

Problem 10.1 Reflectivity of semiconductors

One can calculate the reflectivity of the material using the real(ϵ_r) and imaginary(ϵ_i) parts of the dielectric function. To this end, one defines the complex index of refraction as

$$N(\omega) = \sqrt{\epsilon(\omega)} = \frac{\kappa_1(\omega)}{k} + \frac{i\lambda(\omega)}{k}, \quad (1)$$

where $k = \omega/c$. Expressing λ and κ in terms of the real and the imaginary parts of the dielectric function, we have

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

$$\frac{\lambda(\omega)}{k} = \frac{1}{\sqrt{2}} \sqrt{-\epsilon_r(\omega) + \sqrt{\epsilon_r^2(\omega) + \epsilon_i^2(\omega)}}. \quad (3)$$

The reflectivity is given by the standard formula

$$R(\omega) = \frac{(\kappa(\omega) - k)^2 + \lambda^2(\omega)}{(\kappa(\omega) + k)^2 + \lambda^2(\omega)}. \quad (4)$$

Moreover, since the conductivity and the dielectric function are related as (Lecture 18)

$$\epsilon(\omega) = 1 + \frac{4\pi i\sigma(\omega)}{\omega}. \quad (5)$$

one can calculate reflectivity using conductivity. In this exercise, we calculate conductivity using classical equations of motion of a single charged particle in the presence of a time-dependent electric field and harmonic confinement potential.

The force acting on a particle in a semiconductor is now given by

$$\mathbf{F}(t) = q\mathbf{E}(t) - \frac{\mathbf{p}(t)}{\tau} - m\omega_0^2\mathbf{r}(t) \quad (6)$$

leading to the equation of motion

$$m\ddot{\mathbf{r}}(t) = q\mathbf{E}(t) - \frac{m\dot{\mathbf{r}}(t)}{\tau} - m\omega_0^2\mathbf{r}(t), \quad (7)$$

or in Fourier space

$$-m\omega^2\mathbf{r}(\omega) = q\mathbf{E}_0 + \frac{i\omega m}{\tau}\mathbf{r}(\omega) - m\omega_0^2\mathbf{r}(\omega). \quad (8)$$

Solving for $\mathbf{r}(\omega)$ leads to

$$\mathbf{r}(\omega) = \frac{q}{m(\omega_0^2 - \omega^2 - i\omega/\tau)}\mathbf{E}_0. \quad (9)$$

Using $\mathbf{v}(\omega) = -i\omega\mathbf{r}(\omega)$ and $\mathbf{j} = nq\mathbf{v}$, we obtain the conductivity

$$\sigma(\omega) = \frac{nq^2\tau}{m} \frac{1}{1 - i\omega\tau(1 - (\omega_0/\omega)^2)} = \frac{\omega_p^2}{4\pi} \frac{\tau}{1 - i\omega\tau(1 - (\omega_0/\omega)^2)}. \quad (10)$$

For the reflectivity we still keep the parameter ϵ_∞ to describe the inner shells of the semiconductor. The real and imaginary parts of the dielectric function are given by

$$\epsilon_r = \epsilon_\infty - \frac{\omega_p^2 \tau^2 (1 - (\omega_0/\omega)^2)}{1 + [\omega\tau(1 - (\omega_0/\omega)^2)]^2}, \quad (11a)$$

$$\epsilon_i = \frac{\omega_p^2 \tau / \omega}{1 + [\omega\tau(1 - (\omega_0/\omega)^2)]^2}. \quad (11b)$$

The results are shown in Fig. 1. We note that the region of strong reflectivity shifts from around $\omega = 0$ to a narrow range around the frequency of the harmonic potential, ω_0 . This effect can only be observed for sufficiently clean systems, where $\tau\omega_p \gg 1$. If we now considered multiple harmonic potentials for the different orbitals, this would lead to multiple such resonance lines that could be observed in the reflectivity.

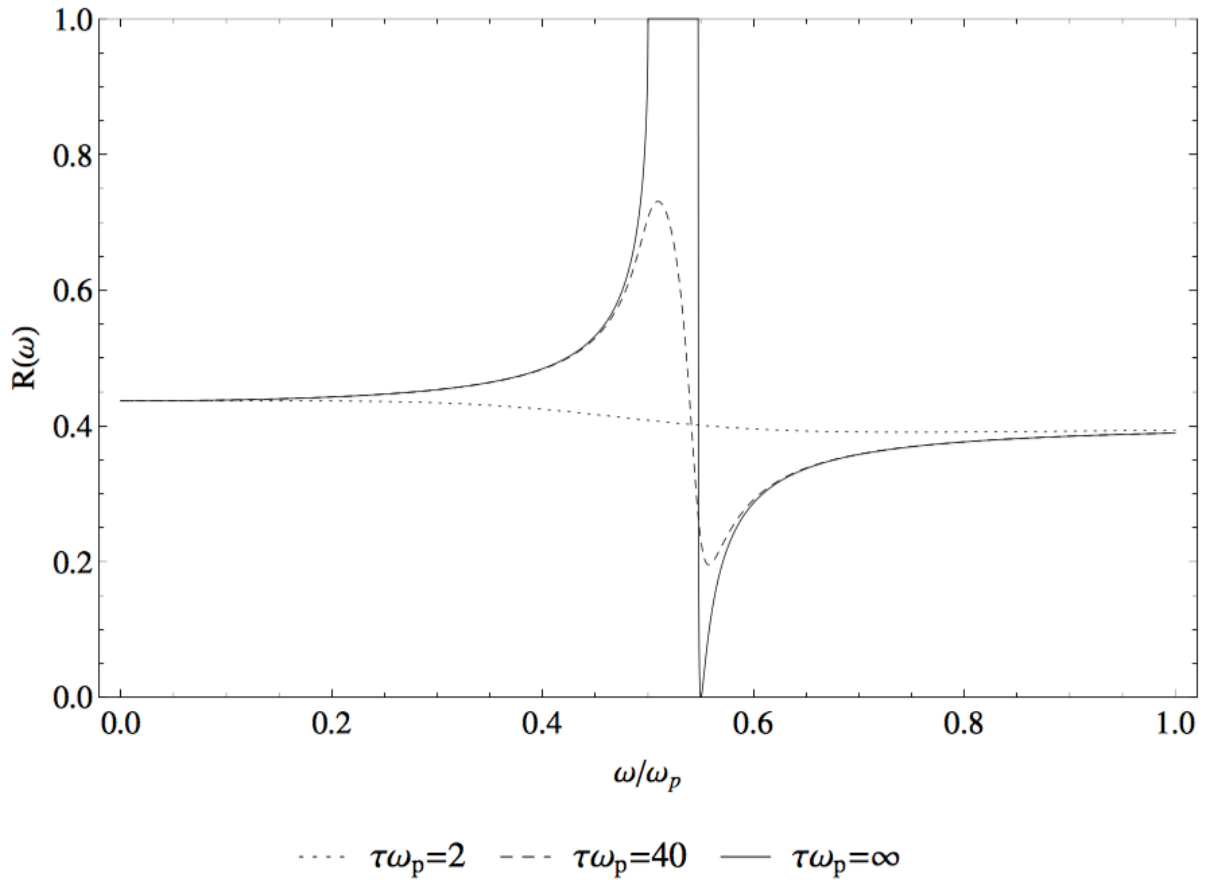


Figure 1: Frequency dependence of the reflectivity for a semiconductor with $\epsilon_\infty = 20$ and $\omega_0 = \frac{1}{2}\omega_p$.

Problem 10.2 Frequency dependence of conductivity

To calculate the frequency dependence of conductivity in a spatially homogeneous system (i.e., $\frac{\partial f}{\partial \mathbf{r}} = 0$), we use the Boltzmann transport in relaxation-time approximation,

$$-i\omega\delta f(\mathbf{k}, \omega) - \frac{e\mathbf{E}(\omega)}{\hbar} \nabla_{\mathbf{k}} f_0(\mathbf{k}) = -\frac{\delta f(\mathbf{k}, \omega)}{\tau(\epsilon_{\mathbf{k}})}, \quad (12)$$

where $f(\mathbf{k}, \mathbf{r}, t) = f_0(\mathbf{k}, \mathbf{r}, t) + \delta f(\mathbf{k}, \mathbf{r}, t)$, and

$$f(\mathbf{k}, t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\mathbf{k}, \omega) e^{-i\omega t} \quad \text{and} \quad E(\mathbf{k}, t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathbf{E}(\mathbf{k}, \omega) e^{-i\omega t}. \quad (13)$$

Solving Eq. 12 for $\delta f(\mathbf{k}, \omega)$, we obtain ¹

$$\delta f(\mathbf{k}, \omega) = \frac{\tau}{(1 - i\omega\tau)} e^{(\mathbf{E}(\omega) \cdot \mathbf{v}_{\mathbf{k}})} \frac{\partial f_0}{\partial \epsilon}, \quad (14)$$

which is the same equation as the one derived for $\delta f(\mathbf{k}, 0)$ in Lecture 19, up to a substitution

$$\frac{1}{\tau} \rightarrow \frac{1}{\tau} - i\omega.$$

Therefore, the conductivity for the isotropic Fermi surface is given by

$$\sigma = \frac{e^2}{3} N(\epsilon_F) |\mathbf{v}_F|^2 \frac{\tau}{1 - i\omega\tau}. \quad (15)$$

Problem 10.3 Umklapp processes

The appearance of resistance due to electron-electron scattering is not quite obvious. The reason is that while the slowing down of electrons due to resistance implies a change in the total momentum of electrons, Coulomb interaction preserves total momentum in a translationally invariant system.

However, in a crystal the continuous translational symmetry is reduced to that of discrete lattice translations. As a result, the quasi-momentum is conserved only up to $\hbar\mathbf{K}$, where \mathbf{K} is a reciprocal lattice vector

$$\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4 = \mathbf{K}. \quad (16)$$

Above k_1, k_2 and k_3, k_4 are the momenta of the initial and the final electrons, respectively. Therefore, in an Umklapp process the initial and final pair of electrons live in different Brillouin zones.

Supposing that the magnitude of the initial momentum k_1 is close the Fermi surface, energy conservation implies that the remaining momenta should also live close to the Fermi surface. Thus, the condition for the Umklapp processes becomes

$$\max(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) = 4 \max |\mathbf{k}_F(\mathbf{n})| > |\mathbf{K}_{\min}|, \quad (17)$$

where \mathbf{K}_{\min} is the shortest reciprocal lattice vector, and \mathbf{n} are possible directions of \mathbf{k}_F . Obviously, for materials where the Fermi surface extends to the edge of the Brillouin zone, the above condition is satisfied.

In fact, even in alkali metals where the Fermi surface never extends to the edge of the Brillouin zone the condition for Umklapp processes is satisfied. Since alkali metals have only a single electron in their valence band, the Fermi surface has half the volume of the first Brillouin zone. Moreover, all alkali metals crystallize in the bcc lattice. We denote the length of a side of the conventional unit cell with a and the length of the corresponding reciprocal lattice vector is $|\mathbf{K}| = \frac{2\pi}{a}$. Since the conventional unit cell includes two equivalent atoms, the volume of the primitive cell is $a^3/2$ and the volume of the Brillouin zone is $2|\mathbf{K}|^3$. Using the periodicity of the Brillouin zone ($\sqrt{2}|\mathbf{K}|$), we find that the condition for the Umklapp process is satisfied,

$$\frac{4\pi|\mathbf{k}_F|^3}{3} = \frac{2}{2}|\mathbf{K}|^3 \quad \rightarrow \quad |\mathbf{k}_F| = \left(\frac{3}{4\pi}\right)^{(1/3)} |\mathbf{K}| = 0.620|\mathbf{K}| > \frac{\sqrt{2}}{4}\mathbf{K} \quad (18)$$

¹Since we are only considering the linear response in \mathbf{E} ; and $\delta f \propto |\mathbf{E}|$ by assumption, the second term in Eq. 12, involves only $f_0(\mathbf{k})$ and not $f(\mathbf{k})$.