^{dim} k = \frac{(2\pi)^{dim}}{V}$

$$\frac{\frac{\int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} d^3k}{\frac{(2\pi)^3}{\cancel{V}}}}{\Delta\varepsilon \cdot \cancel{V}} = \frac{\int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} d^3k}{(2\pi)^3} \cdot \frac{1}{\Delta\varepsilon}$$

cartesian → spherical

$d^3k = dk_x dk_y dk_z = k^2 \sin\theta \, dk \, d\theta \, d\phi$

$= \frac{4\pi}{(2\pi)^3} \int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} k^2 dk \cdot \frac{1}{\Delta\varepsilon}$

convert back to limit

$= \lim_{\Delta\varepsilon \to 0} \frac{4\pi}{(2\pi)^3} k^2(\varepsilon) \frac{dk}{d\varepsilon} \qquad \varepsilon = \frac{\hbar^2 k^2}{2m} \qquad d\varepsilon = \frac{2\hbar^2 k}{2m} dk$

$= \lim_{\Delta\varepsilon \to 0} \frac{4\pi}{(2\pi)^3} k^2(\varepsilon) \frac{m}{\hbar^2 k} = \frac{4\pi}{(2\pi)^3} \frac{k m}{\hbar^2} \qquad d\varepsilon = \frac{\hbar^2 k}{m} dk$

$= \frac{4\pi}{8\pi^3} \frac{m}{\hbar^2} \sqrt{\frac{2m\varepsilon}{\hbar^2}} = \boxed{\frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}} \qquad d\varepsilon/dk = \frac{\hbar^2 k}{m} \qquad \frac{dk}{d\varepsilon} = \frac{m}{\hbar^2 k}$

$k = \sqrt{\frac{2m\varepsilon}{\hbar^2}}$

b) 2D $\lim_{\Delta\varepsilon \to 0} \frac{\#\text{ states}}{\Delta\varepsilon \cdot V}$ $\qquad \frac{\int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} d^2k}{(2\pi)^2} \cdot \frac{1}{\Delta\varepsilon \cdot \cancel{SA}}$

$d^2k = dk_x dk_y \to$ polar

$k\,dk\,d\theta$ $\qquad \frac{1}{(2\pi)^2} \int_0^{2\pi}\int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} k\,dk\,d\theta \cdot \frac{1}{\Delta\varepsilon}$ $\quad 2\pi$

$$= \frac{2\pi}{(2\pi)^2} \int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} k\,dk \cdot \frac{1}{\Delta\varepsilon}$$

back to limit

$$\lim_{\Delta\varepsilon \to 0} \frac{1}{2\pi} k(\varepsilon) \frac{dk}{d\varepsilon} \qquad dk/d\varepsilon = \frac{m}{\hbar^2 k}$$

$$\frac{1}{2\pi} k \frac{m}{\hbar^2 k} = \boxed{\frac{1}{2\pi} \frac{m}{\hbar^2}}$$

c) 1D $\quad \frac{\int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} dk}{\frac{2\pi}{\cancel{L}}} \cdot \frac{1}{\Delta\varepsilon \cdot \cancel{L}} \to \frac{1}{2\pi} \int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} dk \cdot \frac{1}{\Delta\varepsilon}$ $\quad 2$

$$= \frac{1}{\pi} \frac{dk}{d\varepsilon} = \frac{1}{\pi} \frac{m}{\hbar^2 k}$$

$$= \frac{m}{\pi \hbar^2 k} \qquad k = \sqrt{\frac{2m\varepsilon}{\hbar^2}}$$

$$= \frac{m}{\pi\hbar^2} \sqrt{\frac{\hbar^2}{2m\varepsilon}} = \boxed{\frac{1}{\pi} \sqrt{\frac{m}{2\hbar^2 \varepsilon}}}$$

d) dim > 3 $\qquad g_{dim}(\varepsilon) = \lim_{\Delta\varepsilon \to 0} \frac{\#\text{ states within } [\varepsilon, \varepsilon+\Delta\varepsilon]}{\Delta\varepsilon \cdot V_{dim}}$

$$g_{dim}(\varepsilon) = \frac{\int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} d^{dim}k}{(2\pi)^{dim}} \cdot \frac{1}{\Delta\varepsilon \cdot \cancel{V_{dim}}}$$

$d^{dim}k \to r^{dim-1} \left(\frac{2\pi^{n/2}}{\Gamma(n/2)}\right)$

formula for total solid angle in $\uparrow$ space

$$\frac{1}{(2\pi)^{dim}} \left(\frac{2\pi^{dim/2}}{\Gamma(dim/2)}\right) \int_{\varepsilon_k}^{\varepsilon_k+\Delta\varepsilon} k^{dim} \cdot \frac{1}{\Delta\varepsilon}$$

to limit

$$= \lim_{\Delta\varepsilon \to 0} \frac{1}{(2\pi)^{dim}} \cdot \left(\frac{2\pi^{dim/2}}{\Gamma(dim/2)}\right) k^{dim}(\varepsilon) \frac{dk}{d\varepsilon}\Big|_\varepsilon \qquad k = \sqrt{\frac{2m\varepsilon}{\hbar^2}} \qquad \frac{dk}{d\varepsilon}\Big|_\varepsilon = \frac{m}{\hbar^2 k}$$

$$= \frac{1}{(2\pi)^{dim}} \left(\frac{2\pi^{dim/2}}{\Gamma(dim/2)}\right) \left(\frac{2m\varepsilon}{\hbar^2}\right)^{\frac{dim-1}{2}} \frac{m}{\hbar^2} \to \boxed{\frac{1}{(2\pi)^{dim}} \left(\frac{2\pi^{dim/2}}{\Gamma(dim/2)}\right) \left(\frac{2m^3\varepsilon}{\hbar^4}\right)^{\frac{dim-1}{2}}}$$

e) (0D) $g_{0D}(\mathcal{E}) = \sum_n \delta(\mathcal{E} - \mathcal{E}_n)$

$$g_{dim}(\mathcal{E}) = \frac{\int d^{dim}k \cdot \frac{1}{\Delta\mathcal{E} \cdot V_{dim}}}{\cancel{(2\pi)^{dim}}} \rightarrow \frac{1}{(2\pi)^{dim}} \int d^{dim}k \cdot / \Delta\mathcal{E} \rightarrow \frac{1}{(2\pi)^{dim}} \int d^{dim}\vec{k}\, \delta(\mathcal{E} - \mathcal{E}_{\vec{k}})$$

$$\frac{1}{(2\pi)^{dim}} \int d^{dim}\vec{k}\, \delta(\mathcal{E} - \mathcal{E}_k) \rightarrow \frac{1}{(2\pi)^{dim}} \sum_n \delta(\mathcal{E} - \mathcal{E}_n),$$ or call it $\frac{1}{V_{dim}} \sum_n \delta(\mathcal{E} - \mathcal{E}_n)$

for (0D), $(2\pi)^0 \rightarrow 1$, so $g_{0D} = \sum_n \delta(\mathcal{E} - \mathcal{E}_n)$

3) $E_{r,n,k} = \frac{\hbar^2 \pi^2}{2mW^2} n^2 + \frac{\hbar^2 k^2}{2m}$ $\quad m = .067 m_0 \quad m_e = 9.1 \times 10^{-31} kg$

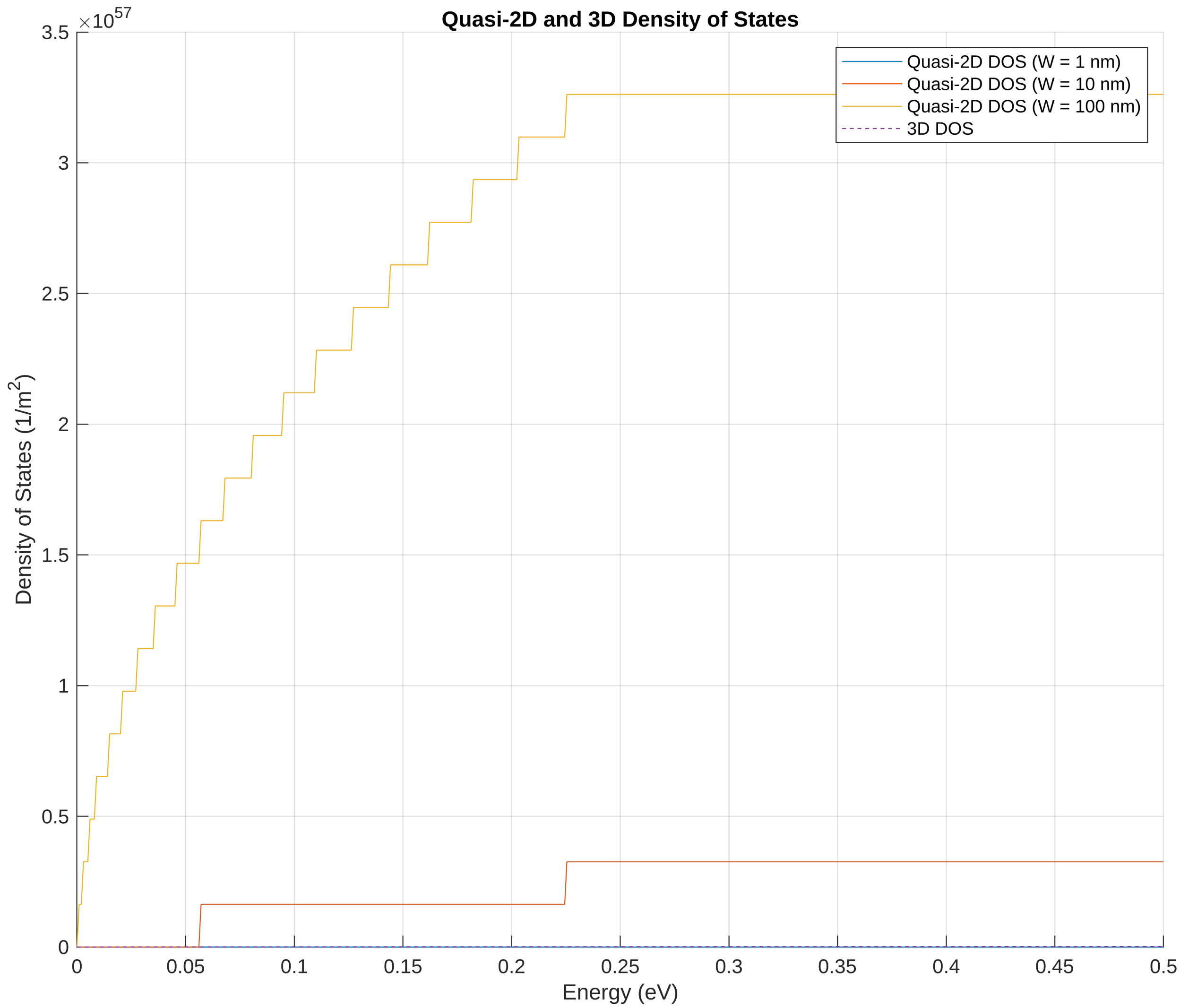
Problem 3

a)

There is a 2D and 3D representation of the energy for this system. $E_{n,k} = \frac{h^2\pi^2}{2mW^2}n^2 + \frac{h^2k^2}{2m}$ for a quasi-2D system, and $E_k = \frac{h^2k^2}{2m}$ for an unbounded 3D system.

```
clc
clear
close all

% Constants
hbar = 1.054e-34;
m = 9.107e-31;
mo = 0.067 * m;
W_values = [1, 10, 100] * 1e-9;  % Quantum well width in meters
W = W_values(1);
q = 1.6e-19;

% Energy range in eV
E = linspace(0, 0.5, 500) * q;  % Convert eV to Joules
n = 1:20;

figure('Position', [100, 100, 1000, 800]); % Increase figure window size
hold on;
grid on;
xlabel('Energy (eV)');
ylabel('Density of States (1/m^2)');
title('Quasi-2D and 3D Density of States');

% Loop over W values to compute quasi-2D DOS
for i = 1:length(W_values)
    g_2D = zeros(size(E));

    % Compute subband energy levels
    E_n = ((hbar * pi * n / W_values(i)).^2) / (2 * mo);

    % Sum contributions of all subbands
    for j = 1:length(n)
        g_2D = g_2D + (m / (pi * hbar^2)) * (E > E_n(j));  % Step function
contribution
    end

    % Plot DOS
    plot(E / q, g_2D / q, 'DisplayName', sprintf('Quasi-2D DOS (W = %.0f
nm)', W_values(i) * 1e9));
end
```

```
% Compute 3D DOS
g_3D = (1 / (4 * pi^2)) * (2 * mo / (hbar^2))^(3/2) .* sqrt(E);
plot(E / q, g_3D * W / q, '--', 'DisplayName', '3D DOS');

legend('show');
hold off;
```

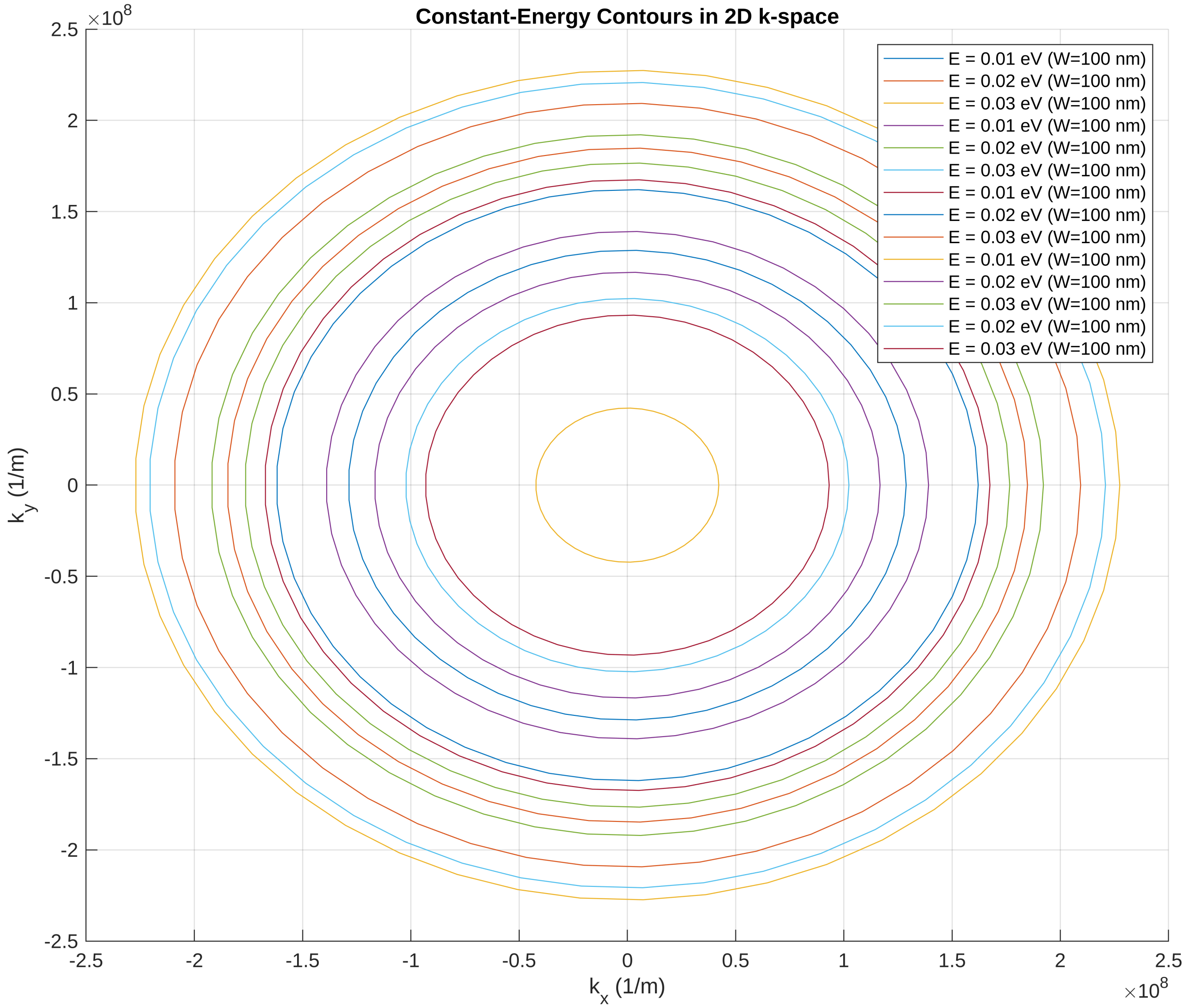


You can see that as the well width increases, the quasi-2D density of states starts to follow the $\propto \sqrt{E}$ relationship, similar to the 3D density of states. This following intuition, as the width increases, the third dimension is becoming less bounded, becoming almost 3D unbounded. When the width is small, it acts similar to the unbounded 2D density of states, where it doesn't depend on energy. If the 3D DOS was of the same magnitude, this would be clear, but I believe they are off by a factor of e4 because of the per volume to per area unit conversion.

b)

All degenerate wavevectors that have the same energy.

```
figure('Position', [100, 100, 1000, 800]); % Increase figure window size
hold on;
grid on;
xlabel('k_x (1/m)');
ylabel('k_y (1/m)');
title('Constant-Energy Contours in 2D k-space');

% Energy values to plot (in eV)
E_plot = [0.01, 0.02, 0.03] * q;
W_values = [1, 10, 100] * 1e-9;  % Quantum well width in meters
W = W_values(1);
n_values = 1:5;

for i = 1:length(W_values)

    for j = 1:length(n_values)
        E_n = (hbar^2 * (pi * n_values(j) / W_values(i))^2) / (2 * mo);

        for k = 1:length(E_plot)
            E = E_plot(k);
            if E > E_n  % Only plot if E > E_n
                k_mag = sqrt((2 * mo / hbar^2) * (E - E_n));
                theta = linspace(0, 2*pi, 50);
                kx = k_mag * cos(theta);
                ky = k_mag * sin(theta);
                plot(kx, ky, 'DisplayName', sprintf('E = %.2f eV (W=%.0f
nm)', E/q, W_values(i)*1e9));
            end
        end
    end
end

legend('show');
hold off;
```

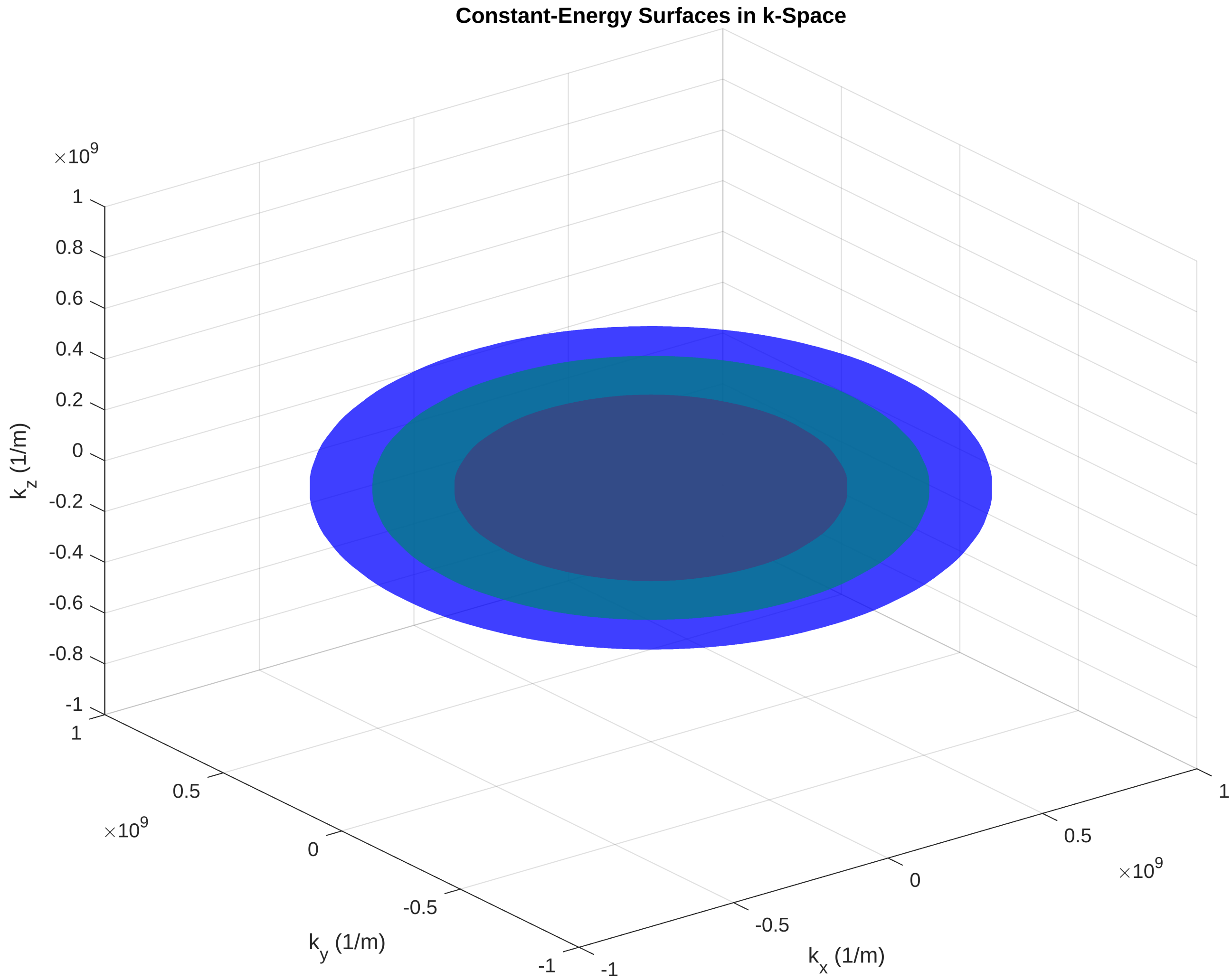


Not quite sure what the problems are with the legend, but not working correctly. You can still get the idea that in 2D, different energies have a grouping of degenerate k values.

Problem 4)

a)

```
% Constants
hbar = 1.0545718e-34;  % Reduced Planck's constant (J·s)
m0 = 9.10938356e-31;   % Free electron mass (kg)
m_xy = 0.98 * m0;      % Effective mass in xy-plane
m_z = 0.19 * m0;       % Effective mass in z-direction
q = 1.6e-19;

% Energy values to plot (in eV)
E_values = [0.01, 0.02, 0.03] * q;

% k-space range
k_max = 1e9;  % Maximum k value in 1/m
k_points = 50; % Grid points in each direction
[kx, ky, kz] = meshgrid(linspace(-k_max, k_max, k_points), ...
                         linspace(-k_max, k_max, k_points), ...
                         linspace(-k_max, k_max, k_points));

% Energy dispersion equation
E_k = (hbar^2 / (2 * m_xy)) * (kx.^2 + ky.^2) + (hbar^2 / (2 * m_z)) * kz.^2;

% Plot constant-energy surfaces
figure('Position', [100, 100, 1000, 800]); % Increase figure window size
hold on;
colors = ['r', 'g', 'b'];

for i = 1:length(E_values)
    E_level = E_values(i);
    fv = isosurface(kx, ky, kz, E_k, E_level);
    p = patch(fv);
    set(p, 'FaceColor', colors(i), 'EdgeColor', 'none', 'FaceAlpha', 0.5);
end

% Plot settings
xlabel('k_x (1/m)');
ylabel('k_y (1/m)');
zlabel('k_z (1/m)');
zlim([-1e9 1e9]);
title('Constant-Energy Surfaces in k-Space');
grid on;
view(3);
hold off;
```



My intution says this isn't entirely correct, because if the effective mass for the z-component is lower, then the slope of its k-component should be steeper. This ellipse stretches towards kx and ky, giving it a greater slope. I honestly can't get this to change though.

b)

This is currently an ellipse, very close to a sphere, so if we can get all k components to have equal weights, a sphere is obtainable. Lets get kz to have the same weight at kx and ky, by setting a new coordinate system. We just need to use the ratio between the two effective masses to get all the k's to equal, and k in the z direction is (supposed to) be steeper, so lets shrink this to kx and ky. Our new kz' is $= \sqrt{\frac{m_z}{m_{\mathrm{xy}}}} * k_z$. Now this is like any previous 3D DOS derivition, with the final answer being $g(E) = \frac{1}{4\pi^2}\left(\frac{2m}{h^2}\right)^{1.5}\sqrt{E}$, BUT, our new m is equal to m_xy, and the new E is proportional to $k'_x{}^2 + k'_y{}^2 + k'_z{}^2$, while k'_z has the effective mass ratio discussed early.

c)

Our new quantized k would be $k_z = \frac{\pi n}{W}$, so we just have a new equation of $E = \frac{h^2}{2m_{\text{xy}}}\left(k_x{}^2 + k_y{}^2\right) + \frac{h^2}{2m_z}\left(\frac{n\pi}{W}\right)^2$

d)

Same as in problem c) but we'll skip to

$$E = \frac{h^2}{2m_{\text{xy}}}\left(k_x{}^2 + \frac{n\pi}{W}^2\right) + \frac{h^2}{2m_z}k_z{}^2$$

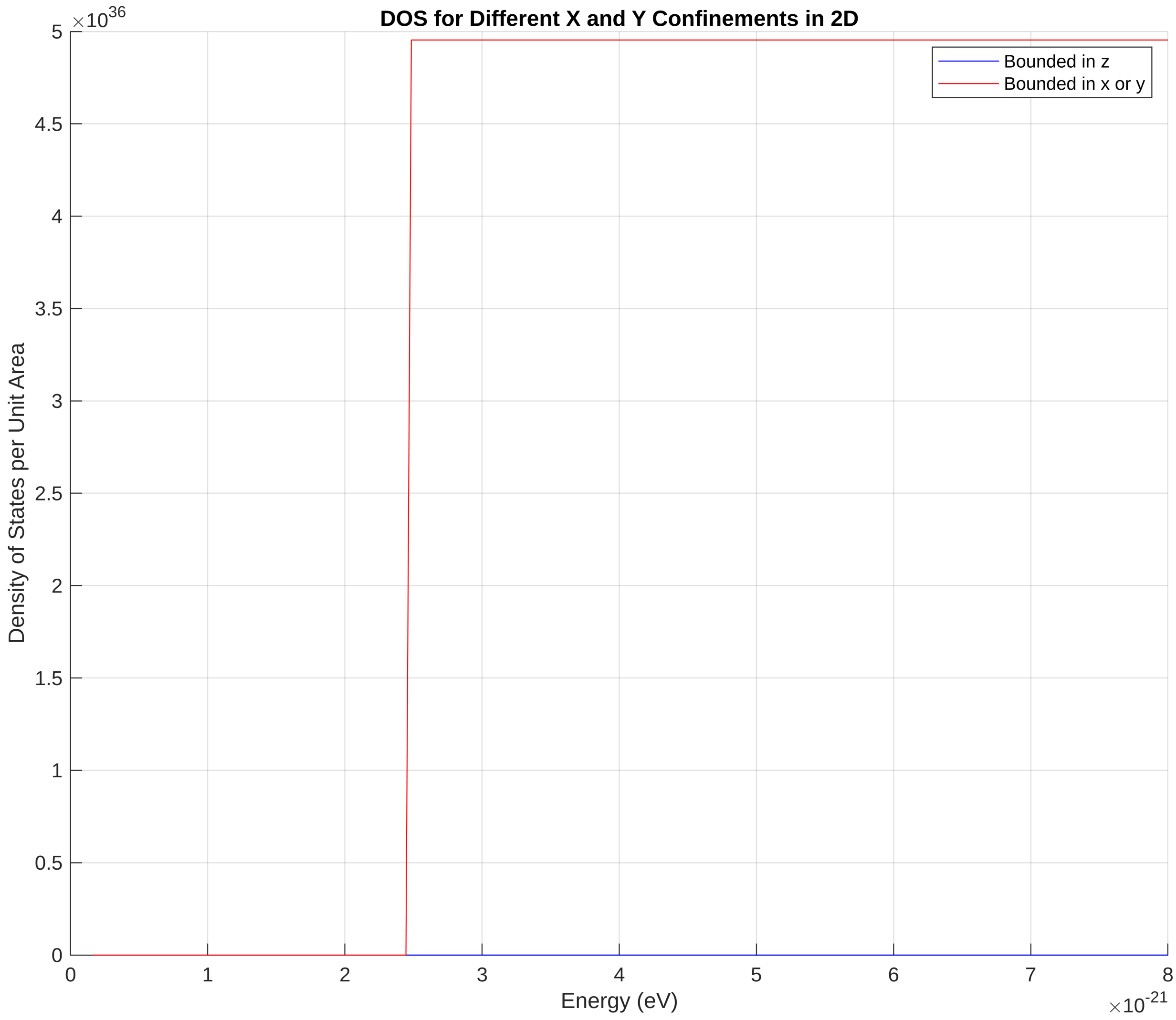
OR

$$E = \frac{h^2}{2m_{\text{xy}}}\left(k_y{}^2 + \frac{n\pi}{W}^2\right) + \frac{h^2}{2m_z}k_z{}^2$$

e)

```
% Constants
hbar = 1.0545718e-34;
m0 = 9.10938356e-31;
m_xy = 0.98 * m0;
m_z = 0.19 * m0;
W = 5e-9;  % Quantum well width (5 nm)

% Energy range in eV
E_range = linspace(0.001, 0.05, 200) * q;

% 2D confinement in z-direction (case c)
g_2D_z = zeros(size(E_range));
for n = 1:5
    E_n = (hbar^2 / (2 * m_z)) * (n * pi / W) ^ 2;
    g_2D_z = g_2D_z + ((2 * m_xy) / (2 * pi * hbar^2)) .* (E_range >= E_n);
end

% 2D confinement in x or y-direction (case d)
g_2D_x = zeros(size(E_range));
for n = 1:5
    E_n = (hbar^2 / (2 * m_xy)) * (n * pi / W) ^ 2;
    g_2D_x = g_2D_x + ((2 * m_z) / (2 * pi * hbar^2)) .* (E_range >= E_n);
end

figure('Position', [100, 100, 1000, 800]); % Increase figure window size
hold on;
plot(E_range, g_2D_z, 'b');
plot(E_range, g_2D_x, 'r');
xlabel('Energy (eV)');
ylabel('Density of States per Unit Area');
title('DOS for Different X and Y Confinements in 2D');
legend('Bounded in z', 'Bounded in x or y');
```

```
grid on;
hold off;
```



This is like problem 3) when we experienced a step function when a 3D system is confined in one dimension. As we calculated in part b) of this problem, the 3D DOS depends on the effective mass, so the step function of the density of states will depend on which dimension we bound the electron in, because its effective mass in the dimension will change the DOS.