ECE 65600 (Electron Transport in Semiconductors) HW #5

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1) The equation of motion for an electron in k-space is $d\left(\hbar\vec{k}\right)/dt = \vec{F}_e$. What assumptions are necessary for this equation to be valid?

   a) Parabolic energy bands.
   b) Non-degenerate conditions.
   c) No quantum mechanical reflections.
   d) No B-field.
   e) No temperature gradients.

The given equation describes the semiclassical transport of electrons in *k*-space. It basically assumes that the conduction band profile, $E_C(x)$ varies slowly compared to the scale of the electron's De Broglie wavelength (~ 10 nm for electrons in Si at 300 K), as shown in Figure 1. Therefore, **wave phenomena such as quantum mechanical reflections and tunneling are ignored in this model**, and electron motion can be described by classical mechanics. Therefore, **the correct answer is (c).**

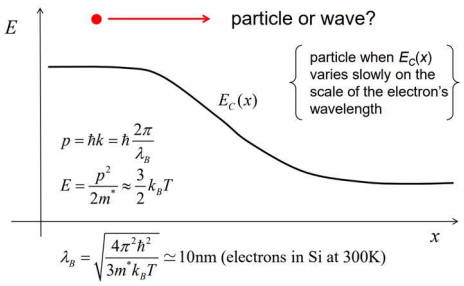


Figure 1. Assumed $E_C(x)$ condition

2) Under what conditions is this equation valid? $\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = 0$

   a) No recombination-generation.
   b) Equilibrium.
   c) No scattering.
   d) Position independent effective mass.
   e) All of the above.

The given equation is a special case of Boltzmann Transport Equation (BTE). It is basically derived by rearranging $df/dt = 0$, as shown in Figure 2, thus **describes the distribution function *f* under the equilibrium condition (b)**. Note that it assumes **the position-independent effective mass (d)**, thus $\hbar v = \nabla_{\mathbf{k}} E(\mathbf{k}, \mathbf{r}) = \nabla_{\mathbf{k}} E(\mathbf{k})$, usually used in semi-classical transports (otherwise, one should solve the equation of motion for effective mass). Additionally, the equilibrium condition naturally means **there is no scattering (c).** Furthermore, it assumes there is **no net recombination-generation (a)**. Note that if they exist, the generalized BTE is described as:

$$f(x, p_x, t) \qquad \frac{df}{dt} = 0$$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial p_x}\frac{dp_x}{dt} = 0$$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\upsilon_x + \frac{\partial f}{\partial p_x}F_x = 0$$

Figure 2. Derivation of BTE under the equilibirum.

$$\frac{\partial f}{\partial t} = -\upsilon_x \frac{\partial f}{\partial x} - F_x \frac{\partial f}{\partial p_x} + \left(\frac{\partial f}{\partial t}\right)_{g-r} + \left(\frac{\partial f}{\partial t}\right)_{coll}$$

where one can clearly check that the recombination-generation term $\partial f/\partial f|_{g-r}$ and collision term (scattering) $\partial f/\partial t|_{coll}$ are zero in the given equation. In summary, **the given equation assumes all (a – d), thus the correct answer is (e).**

3) What is the quantity, $\sum_{\vec{p}'} S(\vec{p}' \to \vec{p}) f(\vec{p}') \left[1 - f(\vec{p})\right]$?

a) The collision integral.
b) The in-scattering rate to state $\vec{p}$.
c) The out-scattering rate from state $\vec{p}$.
d) The relaxation time approximation.
e) The collision operator.

Figure 3 shows that the given quantity is **the in-scattering rate from a state p' to a state p**, as indicated by the direction of the arrow in the scattering potential *S*. Note that the $f(p')$ and $1 - f(p)$ respectively represent the probabilities that the initial state p' is occupied and that the final state p is empty, which is a natural condition that the transition occurs. Thus, **the correct answer is (b).**

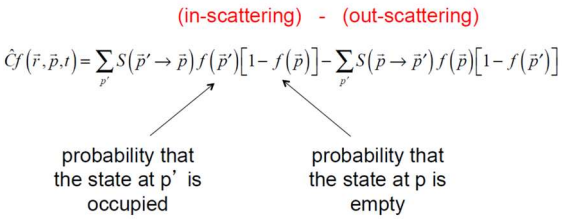


Figure 3. In-scattering and out-scattering terms.

4) What is the quantity, $-\left(\frac{f(\vec{p}) - f_S(\vec{p})}{\tau_m}\right)$?

a) The collision operator.
b) The collision operator in the relaxation time approximation.
c) The solution to the steady-state Boltzmann equation.
d) The in-scattering term of the collision operator.
e) The out-scattering terms of the collision operator.

It is the collision operator, but in the relaxation time approximation (RTA), thus the correct answer is (b). It approximates the collision integral $\hat{C}f = \partial f/\partial t|_{coll}$ as a linear term governed by a momentum relaxation time τ_m, i.e., $\partial f/\partial t|_{coll} \approx -(f - f_S)/\tau_m$. Its underlying mechanism is based on the assumption that the perturbations from equilibrium decay exponentially with the relaxation time.

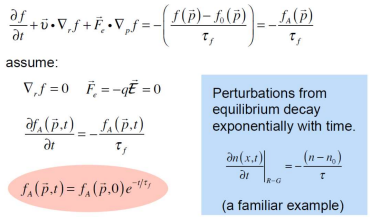


Figure 4. RTA of collision operators.

5) In the solution to the steady-state Boltzmann equation, $\delta f = \tau_m \left(-\partial f_S/\partial E\right) \vec{v} \cdot \vec{E}$, what is the term $\left(-\partial f_S/\partial E\right)$ called?

a) The electrochemical potential.
b) The chemical potential.
c) The Fermi window.
d) The generalized force.
e) The electric field.

It is called the Fermi window, as shown in Figure 5, thus the correct answer is (c). As the name suggests, an electron can transport through the Fermi window, but it can only do so when this window is open, i.e., $-\partial f_S/\partial E > 0$.

The term "Fermi window" becomes clearer in the context of the Landauer approach, as it actually refers to the difference between the Fermi-Dirac distributions of the source and drain contacts, i.e., $f_1 - f_2 = -\partial f_1/\partial E$, under a small bias condition.

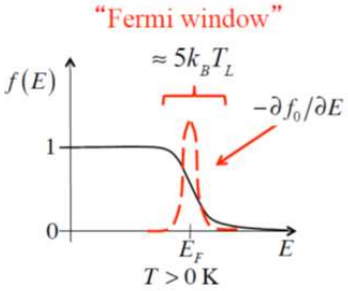


Figure 5. Fermi window.

6) In this equation, $\hat{C}f = -\left(\frac{f(\vec{p}) - f_S(\vec{p})}{\tau_m}\right)$, what is $f_S(\vec{p})$?

a) The distribution function.
b) The equilibrium distribution function.
c) A distribution function with the shape of the equilibrium distribution function.
d) The Bose-Einstein distribution.
e) The anti-symmetric part of the distribution function.

The distribution function f can be written as the summation of its symmetric and anti-symmetric part, i.e., $f = f_S + f_A$, as shown in Figure 6. For the equilibrium case, $f = f_S = f_0$. However, for the near-equilibrium case, $f = f_S + f_A \approx f_0 + f_A$, i.e., the symmetric part f_S is almost similar to f_0. Note that, in this case, f_S is not an equilibrium distribution itself; it is a symmetric part of the near-equilibrium one. However, its shape is almost similar to the equilibrium distribution function.

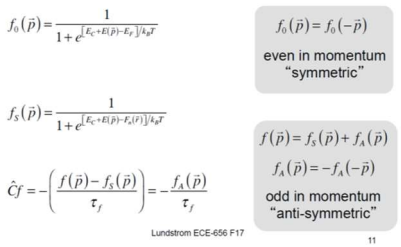


Figure 6. The symmetric and anti-symmetric components of distribution functions.

As a result, the collision operator acting on the non-equilibrium f is rewritten as $\hat{C}f = \partial f/\partial t|_{coll} = \partial f_S/\partial t|_{coll} + \partial f_A/\partial t|_{coll}$, and since $\partial f_S/\partial t|_{coll} \approx \partial f_0/\partial t|_{coll} = 0$, $\partial f/\partial t|_{coll} \approx \partial f_A/\partial t|_{coll} \approx -f_A/\tau_m \Longrightarrow \hat{C}f = \partial f/\partial t|_{coll} \approx -(f - f_S)/\tau_m$. **As mentioned previously, f_S is not an equilibrium distribution, but the symmetric part whose shape is almost identical with the equilibrium distribution function. Thus, the correct answer is (c)**.

7) For spherical bands, how is the near-equilibrium average scattering time, $\langle\langle \tau_m \rangle\rangle$ defined?

a) $\langle v_x^2 \tau_m \rangle / \langle v_x^2 \rangle$.
b) $\langle v^2 \tau_m \rangle / \langle v^2 \rangle$.
c) $\langle (E - E_C)\tau_m \rangle / \langle (E - E_C) \rangle$.
d) All of the above.
e) None of the above.

Basically, the near-equilibrium average scattering time is defined as an energy average of the energy-dependent momentum relaxation time, $\langle\langle \tau_m \rangle\rangle = \frac{\langle E\tau_m \rangle}{\langle E \rangle}$ so **(c) is the most fundamental definition**. However, for the spherical band case, $E = \frac{\hbar^2}{2m^*}\mathbf{k}^2, \mathbf{v} = \frac{1}{\hbar}\nabla_{\mathbf{k}} E = \frac{\hbar}{m^*}\mathbf{k} \Longrightarrow E = \frac{1}{2}m^*\mathbf{v}^2 = \frac{1}{2}m^*(v_x^2 + v_y^2 + v_z^2) = \frac{1}{2}m^*(3v_x^2) \Longrightarrow \mathbf{v}^2 = \frac{2E}{m^*}$, $v_x^2 = \frac{2E}{3m^*}$ holds. Therefore, $\langle\langle \tau_m \rangle\rangle = \frac{\langle E\tau_m \rangle}{\langle E \rangle} = \frac{2\langle E\tau_m \rangle/m^*}{2\langle E \rangle/m^*} = \frac{\langle 2E\tau_m/m^* \rangle}{\langle 2E/m^* \rangle} = \frac{\langle \mathbf{v}^2\tau_m \rangle}{\langle \mathbf{v}^2 \rangle}$, i.e., **(b) = (c)**, and similarly $\langle\langle \tau_m \rangle\rangle = \frac{\langle E\tau_m \rangle}{\langle E \rangle} = \frac{2\langle E\tau_m \rangle/3m^*}{2\langle E \rangle/3m^*} = \frac{\langle 2E\tau_m/3m^* \rangle}{\langle 2E/3m^* \rangle} = \frac{\langle v_x^2\tau_m \rangle}{\langle v_x^2 \rangle}$, i.e., **(a) = (c)**, for the spherical band. Therefore, t**he correct answer is (d).**

8) What is $\frac{1}{\mu_{tot}} = \frac{1}{\mu_1} + \frac{1}{\mu_2}$ called?

a) The Thompson relation.
b) The Kelvin relation.
c) The Wiedemann-Franz law.
d) The Lorenz number.
e) Mathiessen's rule.

It is Matthiessen's rule, an empirical rule that used to describe how different scattering mechanisms contribute to the total mobility of charge carriers. **Thus, the correct answer is (e).**

1) We have discussed $M(E)$ for a 3D semiconductor with parabolic energy bands. Answer the following two questions about a 3D semiconductor with non-parabolic energy bands.

a) Assume that the non-parabolicity can be described by $E(1+\alpha E)=\frac{\hbar^2 k^2}{2m^*(0)}$.

Derive an expression for the corresponding $M(E)$.

Without loss of generality, $E_C = 0$ will be assumed. From the lecture note, one can find that the (area-normalized) number of modes for 3D semiconductors is

$$M(E) = \frac{h}{4}\langle v_x^+(E)\rangle D_{3D}(E) = \frac{hv(E)}{8} D_{3D}(E)\,. \tag{1}$$

Note that the (volume-normalized) DOS for 3D is

$$D_{3D}(E)dE = g_s g_v \frac{1}{8\pi^3} 4\pi k^2 dk^2 = g_s g_v \frac{1}{2\pi^2} k^2 dk^2 = \frac{g_v}{\pi^2} k^2 dk, \tag{2}$$

for the spin degeneracy $g_s = 2$ and valley degeneracy g_v. The non-parabolic band structure gives

$$k^2 = \frac{2m^*(0)}{\hbar^2} E(1+\alpha E),\;\; k = \frac{\sqrt{2m^*(0)E(1+\alpha E)}}{\hbar}, \tag{3}$$

and similarly,

$$\frac{dE}{dk}(1+2\alpha E) = \frac{\hbar^2 k}{m^*(0)},\;\; kdk = \frac{m^*(0)}{\hbar^2}(1+2\alpha E)dE. \tag{4}$$

By putting (3) and (4) into (2), one can get

$$D_{3D}(E)dE = \frac{g_v}{\pi^2} k^2 dk^2 = \frac{g_v m^*(0)}{\pi^2\hbar^3}\sqrt{2m^*(0)E(1+\alpha E)}(1+2\alpha E)dE. \tag{5}$$

Again, from (4), $v(E)$ can be computed as

$$v = \frac{1}{\hbar}\frac{dE}{dk} = \frac{\hbar k}{m^*(0)(1+2\alpha E)} = \frac{\sqrt{2m^*(0)E(1+\alpha E)}}{m^*(0)(1+2\alpha E)}. \tag{6}$$

Finally, by putting (5) and (6) into (1), $M(E)$ is equal to:

$$M(E) = \frac{hv(E)}{8} D_{3D}(E) = \frac{2\pi\hbar}{8}\frac{\sqrt{2m^*(0)E(1+\alpha E)}}{\cancel{m^*(0)(1+2\alpha E)}}\frac{g_v \cancel{m^*(0)}}{\pi^2\hbar^3}\sqrt{2m^*(0)E(1+\alpha E)}\cancel{(1+2\alpha E)}\,. \tag{7}$$

Rearranging (7) gives

$$M(E) = \frac{2\pi\hbar}{8}\frac{g_v}{\pi^2\hbar^3} 2m^*(0)E(1+\alpha E) = \frac{g_v m^*(0)}{2\pi\hbar^2} E(1+\alpha E)\,. \tag{8}$$

If one considers the conduction band minimum is E_C rather than 0, than (8) is expressed as

$$\boxed{M(E) = \frac{g_v m^*(0)}{2\pi\hbar^2}(E-E_C)\big(1+\alpha(E-E_C)\big)}. \tag{9}$$

b) Using the following numbers for GaAs,
$m^*(0) = 0.067\, m_0$
$\alpha = 0.64$,
plot $M(E)$ from the bottom of the Γ valley to $E = 0.3$ eV comparing results from the non-parabolic expression derived in part a) to the parabolic expression.

The code and plot are as follows. $E_C = 0$ and $g_v = 1$ is assumed.

generate_nonparbolic_modes.py

```python
import numpy as np
import matplotlib.pyplot as plt


m_e = 9.109e-31
hbar = 1.054e-34
q = 1.602e-19

def compute_number_of_modes(m_star, alpha, E_min=0, E_max=0.3, non_parabolic=False):  2 usages
    m = m_star * m_e

    E = np.linspace(E_min, E_max,  num: 100)

    if non_parabolic:
        return E, (m / (2 * np.pi * hbar ** 2)) * (q * (E - E_min)) * (1 + (alpha / q) * (q * (E - E_min)))
    else:
        return E, (m / (2 * np.pi * hbar ** 2)) * (q * (E - E_min))

if __name__ == '__main__':
    E, M_para = compute_number_of_modes(m_star=0.067, alpha=0.64, non_parabolic=False)
    E, M_nonpara = compute_number_of_modes(m_star=0.067, alpha=0.64, non_parabolic=True)

    plt.plot( *args: E, M_para, c='k', lw=2.0, label='alpha = 0.0 [1/eV]')
    plt.plot( *args: E, M_nonpara, c='r', lw=2.0, label='alpha = 0.5 [1/eV]')
    plt.xlabel('Energy E [eV]')
    plt.ylabel('Number of modes M [$m^{-2}$]')
    plt.grid()
    plt.legend()
    plt.show()
```

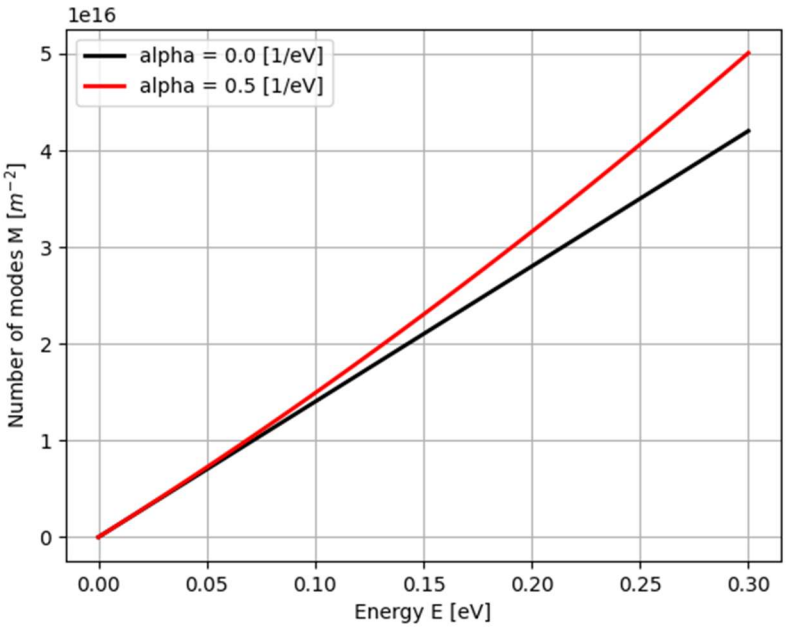
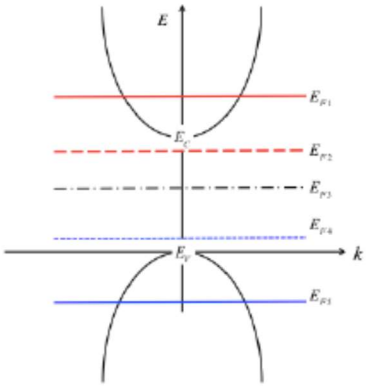


Figure 7. Used code and computation results.

2) **The figure below shows a semiconductor with the Fermi level located in five different locations. If we use the Landauer expression to compute the current:**

$$I=(2q/h)\int_{E_1}^{E_2} T(E)M(E)(f_1-f_2)dE$$

what are appropriate limits of integration, E_1 and E_2, for each case? You may assume room temperature and a bandgap of 1 eV and that $E_{F1} \approx E_{F2} \approx E_F$.



I assume that E_{F1} and E_{F2} in the paragraph refer to the Fermi levels of contract 1 (f_1) and contact 2 (f_2), respectively, while in the figure E_{F1} and E_{F2} simply represent different (channel) Fermi levels E_F. To avoid any ambiguity, I will denote the Fermi levels of contacts (E_{F1} and E_{F2} in the paragraph) as $E_{F1} = E_{FS}$ and $E_{F2} = E_{FD}$, respectively.

Also, I assume that all quantum mechanical transport phenomena such as tunneling can be ignored, and trap states within the band gap are also neglected. That is, it is assumed that $M(E)$ exists only above E_C or below E_V, and does not exist within the band gap.

Because $E_{F1} \approx E_{F2} \approx E_F$, the small voltage approximation can be applied:

$$I \propto \int_{E_1}^{E_2} T(E)M(E)(f_1 - f_2)dE \approx \int_{E_1}^{E_2} T(E)M(E)\left(-\frac{\partial f_1}{\partial E}\right)(qV)dE. \quad (10)$$

The Fermi window $\left(-\frac{\partial f_1}{\partial E}\right)$ typically has a width of $5k_BT$, as shown in Figure 5. Therefore, when estimating an appropriate integration range, the Fermi window function can be approximated as a symmetric rectangular filter with a width of $5k_BT = 0.13\text{eV}$ (at 300 K).

(1) Case $E_F = E_{F1} \gg E_C$

Assume that $E_F = E_{F1}$ is sufficiently higher than E_C (by at least $E_F - E_C > 2.5k_BT$). Then, within the $5k_BT$ range centered around $E_F = E_{F1}$, $M(E)$ is always greater than zero (since the DOS always exists). Therefore, the integration should be performed over the range $\boldsymbol{E_1 = E_F - 2.5k_BT}$ **and** $\boldsymbol{E_2 = E_F + 2.5k_BT}$. Please refer Figure 7 (a) for a graphical representation.

(2) Case $E_F = E_{F2} \leq E_C$

Assume that $E_F = E_{F2}$ is lower than E_C but only slightly (i.e., $E_C - E_F < 2.5k_BT$). In this case, the upper bound of the integral is determined by $E_2 = E_F + 2.5k_BT$, while the lower bound is determined by $E_1 = E_C$, because $M(E) = 0$ below E_C (i.e., DOS = 0 within the band gap). Therefore, the integration should be performed over the range $\boldsymbol{E_1 = E_C}$ **and** $\boldsymbol{E_2 = E_F + 2.5k_BT}$. Please refer Figure 7 (b) for a graphical representation.

(3) Case $E_F = E_{F3} = E_i$

In this case, current will not flow, because there is no available mode $M(E)$ that can be occupied. Therefore, **defining the range of integration becomes meaningless**. Please refer Figure 7 (c) for a graphical representation.

(4) Case $E_F = E_{F4} \geq E_V$

This is exactly the same case with (2), except that the sign should be changed because one must consider the p-type transport. Therefore, the integration should be performed over the range $E_2 = E_V$ **and** $E_1 = E_F - 2.5k_BT$. Please refer Figure 7 (d) for a graphical representation.

(5) Case $E_F = E_{F5} \ll E_V$

This is exactly the same case with (1), except that the sign should be changed because one must consider the p-type transport. Therefore, the integration should be performed over the range $E_2 = E_F + 2.5k_BT$ **and** $E_1 = E_F - 2.5k_BT$. Please refer Figure 7 (e) for a graphical representation.

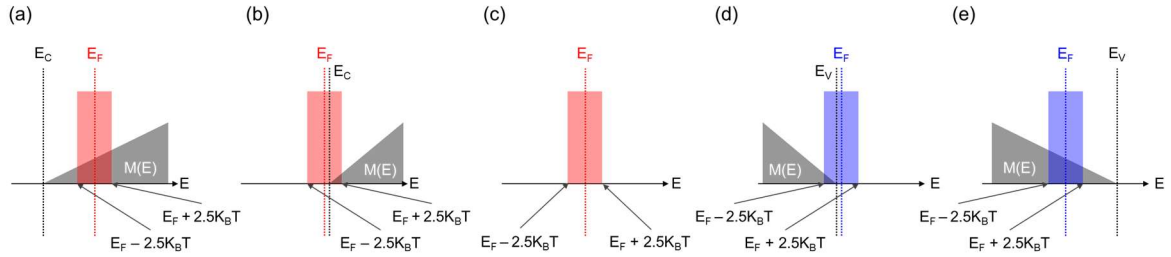


Figure 8. Graphical representation of each situation. Only the region where the Fermi window (red or blue area) overlaps with $M(E)$ (gray triangle) can be meaningful.

References (other than the course material)

[1] M. Lundstrom, *Fundamentals of Carrier Transport*, 2nd ed. Cambridge, U.K.: Cambridge Univ. Press, 2000.