ECE 456 - Problem Set 1

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Question 1

(a)

Beginning with the following two equations:

$$N = \int_{-\infty}^{\infty} \frac{\gamma_1 f_1(E) + \gamma_2 f_2(E)}{\gamma_1 + \gamma_2} D(E - U) dE, \tag{1}$$

$$I = \frac{q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \int_{-\infty}^{\infty} [f_1(E) - f_2(E)] D(E - U) dE, \tag{2}$$

and changing the variable of integration to $E' = E - U$:

$$N = \int_{-\infty}^{\infty} \frac{\gamma_1 f_1(E' + U) + \gamma_2 f_2(E' + U)}{\gamma_1 + \gamma_2} D(E') dE',$$

$$I = \frac{q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \int_{-\infty}^{\infty} [f_1(E' + U) - f_2(E' + U)] D(E') dE'.$$

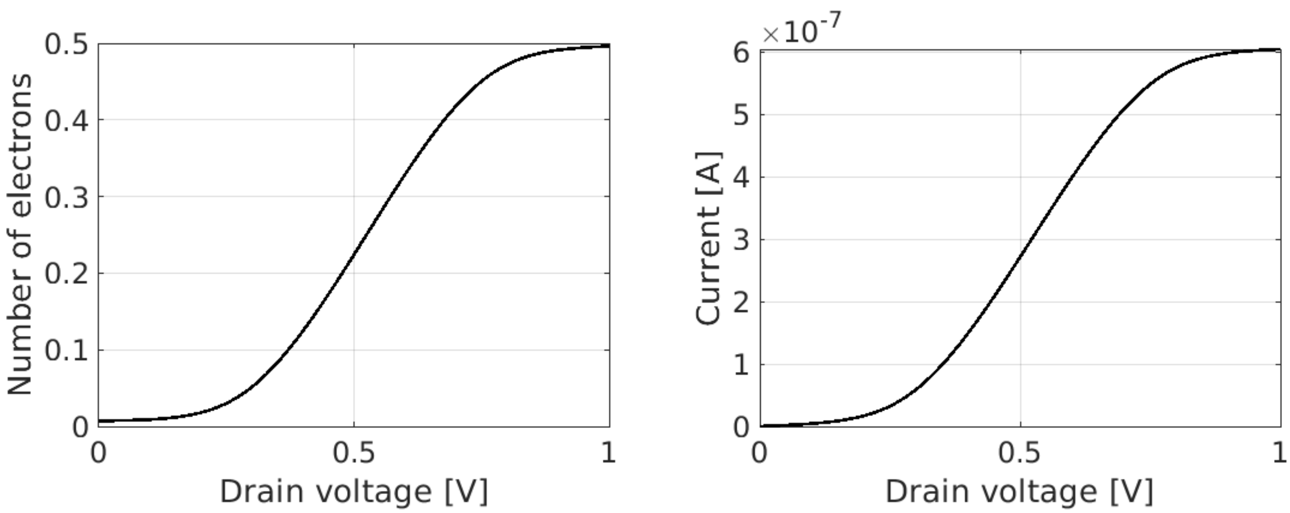
Replacing $E' \to E$, we obtain equations 3 and 4.

$$N = \int_{-\infty}^{\infty} \frac{\gamma_1 f_1(E + U) + \gamma_2 f_2(E + U)}{\gamma_1 + \gamma_2} DE dE, \tag{3}$$

$$I = \frac{q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \int_{-\infty}^{\infty} [f_1(E + U) - f_2(E + U)] DE dE. \tag{4}$$

(b)

For the provided constants, the plots of the number of channel electrons and the channel current follow:



(a) Plot of channel electrons vs. drain voltage.

(b) Plot of channel current vs. drain voltage.

Figure 1: Number of electrons and current versus drain voltage.

Below is our code. Note that some variable names are different from those in the example code.

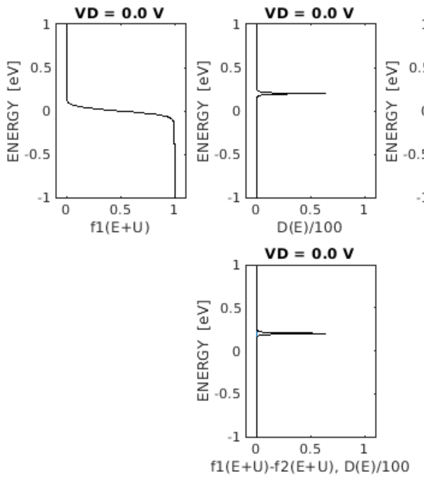
```

clear all;

%% Constants

% Physical constants
hbar = 1.052e-34;
```

```
% Single-charge coupling energy (eV)
U_0 = 0.25;
% (eV)
kBT = 0.025;
% Contact coupling coefficients (eV)
gamma_1 = 0.005;
gamma_2 = gamma_1;
gamma_sum = gamma_1 + gamma_2;
% Capacitive gate coefficient
a_G = 0.5;
% Capacitive drain coefficient
a_D = 0.5;
a_S = 1 - a_G - a_D;

% Central energy level
mu = 0;

% Energy grid, from -1eV to 1eV
NE = 501;
E = linspace(-1, 1, NE);
dE = E(2) - E(1);
% TODO name this better
cal_E = 0.2;

% Lorentzian density of states, normalized so the integral is 1
D = (gamma_sum / (2*pi)) ./ ( (E-cal_E).^2 + (gamma_sum/2).^2 );
D = D ./ (dE*sum(D));

% Reference no. of electrons in channel
N_0 = 0;

voltages = linspace(0, 1, 101);

% Terminal Voltages
V_G = 0;
V_S = 0;

for n = 1:length(voltages)
    % Set varying drain voltage
    V_D = voltages(n);

    % Shifted energy levels of the contacts
    mu_1 = mu - V_S;
    mu_2 = mu - V_D;

    % Laplace potential, does not change as solution is found (eV)
    % q is factored out here, we are working in eV
    U_L = - (a_G*V_G) - (a_D*V_D) - (a_S*V_S);

    % Poisson potential must change, assume 0 initially (eV)
    U_P = 0;

    % Assume large rate of change
    dU_P = 1;

    % Run until we get close enough to the answer
    while dU_P > 1e-6
        % source Fermi function
        f_1 = 1 ./ (1 + exp((E + U_L + U_P - mu_1) ./ kBT));
        % drain Fermi function
        f_2 = 1 ./ (1 + exp((E + U_L + U_P - mu_2) ./ kBT));
```

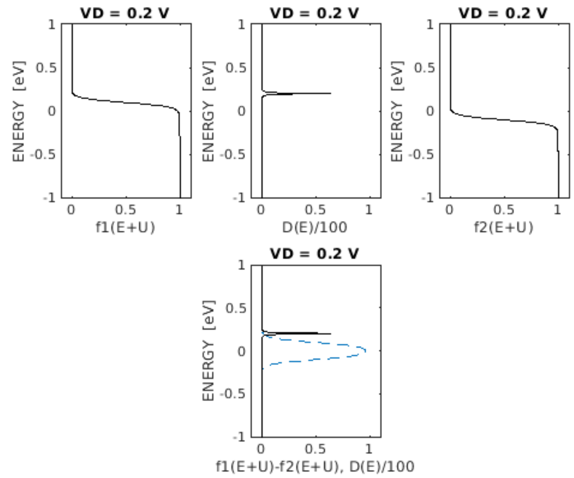
```
        % Update channel electrons against potential
        N(n) = dE * sum( ((gamma_1/gamma_sum) .* f_1 + (gamma_2/gamma_sum) .* f_2) .* D);

        % Re-update Poisson portion of potential
        tmpU_P = U_0 * ( N(n) - N_0);
        dU_P = abs(U_P - tmpU_P);

        % Unsure why U_P is updated incrementally, perhaps to avoid oscillations?
        %U_P = tmpU_P;
        %U_P = U_P + 0.1 * (tmpU_P - U_P);
    end

    % Calculate current based on solved potential.
    % Note: f1 is dependent on changes in U but has been updated prior in the loop
    I(n) = q * (q/hbar) * (gamma_1 * gamma_1 / gamma_sum) * dE * sum((f_1-f_2).*D);

end


%%Plotting commands

figure(1);
h = plot(voltages, N,'k');
grid on;
set(h,'linewidth',[2.0]);
set(gca,'Fontsize',[18]);
xlabel('Drain voltage [V]');
ylabel('Number of electrons');

figure(2);
h = plot(voltages, I,'k');
grid on;
set(h,'linewidth',[2.0]);
set(gca,'Fontsize',[18]);
xlabel('Drain voltage [V]');
ylabel('Current [A]');
```

(c)

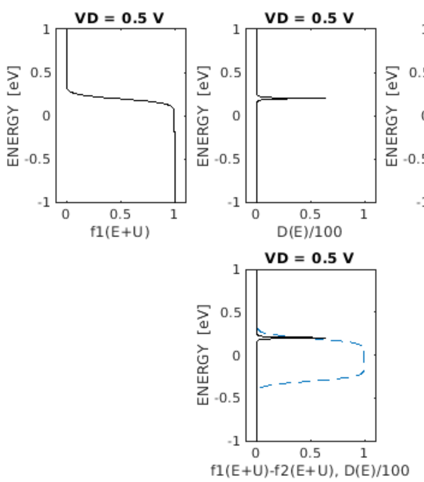
(i)



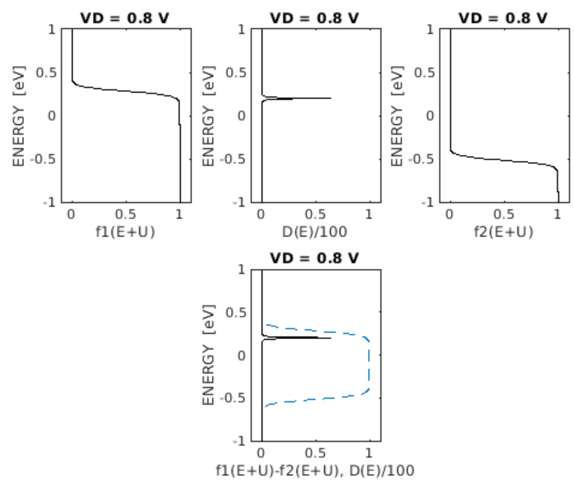
(a) Plot of channel electrons vs. drain voltage.



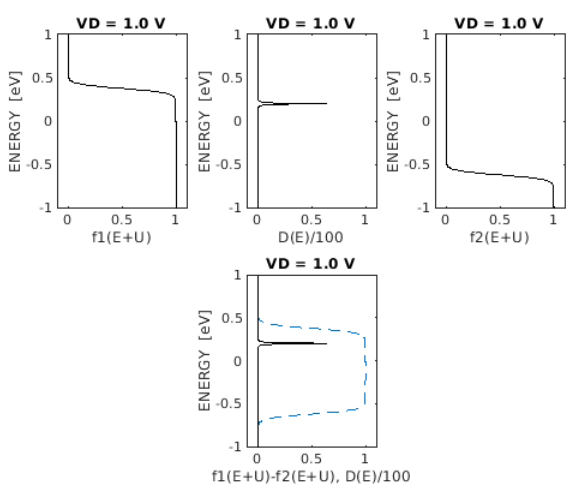
(b) Plot of channel electrons vs. drain voltage.



(c) Plot of channel electrons vs. drain voltage.



(d) Plot of channel electrons vs. drain voltage.



(e) Plot of channel electrons vs. drain voltage.

Figure 2: Visual representation of the Fermi functions of the contacts and channel.

Table 1 shows the variation in the difference between f_1 and f_2 at $E = \varepsilon$, and I at different drain voltages. We compare the differences between values at $V_D = 1.0\,V$ and $V_D = 0.8\,V$:

$$\frac{([f_1(E+U) - f_2(E+U)]|_{E=\varepsilon})|_{V_D=1.0\,V}}{([f_1(E+U) - f_2(E+U)]|_{E=\varepsilon})|_{V_D=0.8\,V}} = 1.0363,$$

$$\frac{I|_{V_D=1.0\,V}}{I|_{V_D=0.8\,V}} = 1.0504,$$

and between values at $V_D = 0.8\,V$ and $V_D = 0.5\,V$:

$$\frac{([f_1(E+U) - f_2(E+U)]|_{E=\varepsilon})|_{V_D=0.8\,V}}{([f_1(E+U) - f_2(E+U)]|_{E=\varepsilon})|_{V_D=0.5\,V}} = 2.1909,$$

$$\frac{I|_{V_D=0.8\,V}}{I|_{V_D=0.5\,V}} = 2.1218.$$

In both comparisons we see that I changes in proportion to $[f_1(E+U) - f_2(E+U)]|_{E=\varepsilon}$, as predicted by Equation (9).

V_D [V]	$[f_1(E+U) - f_2(E+U)]\|_{E=\varepsilon}$	I [nA]
0.0	0.000	0.0
0.2	0.015	17.0
0.5	0.440	271
0.8	0.964	575
1.0	0.999	604

Table 1: Differences in contact Fermi functions evaluated at $E = \varepsilon$ and current I at different drain voltages V_D. Values are taken from Figures 1b and 2a to 2e.

(ii)

Figure 3 has the Fermi functions marked at their "step points", or when they are equal to 0.5. This can be used to find the self-consistant potential U, via the equation for the source Fermi function:

$$f(E+U) = \frac{1}{1 + e^{(E+U-\mu_1)/k_BT}}$$

We could also use the drain Fermi function but since $V_S = 0$, it is simpler to use the source. The function will "step" when $E = \mu_1 - U$, which from Figure 3 occurs at $E = \mu_1 - U = 0.4$ for the source contact. Since $\mu_1 = \mu - qV_S = 0$ We can simply rearrange to find $U = -E = -0.4\,eV$.

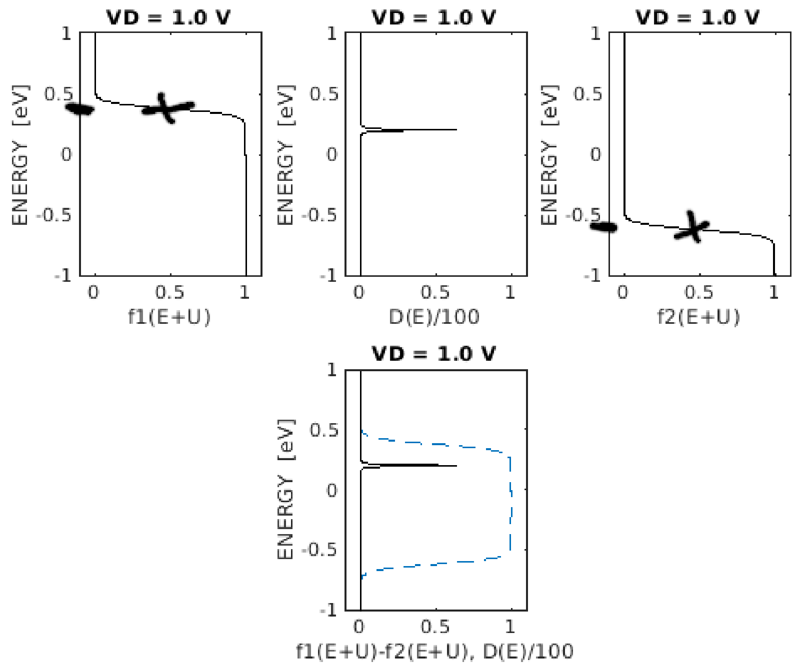


Figure 3: Marked step points of contact Fermi functions.

(iii)

At $V_D = 1V$, the source is trying to *fill* the channel level while the drain is trying to *empty* it. This is because the source has electrons at the channel level, and is filling these in while the drain does not have any and is attempting to bring the channel level back down to where it is.

(iv)

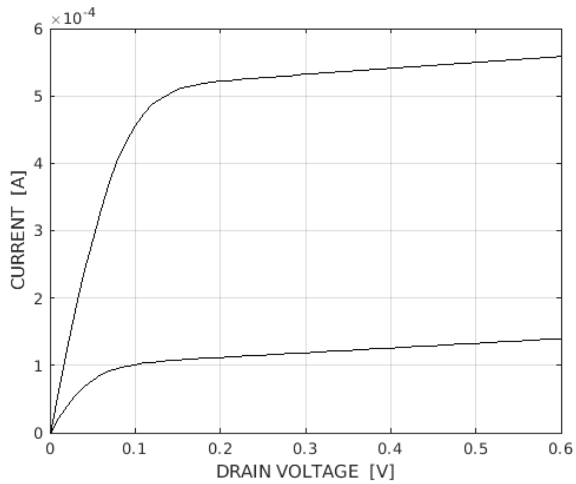
Referring to figure 3 again, we can see the areas where the difference between the Fermi functions of each contact are 1. Roughly, this means that the channel current I would remain the same if the channel energy level was anywhere between $0.3eV$ and $-0.5eV$.

(v)

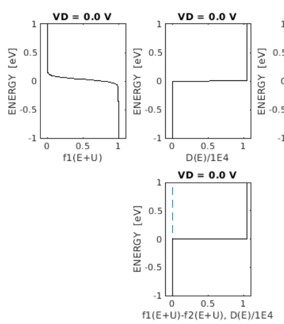
There is no current when $V_D = 0$ because the source does not want to fill the channel. It has no electrons at the channel energy level, and thus there is no impetus to fill the channel. A similar story occurs with the drain, in that it has no electrons at the appropriate energy level, and there are none in the channel for it to pull out.

Question 2

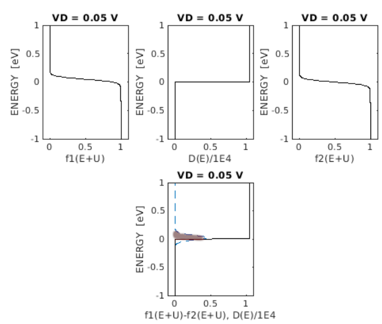
(a)



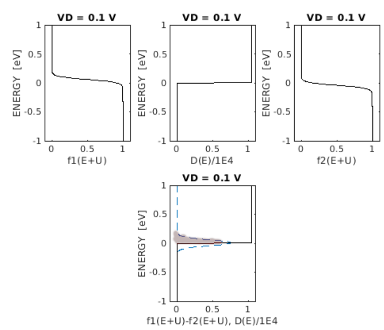
(a) I-V curves.



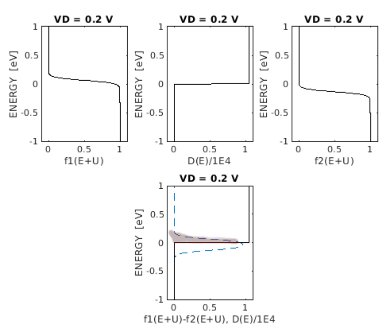
(b) Fermi functions at $0V$.



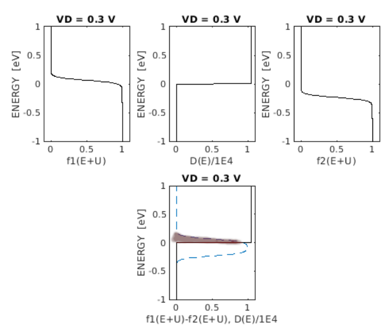
(c) Fermi functions at $0.05V$.



(d) Fermi functions at $0.1V$.



(e) Fermi functions at $0.2V$.



(f) Fermi functions at $0.3V$.

Figure 4: (a) depicts I-V curves at $V_G = 0.5$ V (higher curve) and $V_G = 0.25$ V. (b) through (f) show Fermi functions and $D(E)$ at various drain voltages.

(b)

As the drain voltage increases, we see that the overlapping area under the "curve" of $f_1(E+U) - f_2(E+U)$ and $D(E)$ increases, up until the point where the drain only has electrons below the energy levels available in the channel. The difference function also reaches its maximum height and it widens downward rather than upward. At this point, the overlapping area no longer increases, and therefore the current does not increase either, hitting *saturation current*.

(c)

At $V_D = 0.3V$, the energy levels from approximately 0 to 0.2 eV are being used for electron transport. This is the range where the difference in the contact Fermi functions is more than 0 and the energy is more than 0.
The difference between the two contacts is the greatest at $0eV$, because this is the point at which their Fermi functions have the greatest difference, and thus will be making the most "effort" to equalize the channel potential.

(d)

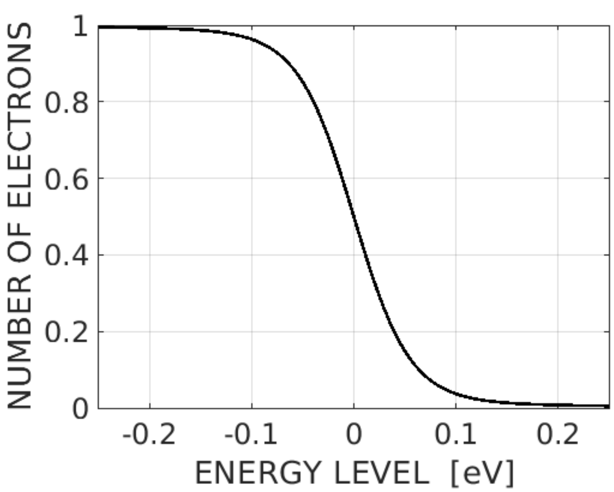
Based on the supposed material changes, we would choose material A to maximize the drain current. The energy levels vanishing at $-0.4eV$ would mean that there is a greater number of energy levels that would be able to be used for conduction. There would be a larger *area* where there is a non-zero difference in the two Fermi functions at the contacts and there are energy levels available in the channel.
This can be contrasted with material B, which would have *no* energy levels in this "conduction" zone and thus no current would be able to flow at all.

Question 3

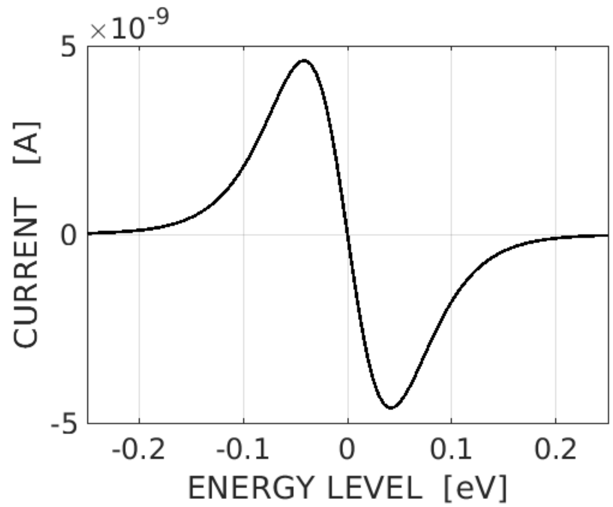
(a)

Below is our code. Note that some variable names are different from those in the example code.

(b)

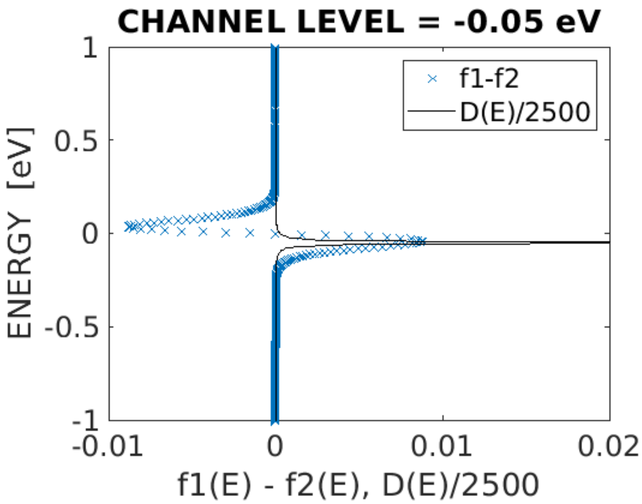


(a) Fermi Functions at $0.3V$.

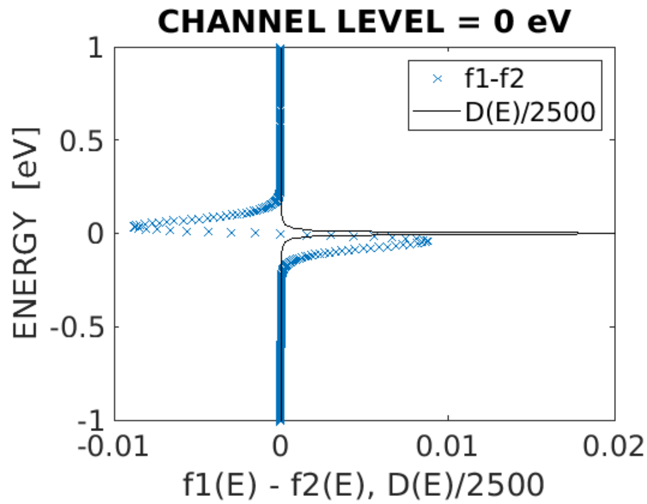


(b) Fermi Functions at $0.3V$.

(c)



(a) Fermi Functions at $0.3V$.



(b) Fermi Functions at $0.3V$.

(d)

The difference in temperature causes a difference in the sharpness of the contact Fermi functions. This in turn leads to the behaviour in $f_1 - f_2$ seen in Figures 6a and 6b. As seen in the previous questions, the current is proportional to the area under the curve of the $D(E) * [f_1 - f_2]$. When the channel level is $\varepsilon = -0.05$ eV, the positive region of $[f_1 - f_2]$ overlaps the non-zero part of $D(E)$, giving a positive current. Alternatively, when $\varepsilon = 0$ eV, half of the area under $D(E)$ overlaps with the negative part of $[f_1 - f_2]$, while half overlaps the positive part. Thus the areas cancel out completely, and the resultant current is 0. A plot of $\varepsilon = +0.05$ eV would show overlap of $D(E)$ with the negative part of $[f_1 - f_2]$, explaining why we get a reverse current flow at that channel level. The maximum current occurs at $\varepsilon = \pm 0.4$ eV (relative to μ).

Question 4

(a)

(i)

$$I = 0, N = 0$$

This is because the only allowed energy level in the channel is at a higher energy level than exists in either of the contacts, thus there are no electrons that would flow into the channel from either contact, thus no current *and* no electrons in the channel.

(ii)

$$I = 608\,nA, N = 0.5$$

Given that we are operating with a single energy level in the channel, we can use the equations 9 and 10 (provided in the assignment) directly.

$$I = \frac{q}{\hbar} \cdot \frac{0.005eV \cdot 0.005eV}{0.005eV + 0.005eV} \cdot [1 - 0] = 608\,nA$$

$$N = \frac{0.005eV \cdot 1 + 0.005eV \cdot 0}{0.005eV + 0.005eV} = 0.5$$

(iii)

$$I = 0\,A, N = 1$$

Given that we are operating with a single energy level in the channel, we can use the equations 9 and 10 (provided in the assignment) directly.

$$I = \frac{q}{\hbar} \cdot \frac{0.005eV \cdot 0.005eV}{0.005eV + 0.005eV} \cdot [1 - 1] = 0\, A$$

$$N = \frac{0.005eV \cdot 1 + 0.005eV \cdot 1}{0.005eV + 0.005eV} = 1$$

(b)

(i)

For $f_1(E+U)$ the step point occurs at $E = \mu_1 - U = 0.25$ eV. Since $U = -0.25$ eV, it follows that $\mu_1 = 0$ eV. Since $\mu_1 = \mu - qV_S$ and $\mu = 0$ eV, $V_S = 0$ V. For $f_2(E+U)$ the step point occurs at $E = \mu_2 - U = -0.25$ eV. Since $U = -0.25$ eV, it follows that $\mu_2 = -0.5$ eV. Since $\mu_1 = \mu - qV_D$ and $\mu = 0$ eV, $V_D = 0.5$ V.

(ii)

For $f_1(E)$ the step point occurs at $E = \mu_1 = 0.25$ eV. Since $\mu_1 = \mu - qV_S$ and $\mu = 0$ eV, $V_S = -0.25$ V. For $f_2(E)$ the step point occurs at $E = \mu_2 = -0.25$ eV. Since $\mu_1 = \mu - qV_D$ and $\mu = 0$ eV, $V_D = 0.25$ V. This assumes $U = 0$ eV.

(c)

(i)

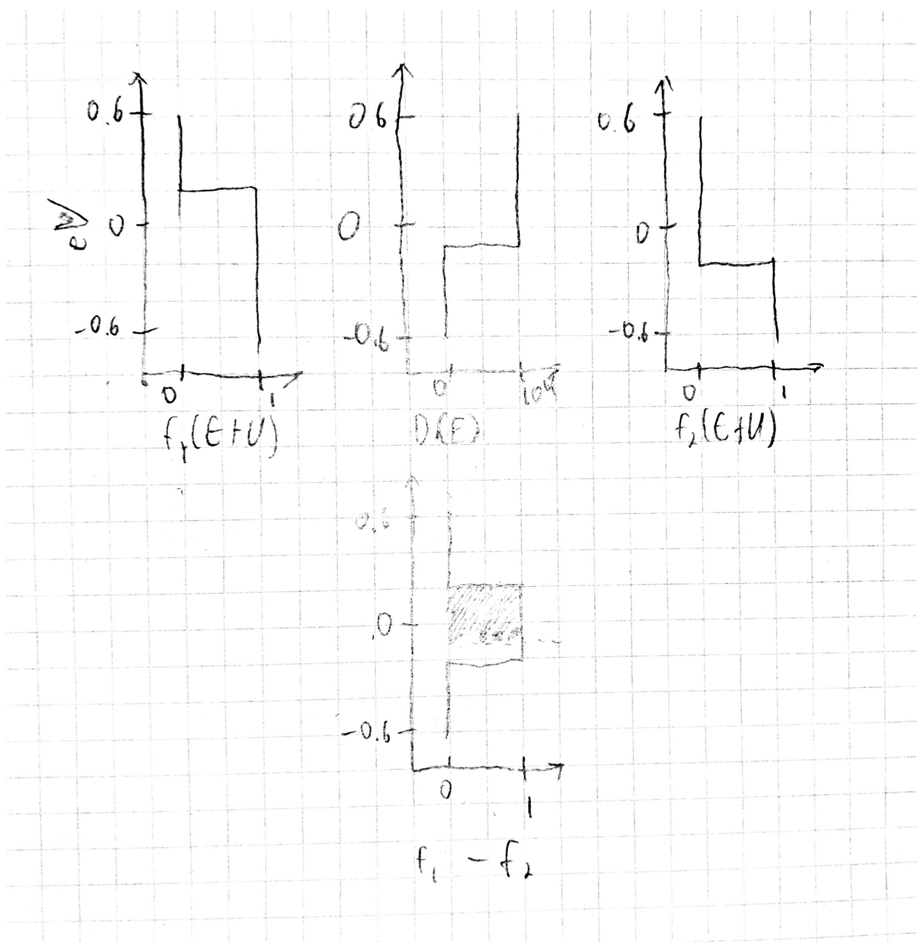


Figure 7: Visualisation of energy levels.

(ii)

Starting with equation 2 in the assignment we get:

$$I = \frac{q}{\hbar} \cdot \frac{0.005^2}{0.01} \cdot \int_{-0.1}^{0.2} [1-0] \cdot 10^4 dE$$
$$I = \frac{q}{\hbar} \cdot \frac{0.005^2}{0.01} \cdot [10^4 \cdot 0.2 - 10^4 \cdot -0.1]$$
$$I = 1.8\, mA$$

(iii)

The graph for the fermi functions at the saturation potentials will look much the same, except that they will be shifted up. This means that there is more area "under" the difference between the fermi functions and thus the bounds of integration can shift and become $[-0.1, 0.3]$.

$$I = \frac{q}{\hbar} \cdot \frac{0.005^2}{0.01} \cdot \int_{-0.1}^{0.3} [1-0] \cdot 10^4 dE$$
$$I = \frac{q}{\hbar} \cdot \frac{0.005^2}{0.01} \cdot [10^4 \cdot 0.3 - 10^4 \cdot -0.1]$$
$$I = 2.4mA$$

(d)

Using equation (5) in the assignment and plugging in the given values we obtain:

$$\begin{aligned}
&U = -q[\frac{C_S V_S + C_G V_G + C_D V_D}{C_E}] + \frac{q^2(N-N_0)}{C_E} \\
&U = -\alpha_S V_S - \alpha_G V_G - \alpha_D V_D + U_0(N-N_0)\ eV \\
&U = -0 \cdot 0 - 0.5 \cdot 0\, eV - 0.5 \cdot 0.6\, eV + 0.25\, eV \cdot (0.325 - 0)\ eV \\
&U = -0.21875\, eV
\end{aligned}$$

Then, starting with Equation 3 and plugging in $D(E-U) = \delta(E-\varepsilon)$, we obtain

$$N = \frac{\gamma_1 f_1(\varepsilon + U) + \gamma_2 f_2(\varepsilon + U)}{\gamma_1 + \gamma_2}$$

Recalling that the expressions for the contact Fermi functions are (with $\mu = 0$ eV):

$$\begin{aligned}
f_1(\varepsilon + U) &= \frac{1}{1 + e^{(\varepsilon + U + qV_S)/k_B T}} = \frac{1}{1 + e^{(0.2 - 0.21875 + 0)/0.025}} = 0.679 \\
f_2(\varepsilon + U) &= \frac{1}{1 + e^{()\varepsilon + U + qV_D)/k_B T}} = \frac{1}{1 + e^{(0.2 - 0.21875 + 0.6)/0.025}} \simeq 0
\end{aligned}$$

Then, solving for γ_2:

$$\gamma_2 = \gamma_2 \frac{N - f_1(\varepsilon + U)}{f_2(\varepsilon + U) - N} = 5.45 \times 10^{-3}\, eV$$

(e)

Assuming the density of states for each molecule can be modeled by $D(E) = \delta(E-\varepsilon)$, Equation (12) in the assignment is valid here. Thus the current will be maximized when $[f_1(E) - f_2(E)]|_{E=\varepsilon}$ is maximized. Solving $[f_1(E) - f_2(E)]|_{E=\varepsilon}$ for each molecule, we obtain:

Molecule A:

$$[f_1(E) - f_2(E)]|_{E=\varepsilon_A} = \frac{1}{1+e^{\frac{\varepsilon_A}{k_B T_1}}} - \frac{1}{1+e^{\frac{\varepsilon_A}{k_B T_2}}} = \frac{1}{1+e^{\frac{0}{0.024}}} - \frac{1}{1+e^{\frac{0}{0.027}}} = 0$$

Molecule B:

$$[f_1(E) - f_2(E)]|_{E=\varepsilon_B} = \frac{1}{1+e^{\frac{\varepsilon_B}{k_B T_1}}} - \frac{1}{1+e^{\frac{\varepsilon_B}{k_B T_2}}} = \frac{1}{1+e^{\frac{-0.05}{0.024}}} - \frac{1}{1+e^{\frac{-0.05}{0.027}}} = 0.02493$$

Molecule C:

$$[f_1(E) - f_2(E)]|_{E=\varepsilon_C} = \frac{1}{1+e^{\frac{\varepsilon_C}{k_B T_1}}} - \frac{1}{1+e^{\frac{\varepsilon_C}{k_B T_2}}} = \frac{1}{1+e^{\frac{-0.1}{0.024}}} - \frac{1}{1+e^{\frac{-0.1}{0.027}}} = 0.00877$$

Molecule B should be chosen.

(f)

Referring again to equation 2 in the assignment, we know that $D(E)$ is valid for all E, however since γ_1 is dependant on the energy level, we can use it to reduce our limits. For material A, this means we only care about E above $0eV$, and for B, E below $0eV$. Since we know the voltages on the contacts, we can calculate the effective fermi level at each.

$$\mu_1 = \mu_0 - V_S = 0 - (-2V) = 2\,eV$$

$$\mu_2 = \mu_0 - V_D = 0 - 1V = -1\,eV$$

With the fermi levels of each contact, we can adjust the limits of integration further for each material. Material A can be evaluated on $[0eV, 2eV]$, and material B can be evaluated on $[-1eV, 0eV]$.

$$I_A = \frac{q}{\hbar} \cdot \frac{0.005^2}{0.01} \cdot \int_0^2 [1-0] \cdot 10^4 dE$$

$$I_A = 12.2\,mA$$

$$I_B = \frac{q}{\hbar} \cdot \frac{0.005^2}{0.01} \cdot \int_0^2 [1-0] \cdot 10^4 dE$$

$$I_A = 6.1\,mA$$

Material A should be chosen.

(g)

Using Ohm's law we find the corresponding conductance:

$$\sigma_{max} = \frac{I_{max}}{V} = \frac{500\,nA}{4.3\,mV} = 116\,\mu S.$$

We expect this result to be an integer multiple of $G_0 = 38.76\,\mu S$, the quantum of conductance. We find

$$\frac{\sigma_{max}}{G_0} = 3.$$

We conclude there are 3 levels.