Dispersion Formulas of the Quantum Optics of Metals in the Many-electron Theory with Consideration of Electron Damping

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The general dispersion formulas of the quantum optics of metals with consideration of electron damping have been derived for the aggregate of interacting electrons which can be described by the general wave function.

IN reference (1) there were obtained some dispersion formulas of the quantum optics of metals based on the many-electron theory. However, they are correct in the visible and ultra-violet regions of the spectrum only when the damping of electron motion is not taken into account. It is of interest to consider the general case, which includes electron damping.

In the general case the effect of the alternating field of a light wave on the electrons in a metal can be twofold. Correspondingly the quantum optics of metals differentiates between two types of processes — acceleration, and the transition of electrons into higher energy states. In the first case the electrons can lose the acquired acceleration by virtue of their interaction with the elastic vibrations of the lattice (phonons); in the second case the electron system in general does not remain in the excited state, but "jumps back", with the phonon-lattice interaction having an influence, among other causes, on the duration of the excited state. This interaction can be taken into account by introducing a damping factor of electron motion $\Gamma_{\vec{\xi}'_1 \vec{\xi}'_2 \cdots \vec{\xi}'_N} = \Gamma'$.

In considering the interaction of the electron system with the lattice vibrations, the principle of conservation of energy and the interference condition will assume the form:

$$E(\vec{\xi}'_1, \ldots, \vec{\xi}'_N) = E(\vec{\xi}_1, \ldots, \vec{\xi}_N) \pm \hbar\omega \mp \hbar\omega_{\mathbf{q}}, \qquad (1)$$

$$\sum \mathbf{k}'_i = \sum \mathbf{k}_i + \mathbf{K} \mp \mathbf{q} + 2\pi \mathbf{g}, \qquad (2)$$

where $\mathbf{q}$ is the wave vector and $\hbar\omega_{\mathbf{q}}$ is the energy of the phonon being absorbed or emmited.

If it were possible to neglect the interaction of the electron system with the lattice vibrations, then the electron system would be in the excited state for a long time (stationary state). However, if the interaction is large, then the electron system, being in an excited state, will give up its energy to the lattice vibrations (nonstationary states). During this process the energy of lattice vibrations will grow, and with time, become uniformly distributed among all frequencies, i.e., there will finally result a rise in the lattice temperature.

The effect of the lattice vibrations on the electron system can be expressed by a decrease in the duration of electron occurence in the excited state. Mathematically this is developed by replacing the energy of the electron system in the excited state $(\vec{\xi}'_1, \ldots, \vec{\xi}'_N, s')$ by the complex quantity

$$E(\xi'_1, \xi'_2, \ldots, \xi'_N, s') \to E(\xi'_1 \xi'_2, \ldots, \xi'_N, s') - i\hbar\Gamma_{\vec{\xi}'_1, \ldots, \vec{\xi}'_N},$$

where $\Gamma_{\vec{\xi}'_1, \ldots, \vec{\xi}'_N}$ is the damping factor of electron motion. To derive dispersion formulas which take into consideration the interaction of the electron system with the lattice vibrations it is necessary, therefore, to make the aforementioned substitution; the formulas (2.6), [1] expressing the law of conservation of energy and the interference condition, are to be replaced by formulas (1) and (2) of this paper. However, in as much as the wave vectors of the photon and the phonon can be neglected in comparison with the generalized vector of the entire electronic system, the interference condition will have the same expression as in reference (1). As in the one-electron theory, the lattice quantum energy can be neglected in comparison with the energy of the entire electron system, and therefore, instead of equation (1) we shall have the previous form of the law of conservation of energy (2.6) [1]. In taking into account the above

[1] A. V. Sokolov, J. Exper. Theoret. Phys. USSR **25**, 341 (1953)

considerations, the expression for the current density (3.17) in reference (1) takes the form:

$$\mathbf{j} = \frac{e^2}{m^2 c\hbar (Ga)^{3N}} \tag{3}$$

$$\times \sum_{s,s'} \int d\vec{\xi}_1 \dots d\vec{\xi}_N [\rho_0 (\vec{\xi}_1, \dots, \vec{\xi}_N, s')$$

$$- \rho_0 (\vec{\xi}_1, \dots, \vec{\xi}_N, s)]$$

$$\times (\vec{\xi}_1, \dots, \vec{\xi}_N, s' | \sum \hat{\mathbf{p}}_i | \vec{\xi}_1, \dots, \vec{\xi}_N, s)$$

$$\times \left\{ \mathbf{B} e^{i\omega t} \frac{1 - [\exp - (\omega' + \omega - i\Gamma') t]}{\omega' - \omega - i\Gamma'} \right.$$

$$\left. + \mathbf{B}^* e^{-i\omega t} \frac{1 - \exp[- i(\omega' - \omega - i\Gamma') t]}{\omega' - \omega - i\Gamma'} \right\}$$

$$\times (\vec{\xi}_1, \dots, \vec{\xi}_N, s | \sum \hat{\mathbf{p}}_i | \xi_1, \dots, \xi_N, s')$$

$$- \frac{e^2}{mc (Ga)^{3N}} \mathbf{A} \sum_s \int \rho_0 (\vec{\xi}_1, \dots, \vec{\xi}_N, s)$$

$$\times e^{-\Gamma' t} d\vec{\xi}_1, \dots, d\vec{\xi}_N,$$

where $\omega' = \omega_{\vec{\xi}_1, \dots, \vec{\xi}_N, s; \vec{\xi}'_1, \dots, \vec{\xi}'_N, s'}$.

This expression has a simple physical meaning. Immediately after the application of the field at $t \approx 0$ this expression gives the displacement current, specified by the original distribution of the electrons among the states $\rho_0(\vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_N, s)$. Afterwards with $t > 0$, there appear two more types of terms as a result of the redistribution of electrons among the states by the action of the field: those harmonically dependent on t with the frequency ω of the external electro magnetic field and terms containing function of t with frequencies ω' and damping out with time. The first refer to the forced vibrations of the system, while the second describe its natural oscillations, set up at the starting time of field application and damped out exponentially with time. The current, determined by the initial electron distribution is also damped out with time. With strong damping, as in the case of large t one can completely neglect the natural vibrations of the system and the initial current. However, when damping is absent ($\Gamma' = 0$), or when it is weak ($\Gamma' \gtrsim 0$), the natural oscillations of the system must also be taken into account.

For the convenience of subsequent calculations, Eq. (3) may be rearranged as

$$\mathbf{j} = \mathbf{j}_1 + i\,\mathbf{j}_2, \tag{4}$$

where

$$\mathbf{j}_1 = \frac{e^2}{m^2 c\hbar (Ga)^{3N}} \sum_{s,s'} \int d\vec{\xi}_1, \dots, d\vec{\xi}_N \tag{4a}$$

$$[\rho_0 (\vec{\xi}_1, \dots, \vec{\xi}_N, s')$$

$$- \rho_0 (\vec{\xi}_1, \dots, \vec{\xi}_N, s)]$$

$$\times (\vec{\xi}_1, \dots, \vec{\xi}_N, s' | \sum \mathbf{p}_i | \vec{\xi}_1, \dots, \vec{\xi}_N, s)$$

$$\times \left\{ \mathbf{B} e^{i\omega t} \frac{1}{\omega' + \omega - i\Gamma'} + \mathbf{B}^* e^{-i\omega t} \frac{1}{\omega' - \omega - i\Gamma'} \right\}$$

$$\times (\vec{\xi}_1, \dots, \vec{\xi}_N, s | \sum \hat{\mathbf{p}}_i | \vec{\xi}_1, \dots, \vec{\xi}_N, s')$$

$$- \frac{e^2}{mc (Ga)^{3N}} \mathbf{A} \sum_s \int \rho_0 (\vec{\xi}_1, \dots, \vec{\xi}_N, s)$$

$$\times e^{-\Gamma' t} d\vec{\xi}_1, \dots, d\vec{\xi}_N,$$

$$\mathbf{j}_2 = \frac{e^2}{m^2 c\hbar (Ga)^{3N}} \sum_{s,s'} \int d\vec{\xi}_1, \dots, d\vec{\xi}_N \tag{4b}$$

$$\times [\rho_0 (\vec{\xi}_1, \dots, \vec{\xi}_N, s') - \rho_0 (\vec{\xi}_1, \dots, \xi_N, s)]$$

$$\times (\vec{\xi}_1, \dots, \vec{\xi}_N, s' | \sum \hat{\mathbf{p}}_i | \vec{\xi}_1, \dots, \vec{\xi}_N, s)$$

$$\times \left\{ \mathbf{B} e^{i\omega t} \frac{\exp[- i(\omega' + \omega - i\Gamma') t]}{- i(\omega' + \omega - i\Gamma')} \right.$$

$$\left. + \mathbf{B}^* e^{-i\omega t} \frac{\exp[- i(\omega' - \omega - i\Gamma') t]}{- i(\omega' - \omega - i\Gamma')} \right\}$$

$$\times (\vec{\xi}_1, \dots, \vec{\xi}_N, s | \sum \hat{\mathbf{p}} | \vec{\xi}_1, \dots, \vec{\xi}_N, s').$$

In (4a) the sum over s, s' is broken up into two parts, corresponding to $\rho_0(\vec{\xi}_1, \dots, \vec{\xi}_N, s')$ and $\rho_0(\vec{\xi}_1, \dots, \vec{\xi}_N, s)$ and in the first of them the summation indices $s \rightleftarrows s'$ are interchanged so that

$$\omega_{\vec{\xi}_1, \dots, \vec{\xi}_N, s; \vec{\xi}_1, \dots, \vec{\xi}_N, s'} \to - \omega_{\vec{\xi}_1, \dots, \vec{\xi}_N, s; \vec{\xi}_1, \dots, \vec{\xi}_N, s'} \tag{5}$$

and $\Gamma_{\vec{\xi}_1, \dots, \vec{\xi}'_N} \to \Gamma_{\vec{\xi}'_1, \dots, \vec{\xi}'_N}$.

Collecting again all the terms into a single sum, instead of the expression in the braces of (4a), we shall have

$$\Big\{\mathbf{B}\,e^{i\omega t}\frac{1}{-\omega'+\omega-i\Gamma'}+\mathbf{B}^*\,e^{-i\omega t}\frac{1}{-\omega'-\omega-i\Gamma'}.$$

$$-\mathbf{B}\,e^{i\omega t}\frac{1}{\omega'+\omega-i\Gamma'}-\mathbf{B}^*\,e^{-i\omega t}\frac{1}{\omega'-\omega-i\Gamma'}\Big\}.$$

Grouping in pairs the terms of this parenthesis, the first with the fourth, and the second with the third, and taking into account that

$$\mathbf{B}\,e^{i\omega t}+\mathbf{B}^*e^{-i\omega t}=\mathbf{A},$$

$$\mathbf{B}\,e^{i\omega t}-\mathbf{B}^*\,e^{-i\omega t}=(1/i\omega)\,\dot{\mathbf{A}},$$

the parenthesis in question can be represented by

$$\Big\{-\left[\frac{\omega'-\omega}{(\omega'-\omega)^2+\Gamma'^2}+\frac{\omega'+\omega}{(\omega'+\omega)^2+\Gamma'^2}\right]\mathbf{A}$$

$$+\frac{1}{\omega}\left[\frac{\Gamma'}{(\omega'-\omega)^2+\Gamma'^2}-\frac{\Gamma'}{(\omega'+\omega)^2+\Gamma'^2}\right]\dot{\mathbf{A}}\Big\}.$$

Separating (4b) into two parts, and entering $\mathbf{B}$ into one, and $\mathbf{B}^*$ into the other, the following transformation can be made:

$$\frac{\exp[-i(\omega'+\omega-i\Gamma')t]}{-i(\omega'+\omega-i\Gamma')} \tag{6}$$

$$=e^{-\Gamma' t}\,\frac{\exp[-i(\omega'+\omega)t]}{-i(\omega'+\omega)}\,\frac{1}{1+\left(\dfrac{\Gamma'}{i(\omega'+\omega)}\right)}$$

$$=e^{-\Gamma' t}\,\frac{\exp[-i(\omega'+\omega)t]}{-i(\omega'+\omega)}$$

$$\times\left(1-\frac{\Gamma'}{i(\omega'+\omega)}-\frac{\Gamma'^2}{(\omega'+\omega)^2}-\ldots\right).$$

Before making the analogous transformation for the expression

$$\exp[-i(\omega'-\omega-i\Gamma')t]\,/-i(\omega'-\omega-i\Gamma')$$

in that part of Eq. (4b) which contains $\mathbf{B}^*$, the indices $s\rightleftarrows s'$ are interchanged and, taking into account (5), we obtain

$$\frac{\exp[-i(-\omega'-\omega-i\Gamma')t]}{-i(-\omega'-\omega-i\Gamma')} \tag{7}$$

$$=e^{-\Gamma' t}\,\frac{\exp[-i(-\omega'-\omega)t]}{-i(-\omega'-\omega)}\,\frac{1}{1+[\Gamma'/i(-\omega'-\omega)]}$$

$$=e^{-\Gamma' t}\,\frac{\exp[-i(-\omega'-\omega)]\,t}{-i(-\omega'-\omega)}$$

$$\times\left(1+\frac{\Gamma'}{i(\omega'+\omega)}-\frac{\Gamma'^2}{(\omega'+\omega)^2}\ldots\right).$$

Making then a transition in the expression (4b) from the integration variables $\vec{\xi}_1\,(\xi_1\,\eta_1\zeta_1)\ldots.\ \vec{\xi}_N\,(\xi_N\,\eta_N\zeta_N)$ to variables ω', $u_1,\ldots,u_{3N-1}$ in a manner analogous to that of reference 1, and neglecting in (6) and (7) the terms in $\Gamma'/(\omega'+\omega)$, i.e., considering the damping small*, we obtain in place of (4b) the following expression:

$$\frac{\pi e^2}{m^2 c\,\hbar\,\omega\,(Ga)^{3N}}\sum_{s,s'}\int du_1,\ldots,\ du_{3N-1}\,e^{-\Gamma' t}$$

$$\times\ \frac{\rho_0(\vec{\xi}_1,\ldots,\vec{\xi}_N,\ s')-\rho_0(\vec{\xi}_1,\ldots,\vec{\xi}_N,\ s)}{\left|\operatorname{grad}_{\vec{\xi}_1,\ldots,\vec{\xi}_N}\omega'\right|}$$

$$\times\,(\vec{\xi}_1,\ldots,\vec{\xi}_N,\ s'\,|\sum\hat{\mathbf{p}}_i\,|\,\vec{\xi}_1,\ldots,\vec{\xi}_N,\ s)$$

$$\times\ (\vec{\xi}_1,\ldots,\vec{\xi}_{1N},\ s\,|\,\sum\hat{\mathbf{p}}_i\,|\,\vec{\xi}_1,\ldots,\vec{\xi}_N,\ s').$$

The final expression for the total current density in the metal will have the form:

$$\mathbf{j}=-\frac{e^2}{mc\,(Ga)^{3N}}\sum_s\int d\vec{\xi}_1,\ldots,\ d\vec{\xi}_N,\rho_0$$

$$\times\,(\vec{\xi}_1,\ldots,\ \vec{\xi}_N,\ s)\ \times\Big\{\mathbf{A}\,e^{-\Gamma' t}$$

$$+\frac{1}{m\hbar}\sum_{s'}\left(\frac{\omega'-\omega}{(\omega'-\omega)^2+\Gamma'^2}+\frac{\omega'+\omega}{(\omega'+\omega)^2+\Gamma'^2}\right)$$

$$\times\,\mathbf{D}_{\vec{\xi}_1,\ldots,\vec{\xi}_N,\ s\ \vec{\xi}_1',\ldots,\vec{\xi}_N',\ s'}\,\mathbf{A}\Big\}-\frac{e^2}{m^2\,c\hbar\,\omega\,(Ga)^{3N}}$$

$$\times\sum_{s,s'}\int d\,\vec{\xi}_1,\ldots,\ d\vec{\xi}_N,\ \ \rho_0(\vec{\xi}_1,\ldots,\vec{\xi}_N,\ s)$$

$$\times\left(\frac{\Gamma'}{(\omega'+\omega)^2+\Gamma'^2}-\frac{\Gamma'}{(\omega'-\omega)^2+\Gamma'^2}\right)$$

$$\times\mathbf{D}_{\vec{\xi}_1,\ldots,\vec{\xi}_N',\ s;\ \vec{\xi}_1',\ldots,\vec{\xi}_N',\ s}\ \dot{\mathbf{A}}\ +\frac{\pi e^2}{m^2 c\hbar\omega(Ga)^{3N}}$$

$$\times\ \sum_{s,s'}\int du_1\ldots\ du_{3N-1}\,e^{-\Gamma' t}$$

$$\times\,\frac{\rho_0(\xi_1,\ldots,\ \xi_N,\ s')-\rho_0(\xi_1,\ldots,\ \xi_N,\ s)}{\operatorname{grad}_{\vec{\xi}_1,\ldots,\vec{\xi}_N}\omega'}$$

$$\times\,\mathbf{D}_{\vec{\xi}_1,\ldots,\vec{\xi}_N,\ s\ \vec{\xi}_1',\ldots,\vec{\xi}_N',\ s}\,\dot{\mathbf{A}}.$$

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* This case is of particular interest to us since we wish to prove that with $\Gamma'\doteq 0$ our final formulas for ϵ and σ become the formulas of reference (1). In the presence of strong damping the entire expression (4b) vanishes because of the presence of $e^{-\Gamma' t}$

A comparison of this expression with the current calculated from classical theory

$$\mathbf{j} = \frac{\varepsilon - 1}{4\pi}\frac{\omega^2}{c}\mathbf{A} - \frac{\sigma}{c}\dot{\mathbf{A}},$$

gives the following expressions for the dielectric constant ϵ and the electrical conductivity σ

$$\varepsilon = 1 - \frac{4\pi e^2}{m\omega^2 (Ga)^{3N}}$$

$$\times \sum_s \int \Big[e^{-\Gamma' t} + \frac{1}{m\hbar} \sum_{s'} \Big(\frac{\omega' - \omega}{(\omega' - \omega)^2 + \Gamma'^2}$$

$$+ \frac{\omega' + \omega}{(\omega' + \omega)^2 + \Gamma'^2} \Big) \mathbf{D}_{\vec{\xi}_1, \ldots, \vec{\xi}_N, s\, \vec{\xi}'_1 \ldots \vec{\xi}'_N, s'} \Big]$$

$$\times \rho_0(\vec{\xi}_1, \ldots, \vec{\xi}_N, s)\, d\vec{\xi}_1, \ldots, d\vec{\xi}_N;$$

$$\sigma = - \frac{\pi e^2}{m^2 \hbar \omega (Ga)^{3N}}$$

$$\times \sum_{s,s'} \int e^{-\Gamma' t} \frac{\rho_0(\vec{\xi}_1, \ldots, \vec{\xi}_N, s') - \rho_0(\vec{\xi}_1, \ldots, \vec{\xi}_N, s)}{\operatorname{grad}_{\vec{\xi}_1 \ldots \vec{\xi}_N} \omega'}$$

$$\times \mathbf{D}_{\vec{\xi}_1, \ldots, \vec{\xi}_N; \vec{\xi}'_1, \ldots, \vec{\xi}'_N} du_1 \ldots du_{3N-1}$$

$$+ \frac{e^2}{m^2 \hbar \omega (Ga)^{3N}} \sum_{s,s'} \int \Big(\frac{\Gamma'}{(\omega' + \omega)^2 + \Gamma'^2} - \frac{\Gamma'}{(\omega' - \omega)^2 + \Gamma'^2} \Big)$$

$$\times \rho_0(\vec{\xi}_1, \ldots, \vec{\xi}_N, s)\, \mathbf{D}_{\vec{\xi}_1, \ldots, \vec{\xi}_N; \vec{\xi}'_1, \vec{\xi}'_N} d\vec{\xi}_1, \ldots, d\vec{\xi}_N.$$

As we expected, with $\Gamma' = 0$ the expressions for ϵ and σ become Eqs. (3.23) and (3.24) of reference 1, whereas with $\Gamma' \neq 0$, the terms containing $\exp(-\Gamma' t)$ vanish and, finally, we obtain

$$\varepsilon = 1 - \frac{4\pi e^2}{m\omega^2 (Ga)^{3N}} \sum_s \int \Big[\frac{1}{m\hbar} \sum_{s'} \Big(\frac{\omega' - \omega}{(\omega' - \omega)^2 + \Gamma'^2}$$

$$+ \frac{\omega' + \omega}{(\omega' + \omega)^2 + \Gamma'^2} \mathbf{D}_{\vec{\xi}_1, \ldots, \vec{\xi}_N; \vec{\xi}'_1, \ldots, \vec{\xi}'_N} \Big]$$

$$\times \rho_0(\vec{\xi}_1, \ldots, \vec{\xi}_N, s)\, d\vec{\xi}_1, \ldots, d\vec{\xi}_N,$$

$$\sigma = + \frac{e^2}{m^2 \hbar \omega (Ga)^{3N}} \sum_{s,s'} \int \Big(\frac{\Gamma'}{(\omega' + \omega)^2 + \Gamma'^2}$$

$$- \frac{\Gamma'}{(\omega' - \omega)^2 + \Gamma'^2} \Big) \rho_0(\vec{\xi}_1, \ldots, \vec{\xi}_N, s)$$

$$\times \mathbf{D}_{\vec{\xi} \ldots, \vec{\xi}_N; \vec{\xi}'_1 \ldots, \vec{\xi}'_N} d\vec{\xi}_1, \ldots, d\vec{\xi}_N.$$

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