

Exercise 11.1 Relaxation time approximation

- a) The transition rates are computed by use of Fermi's golden rule, relating the probability for a process to occur to the quantum mechanical matrix elements of scattering off a single impurity a weighting with the impurity density (cf. section 6.3 of the lecture notes)

$$W(\mathbf{k}, \mathbf{k}') = \frac{2\pi n_{\text{imp}}}{\hbar} |\langle \mathbf{k}' | \hat{V}_{\text{imp}} | \mathbf{k} \rangle|^2 \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) \quad (1)$$

The matrix elements¹ $\langle \mathbf{k}' | \hat{V} | \mathbf{k} \rangle = V(\mathbf{k} - \mathbf{k}')$ are given by the Fourier transform of the potential $V(\mathbf{r}) \sim \delta(\mathbf{r})$

$$\begin{aligned} V(\mathbf{k} - \mathbf{k}') &= \frac{1}{2\pi} \int d^2r e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}} V_0 \delta(\mathbf{r}) \\ &= \frac{1}{2\pi} V_0. \end{aligned} \quad (2)$$

Thus, the transition rates are given as

$$W(\mathbf{k}, \mathbf{k}') = \underbrace{\frac{n_{\text{imp}}}{2\pi\hbar} V_0^2}_{W_0} \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}), \quad (3)$$

and given the isotropy of the energy $\varepsilon_{\mathbf{k}} \sim k^2$ they do not depend on \mathbf{k} or \mathbf{k}' as long as the energy is conserved.

- b) In the static limit, the left hand side of the Boltzmann equation

$$\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} + \nabla_{\mathbf{r}} f(\mathbf{r}, \mathbf{k}, t) \cdot \frac{d\mathbf{r}}{dt} + \nabla_{\mathbf{k}} f(\mathbf{r}, \mathbf{k}, t) \cdot (e\mathbf{E}/\hbar) \quad (4)$$

reduces with $f(\mathbf{r}, \mathbf{k}, t) = f(\mathbf{k})$ to the third term proportional to the driving external field. We restrict our considerations to linear order in \mathbf{E} since we are interested in linear response to the driving force. In consequence, we must replace $\nabla_{\mathbf{k}} f$ with $\nabla_{\mathbf{k}} f_0$ because δf is already of order $\mathcal{O}(\mathbf{E})$.

This term represents the so-called drift term. The right hand side of the Boltzmann equation is the collision integral, which for impurity scattering acquires the form (cf. Eq. (6.23) in the lecture notes)

$$\begin{aligned} \left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_{\text{coll}} &= - \int \frac{d^2k'}{(2\pi)^2} W(\mathbf{k}, \mathbf{k}') (f(\mathbf{k}) - f(\mathbf{k}')) \\ &= - \int \frac{d^2k'}{(2\pi)^2} W_0 \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'} (f_0(\mathbf{k}) + \delta f(\mathbf{k}) - f_0(\mathbf{k}') - \delta f(\mathbf{k}')) \\ &= - \int \frac{d\theta' dk' k'}{(2\pi)^2} W_0 \frac{m}{\hbar^2 k} \delta(k - k') (f_0(\mathbf{k}) + \delta f(\mathbf{k}) - f_0(\mathbf{k}') - \delta f(\mathbf{k}')) \\ &= - \frac{m}{\hbar^2} \int \frac{d\theta'}{(2\pi)^2} W_0 [\delta f(k, \theta) - \delta f(k, \theta')]. \end{aligned} \quad (5)$$

¹Note that the potential only depends on the difference between \mathbf{k} and \mathbf{k}' due to the homogeneity of the system.

The LHS can be written as

$$\nabla_{\mathbf{k}} f_0 \cdot (e\mathbf{E}/\hbar) = \frac{\hbar e}{m} \mathbf{E} \cdot \mathbf{k} \frac{\partial f_0}{\partial \epsilon_k} = \frac{\hbar e E k}{m} \frac{\partial f_0}{\partial \epsilon_k} \cos \theta, \quad (6)$$

where θ is the angle between the \mathbf{k} and the electric field, which points into the x -axis.

Taking (6) and (5) together we arrive at

$$\frac{\hbar e E k}{m} \frac{\partial f_0}{\partial \epsilon_k} f_0 \cos \theta = - \int d\theta' \tilde{W}_0 [\delta f(k, \theta) - \delta f(k, \theta')], \quad (7)$$

where $\tilde{W}_0 = mW_0/(2\pi\hbar)^2$. This equation can be considered for every k independently.

- c) As the left hand and right hand side of Eq. (7) for every fixed k depend only on θ which is 2π -periodic, we expand both sides in terms of Fourier modes as given in the exercise sheet.

We start with the Boltzmann equation,

$$\sum_l d_l e^{il\theta} = - \int d\theta' \tilde{W}_0 \left(\sum_l f_l e^{il\theta} - \sum_l f_l e^{il\theta'} \right), \quad (8)$$

which we project onto the m -th Fourier mode with multiplication of both sides with $\exp(-im\theta)$ and integration over θ

$$\int d\theta e^{-im\theta} \sum_l d_l e^{il\theta} = - \int d\theta e^{-im\theta} \int d\theta' \tilde{W}_0 \left(\sum_l f_l e^{il\theta} - \sum_l f_l e^{il\theta'} \right). \quad (9)$$

This equation can be easily evaluated by using the relation

$$\int d\theta e^{in\theta} = 2\pi \delta_{n,0}, \quad (10)$$

and leaves us with

$$\begin{aligned} 2\pi d_m &= -\tilde{W}_0 \sum_l \int d\theta d\theta' \left(e^{-im\theta} e^{il\theta} - e^{-im\theta} e^{il\theta'} \right) f_l \\ &= -(2\pi)^2 \tilde{W}_0 \sum_l (\delta_{m,l} - \delta_{m,0} \delta_{l,0}) f_l. \end{aligned} \quad (11)$$

With the expression (11) we have reduced the problem of finding a solution to the Boltzmann equation to solving a system of linear equations. In general, the system of equations is infinitely large, but often this does not prevent one from finding an exact solution. In our case, relating the equation (11) to the matrix equation on the exercise sheet, we find that the matrix L has the following diagonal form

$$L_{m,n} = -2\pi \tilde{W}_0 \begin{pmatrix} \ddots & & & & & & \\ & 1 & & & & & \\ & & \ddots & & & & \\ & & & 1 & & & \\ & & & & 0 & & \\ & & & & & 1 & \\ & & & & & & \ddots \\ & & & & & & & 1 \\ & & & & & & & & \ddots \end{pmatrix}. \quad (12)$$

- d) We have reduced the problem to a simple matrix equation $d_l = L_{l,m} f_m$, where summation over dummy indices is implied. By symmetry, the matrix must be symmetric and thus diagonal. The eigenvectors of L represent the Fourier decomposition of eigenfunctions of the collision operator and the eigenvalues represent inverse relaxation times. A vanishing eigenvalue represents an infinite relaxation time, the corresponding eigenfunction defines then a conserved quantity. Any quantity that cannot be changed due to collisions will be preserved. In our case, we have only one conserved quantity left, because the energy, that can also not be changed within collisions has explicitly been projected out. This conserved quantity, which as we can see from (12), corresponds to the zeroth Fourier component. This constant shift of δf corresponds to the total particle number of the system and can of course not be changed during collisions.
- e) From the expression for $\nabla_{\mathbf{k}} f_0 \cdot (e\mathbf{E}/\hbar)$ given in Eq. 6, we can directly find its Fourier decomposition as

$$\sum_l d_l e^{il\theta} = \frac{e\hbar k E}{2m} \frac{\partial f_0}{\partial \epsilon_k} (e^{i\theta} + e^{-i\theta}) \Rightarrow d_l = \begin{cases} \frac{e\hbar k E}{2m} \frac{\partial f_0}{\partial \epsilon_k}, & l = \pm 1 \\ 0, & \text{else} \end{cases}. \quad (13)$$

Because the matrix L is diagonal, it is trivial to find a solution to the Boltzmann equation,

$$f_l = \begin{cases} -\frac{e\hbar k E}{2m} \frac{1}{2\pi\tilde{W}_0} \frac{\partial f_0}{\partial \epsilon_k}, & l = \pm 1 \\ 0, & \text{else} \end{cases}. \quad (14)$$

Comparing our result to the single relaxation time approximation, we have for the collision integral

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = -(2\pi\tilde{W}_0)\delta f = -(2\pi\tilde{W}_0)(f - f_0), \quad (15)$$

which we can directly relate to the single relaxation time approximation, Eq. (1) on the exercise sheet by identifying the relaxation time τ with the value $1/(2\pi\tilde{W}_0)$.

Exercise 11.2 Reflectivity of Simple Metals and Semiconductors

Using the relation between conductivity and dielectric function we obtain

$$\epsilon(\omega) = \epsilon_\infty + \frac{i}{\omega\epsilon_0} \sigma(\omega) = \epsilon_\infty - \frac{\omega_p^2 \tau^2}{1 + \omega^2 \tau^2} + i \frac{\omega_p^2 \tau / \omega}{1 + \omega^2 \tau^2}. \quad (16)$$

Parametrizing the complex index of refraction by

$$N(\omega) = \sqrt{\epsilon(\omega)} = n(\omega) + ik(\omega), \quad (17)$$

we find with the abbreviations

$$\begin{aligned} \epsilon_r(\omega) &= \epsilon_\infty - \frac{\omega_p^2 \tau^2}{1 + \omega^2 \tau^2} \\ \epsilon_i(\omega) &= \frac{\omega_p^2 \tau / \omega}{1 + \omega^2 \tau^2} \end{aligned}$$

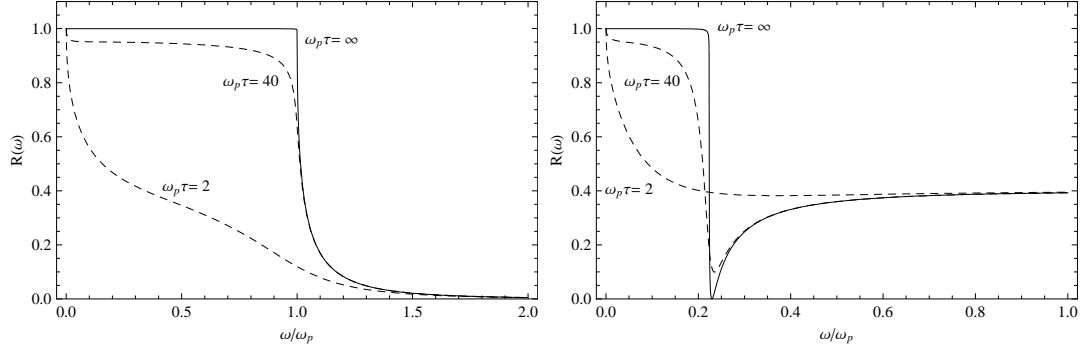


Figure 1: Frequency dependence of the reflectivity. Left: $\epsilon_\infty = 1$, Right: $\epsilon_\infty = 20$.

that

$$n(\omega) = \frac{1}{\sqrt{2}} \sqrt{\epsilon_r(\omega) + \sqrt{\epsilon_r^2(\omega) + \epsilon_i^2(\omega)}}$$

$$k(\omega) = \frac{1}{\sqrt{2}} \sqrt{-\epsilon_r(\omega) + \sqrt{\epsilon_r^2(\omega) + \epsilon_i^2(\omega)}}.$$

The reflectivity is then given by the standard formula

$$R(\omega) = \frac{(n(\omega) - 1)^2 + k^2(\omega)}{(n(\omega) + 1)^2 + k^2(\omega)}. \quad (18)$$

Plots of the reflectivity for different values of ϵ_∞ and $\tau\omega_p$ are shown in fig. 1.

The reason why ϵ_∞ is usually larger in semiconductors than in metals relates to the different electron densities in these two classes of materials: In the formulae above, everything is measured in terms of $\omega_p \propto \sqrt{n_c}$, where n_c is the density of charge carriers. For metals, $n_c \sim 10^{22} \text{cm}^{-3}$, whereas for doped semiconductors, $n_c \sim 10^{13} - 10^{18} \text{cm}^{-3}$. Correspondingly, $\hbar\omega_p \sim 10 \text{eV}$ for metals and $\hbar\omega_p \lesssim 100 \text{meV}$ for heavily doped semiconductors. The simple solution to why ϵ_∞ is higher in semiconductors is that the 'value of ∞ ' depends on the energy range one is interested in, so that also ϵ_∞ varies, as it incorporates the response of all excitations with energies higher than the energy range under investigation. For higher frequency cutoff there is a smaller number of excitations above this cutoff, so that ϵ_∞ decreases with increasing ω_p (as $\omega_{\text{cutoff}} \sim \omega_p$) and ultimately drops to unity for very large cutoff.