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Corrections to the Articles "Dispersion Formulas of the Quantum Optics of Metals in the Many-Electron Theory"

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IN PREVIOUS WORKS[1-3] the dispersion formulas of the quantum optics of metals were obtained both without taking account of electron damping and with taking it into account for the infrared, visible, and ultra-violet regions of the spectra. The present note is intended to indicate errors in the above works, as well as finally to give the correct dispersion formulas for ε and σ.

The many-electron wave function of the crystal used in the cited works was taken from Seitz[4] and is of the form

$$\psi(\mathbf{r}_1 \ldots \mathbf{r}_N, s) = \chi_{\mathbf{k}_1 \ldots \mathbf{k}_N}(\mathbf{r} \ldots \mathbf{r}_N, s) \exp\left(i \sum_{j=1}^{N} \mathbf{k}_j \mathbf{r}_j\right), \tag{1}$$

where χ is a periodic function with period a. It should be noted that the use of the wave function of Eq. (1) for a set of interacting electrons in a crystal is inconsistent, since it gives the total quasimomentum of the system (a conserved quantity) as the sum of the quasimomenta of the separate electrons; this is true, strictly speaking, only for a system of noninteracting electrons.

As was pointed out by Volz and Haken[5,6], if the independent variables are chosen as the coordinates of the center of gravity of the system $\mathbf{R}(X, Y, Z)$ and the appropriate number of relative coordinates, the wave function of a system of interacting electrons in the crystal may be written in the form

$$\psi_{\mathbf{K}, I, s}(\mathbf{R}, \mathbf{r}_{jk}) = \chi_{\mathbf{K}, I, s}(\mathbf{R}, \mathbf{r}_{jk}) \exp(i \mathbf{K}\mathbf{R}), \tag{2}$$

where the three quantum numbers K_x, K_y, and K_z give total quasimomentum of the system and characterize the motion of the center of mass $\mathbf{R}$ of the total electron system, and I is a continuous quantum number related to the relative motion of the electrons, that is, to the relative coordinates $\mathbf{r}_{jk} = \mathbf{r}_j - \mathbf{r}_k$, and characterizes changes in the configuration of the electron systems; s denotes the number of the band together with the other discrete quantum numbers of the system. The function χ is periodic with respect to translation of the center of mass of the system along the lattice vector a.

The use of wave functions such as those of Eq. (2) is more correct, since in this case the total quasimomentum $\mathbf{K}$ of the system of interacting electrons uniquely characterizes the system as a whole.

If we calculate the matrix element for the probability of optical transition, using the wave function of Eq. (3), in the same way as previously[1], we obtain the energy conservation law and interference condition for the whole system of interacting electrons, namely

$$\begin{gathered} E(\mathbf{K}', I', s') = E(\mathbf{K}, I, s) \pm \hbar\omega, \\ \mathbf{K}' = \mathbf{K} + \mathbf{K}_0 + 2\pi\mathbf{g}, \end{gathered} \tag{3}$$

where $\mathbf{K}_0$ is the wave vector of the electromagnetic wave, and g is the reciprocal lattice vector. For selection rules, see also Haken[7].

In connection with this, we note that in the previous works[1-3], essentially single-electron selection rules $\xi_i' = \xi_i$ were used. In actuality, however, the set[8] of quantum numbers $(\mathbf{K}', I')$ need not necessarily be the same as the set $(\mathbf{K}, I)$, but must merely satisfy Eq. (3). The use of the correct wave functions of Eq. (2) in the derivation of the dispersion formulas leads to the following expressions for ε and σ:

$$\varepsilon(\omega) = 1 - \frac{4\pi e^2}{m^2\omega^2 G^3 a^3} \sum_s \int d\xi \rho_0(\xi,s) \left\{ e^{-\Gamma t} + \frac{1}{m\hbar} \sum_{s'} \int d\xi' \left[\frac{\omega' - \omega}{(\omega' - \omega)^2 + \Gamma^2} + \right.\right.$$

$$\left.\left. + \frac{\omega' + \omega}{(\omega' + \omega)^2 + \Gamma^2} \right] \tilde{D}(\xi s;\ \xi' s') \right\}, \tag{4}$$

$$\sigma(\omega) = -\frac{e^2}{m^2 \hbar\, \omega\, G^3 a^3} \sum_{s,s'} \left\{ \int\int\int d\xi d\xi' \rho_0(\xi,s) \left[\frac{\Gamma}{(\omega' - \omega)^2 + \Gamma^2} - \frac{\Gamma^*}{(\omega + \omega)^2 + \Gamma^2} \right] \tilde{D}(\xi s;\ \xi' s') \right.$$

$$\left. + \pi \int du_1 \ldots du_{6+2p-1} \frac{\rho_0(\xi',s') - \rho_0(\xi, s)}{|\operatorname{grad}_{\xi\xi'} \omega'|} \tilde{D}(\xi s; \xi' s') \right\}, \tag{5}$$

where we have introduced the notation

$$\xi = (K, I),\ \hbar\omega' = \hbar\omega'(\xi' s';\ \xi s) = E(\xi', s') - E(\xi, s),$$

p is the number of continuous quantum numbers I, and $\tilde{D}$ is a tensor with components

$$\{\tilde{D}(\xi s;\ \xi' s')\}_{\alpha,\beta} = (\xi' s' | \sum_j \mathbf{P}_{j\alpha} | \xi s)(\xi s | \sum_j \mathbf{P}_{j\beta} | \xi' s'),$$

$$(\alpha, \beta = x, y, z).$$

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