

DIELECTRIC CONSTANT OF BISMUTH-TYPE METALS IN THE INFRARED REGION

A. A. ABRIKOSOV

Institute of Physics Problems, Academy of Sciences, U.S.S.R.

Submitted to JETP editor January 15, 1963

J. Exptl. Theoret. Phys. (U.S.S.R.) 44, 2039-2057 (June, 1963)

The dielectric constant of bismuth-type metals is obtained on the basis of their electron spectrum. It is shown that the dielectric tensor has in a large frequency region real positive frequency-independent principal values on the order of 100, and becomes complex starting with several hundredths or one-tenth of an electron volt. The components of ϵ_{jk} have singularities at some values of the frequency. It is shown at the end of the article that the large dielectric constant leads to an appreciable decrease in the electron-electron and electron-phonon interactions. This makes it possible to apply the gas model to these metals.

In a preceding paper^[1] we have already considered the influence exerted on the number of "free carriers" by the deep electron energy levels corresponding to open equal-energy surfaces. The possibility of observing the effect was appreciably limited there by the exponential temperature dependence of the added carriers and by the low melting temperature. It is much more convenient in this respect to investigate the infrared properties of these metals, a study which incidentally has already begun^[2,3]. Moreover, as will be shown later, the entire frequency dependence of the dielectric tensor ϵ_{jk} is determined only by one constant in addition to the constants characterizing the Fermi surface. When the determination of these constants from the de Haas-van Alphen effect and from cyclotron resonance is completed, infrared measurements will serve as a splendid means of quantitatively verifying the theory.

1. GENERAL EXPRESSION FOR THE DIELECTRIC CONSTANT

We obtain an expression for the current induced by the external electromagnetic field. Let the potential gauge be such that $\varphi = 0$ and $\text{div } \mathbf{A} = 0$, so that $\mathbf{E} = -c^{-1} \partial \mathbf{A} / \partial t$ and $\mathbf{H} = \text{curl } \mathbf{A}$. The current-density operator has the form

$$\hat{j}_i = e \hat{v}_{ix}^+ \hat{\psi}_i^+(x') \hat{\psi}_i(x) - \frac{e^2}{c} (\hat{m}_{xx'}^{-1})^{ik} \hat{\psi}_i^+(x') \hat{\psi}_i(x) A_k, \quad x' \rightarrow x, \quad (1)$$

where $\hat{v}_{xx'}^i$ and $(\hat{m}_{xx'}^{-1})^{ik}$ are operators acting on the variables \mathbf{x} and \mathbf{x}' in the Heisenberg field operators $\hat{\psi}(\mathbf{x})$. The Hamiltonian of the interaction between the electrons and the field is

$$H = - \frac{e}{c} \int \hat{v}_{xx'} \hat{\psi}_i^+(x') \psi_i(x) \mathbf{A}(x) dV, \quad x' \rightarrow x. \quad (2)$$

Taking the average value of the current operator and confining ourselves to the first approximation in \mathbf{A} , we obtain

$$\langle \hat{j}_i(x) \rangle = \frac{ie^2}{c} \int_{-\infty}^{t_x} dt_y \int dy \hat{v}_{xx'}^i \hat{v}_{yy'}^k \langle [\psi_i^+(x') \psi_i(x), \psi_i^+(y') \psi_i(y)] \rangle A_k(y) - \frac{e^2}{c} (\hat{m}_{xx'}^{-1})^{ik} \langle \psi_i^+(x') \psi_i(x) \rangle A_k(x), \quad x' \rightarrow x, \quad y' \rightarrow y. \quad (3)$$

We confine ourselves to the case $T = 0$. The integrand contains here the so-called retarded commutator. As is well known, this quantity can be obtained from the time-ordered mean by reversing the sign of the imaginary part of the Fourier component at negative frequencies. Bearing this in mind, we replace the expression under the integral sign by

$$\langle T (\psi_i^+(x') \psi_i(x) \psi_i^+(y') \psi_i(y)) \rangle.$$

In the model of non-interacting electrons in an external field, this expression is equal to

$$G_{\alpha\beta}(x, y') G_{\beta\alpha}(y, x') - G_{\alpha\alpha}(x, x') G_{\beta\beta}(y, y').$$

The last term yields zero in (3) and will therefore be disregarded. When account is taken of the electron-electron and electron-phonon interactions, additional terms appear, containing electron-electron and electron-phonon vertices. A remarkable property of bismuth-type metals is the fact that all the "Fermi-liquid" corrections, which usually have the same order as the main effect, are exceedingly small here. This problem will be the subject of the last section of the present article. At present, on the basis of this property, we simply consider the model of non-interacting quasi-

particles (gas) in a periodic field. In such a model the Green's function of the electrons can obviously be the pole part of the previously obtained function^[4] (with the coefficient a replaced by unity).

Let us transform expression (3) as follows. Since we are interested in the case when the radiation wave vector is small compared with the period of the reciprocal lattice, we can take the integral with respect to dy and average with respect to dx over the lattice period, regarding j and A as constant. The kernel in the integral of (3) is then of the difference type, and the second term assumes the form $\text{const}_{jk} A_k$. Consequently, Eq. (3) can be written in terms of Fourier components in the form

$$j_i(\kappa, \omega) = K_{ik}(\kappa, \omega) A_k(\kappa, \omega). \quad (4)$$

If A is constant, then $E = H = 0$ and consequently there is no current. We should have therefore $K_{jk}(0, 0) = 0$ ¹⁾. In view of this, we can subtract $K_{jk}(0, 0)$ from the Fourier component of the kernel K_{jk} determined from formula (3). This cancels, in particular, the contribution from the second term in (3).

The expression for the pole part of G was obtained in^[4] and has the form

$$\begin{aligned} G_{\alpha\beta}(x, x') &= \int G_{\alpha\beta}(\varepsilon, k, x, x') \exp\{-i\varepsilon(t-t')\} \\ &+ ik(x-x') \frac{d\varepsilon}{2\pi} \frac{dk}{(2\pi)^3}, \\ G_{\alpha\beta}(\varepsilon, k, x, x') &= \sum_{s, s'} [\varepsilon - \hat{D}(k) \\ &+ i\delta \text{sign}(\varepsilon - \mu)]_{ss'}^{-1} u_s(x, \alpha) u_{s'}(x', \beta), \end{aligned} \quad (5)$$

where u_s are periodic function that realize an irreducible representation of the small group of the point k_0 , in the vicinity of which there is situated the point k . Substituting (5) in the integral (3), in which the retarded commutator is replaced by $G_{\alpha\beta}(x, y') G_{\beta\alpha}(y, x')$, we integrate with respect to y and average with respect to x over the lattice period. Then the kernel in the integral (3) really becomes of the difference type. Taking the Fourier component, we arrive at a formula similar to (4), where K_{jk} is replaced by

¹⁾It can be shown that this actually takes place, provided we take the limit $\omega/\kappa \rightarrow 0$, $\kappa \rightarrow 0$. The physical meaning of this limit can be explained by considering that when $\omega \rightarrow 0$ and $\kappa \rightarrow 0$ the current can be proportional either to E , i.e., ωA , or to $\text{curl } H$, i.e., $\kappa^2 A$. The decrease of ω should therefore be faster than the decrease of κ .

$$\begin{aligned} Q_{ik}(\kappa, \omega) &= \frac{ie^2}{c} \int \frac{d\varepsilon}{2\pi} \frac{dk}{(2\pi)^3} \text{Sp} \left\{ \left[\varepsilon + \frac{\omega}{2} - \hat{D}(k + \frac{\kappa}{2}) \right. \right. \\ &+ i\delta \text{sign}(\varepsilon + \frac{\omega}{2} - \mu) \left. \right]^{-1} \hat{v}^i \left[\varepsilon - \frac{\omega}{2} - \hat{D}(k - \frac{\kappa}{2}) \right. \\ &+ i\delta \text{sign}(\varepsilon - \frac{\omega}{2} - \mu) \left. \right]^{-1} \hat{v}_k \left. \right\}. \end{aligned} \quad (6)$$

From this, in accordance with the preceding, we must subtract $Q_{jk}(0, 0)$ (and the limit must be taken such that $\omega/\kappa \rightarrow 0$) and reverse the sign of the imaginary part of Q_{jk} for $\omega < 0$.

The velocity operator in the model of non-interacting quasiparticles in a periodic field has the form

$$\hat{v} = \partial \hat{D}(k) / \partial k. \quad (7)$$

Since, according to the foregoing, the matrix \hat{D} depends linearly on the components k , v is independent of k .

If the spatial dispersion is negligible, i.e., if we can assume that $\kappa = 0$ in Q_{jk} , then, recalling the relation $j_i = \varepsilon_{ijk} \omega^2 A_k / 4\pi c$ obtained from Maxwell's equations, we get

$$\varepsilon_{ik}(\omega) = \frac{4\pi c}{\omega^2} [Q_{ik}^R(0, \omega) - Q_{ik}^R(0, 0)], \quad (8)$$

where the index R denotes the retarded function, i.e., Q_{jk} with changed imaginary part.

Of course, the foregoing formulas are valid also when the spatial dispersion is significant. In this case the connection between j and A should be substituted in the Maxwell's equations, and A should be either continued symmetrically outside the metal (specular reflection) or assumed equal to zero outside the metal (diffuse reflection).

2. TRANSITIONS INSIDE THE BAND

We consider first the contribution to ε_{jk} due to the electronic transitions within the band [which we denote by $(\varepsilon_{jk})_I$]. We assume here that $\omega \gg v\kappa$, where v is the electron velocity (10^8 cm/sec). We shall see later on that for frequencies that are not too low this criterion is indeed satisfied.

Formula (6) contains the trace operation. According to the properties of the trace, it can be taken over arbitrary functions. We choose these functions to be the eigenfunctions of the matrix $\hat{D}(k)$. If we assume that $\kappa = 0$ and disregard inter-band transitions, then the poles of both denominators in (6) always have imaginary parts of the same sign, and consequently $Q_{jk}(\omega, 0) = 0$. According to formula (8), we obtain

$$(\varepsilon_{ik})_I = -4\pi c / \omega^{-2} Q_{ik}^R(0, 0), \quad (9)$$

where, as already mentioned, the limit in Q_{ik} is taken such that $\omega/\kappa \rightarrow 0$.

Let us assume that $\omega = 0$ and κ is small but different from zero. The integral (6) is taken over the vicinities of the electronic regions $\mathbf{k} = \mathbf{k}_i$ and the hole region $\mathbf{k} = 0$. Let us take one such region, say $\mathbf{k} = 0$. The matrix elements G contained in the integral can be written in the form

$$G_{ik} = \Delta_{ik} \left(\epsilon, \mathbf{k} \pm \frac{\boldsymbol{\kappa}}{2} \right) / \prod_{n=1}^4 \left[\epsilon - \epsilon_n \left(\mathbf{k} \pm \frac{\boldsymbol{\kappa}}{2} \right) + i\delta \operatorname{sign} \left(\epsilon_n \left(\mathbf{k} \pm \frac{\boldsymbol{\kappa}}{2} \right) - \mu \right) \right],$$

where Δ_{ik} is the minor of the matrix $\epsilon - \hat{D}(\mathbf{k} \pm \boldsymbol{\kappa}/2)$, and ϵ_n are the eigenvalues of the matrix \hat{D} . In the vicinity of $\mathbf{k} = 0$ there converge four bands (see [1]²), with the holes corresponding to the second band. In view of the smallness of κ we can put $\kappa = 0$ in all the Δ_{ik} , and also in all the factors of the denominators, except $n = 2$. Then Δ_{ik} becomes a diagonal matrix with elements containing products of the same factors as in the denominators. The signs of $i\delta$ in all the factors of the denominator are definite, except $n = 2$.

As a result of substitution in (6), we get

$$Q_{ik}^{(0)}(\boldsymbol{\kappa}, 0) = \frac{ie^2}{c} \int \frac{d\epsilon}{2\pi} \frac{d\mathbf{k}}{(2\pi)^3} (\hat{v}^i)_{22} (\hat{v}^k)_{22} \left[\epsilon - \epsilon_2^{(0)} \left(\mathbf{k} + \frac{\boldsymbol{\kappa}}{2} \right) + i\delta \operatorname{sign} \left(\epsilon_2^{(0)} \left(\mathbf{k} + \frac{\boldsymbol{\kappa}}{2} \right) - \mu \right) \right]^{-1} \left[\epsilon - \epsilon_2^{(0)} \left(\mathbf{k} - \frac{\boldsymbol{\kappa}}{2} \right) + i\delta \operatorname{sign} \left(\epsilon_2^{(0)} \left(\mathbf{k} - \frac{\boldsymbol{\kappa}}{2} \right) - \mu \right) \right]^{-1}.$$

Recognizing that

$$(\hat{v}^i)_{22} = \partial \epsilon^{(0)}(\mathbf{k}) / \partial k_i = v_i^{(0)}(\mathbf{k}),$$

we take the integral, then put $\kappa = 0$ and substitute in (7), obtaining

$$(\epsilon_{ik}^{(0)})_I = - \frac{4\pi e^2}{\omega^2} \int v_i^{(0)}(\mathbf{k}) v_k^{(0)}(\mathbf{k}) \frac{dS}{(2\pi)^3 |v^{(0)}(\mathbf{k})|},$$

where dS is the area element of the "hole" Fermi surface. The electrons make a perfectly analogous contribution.

We shall not go here through the rather complicated calculations of the tensor $(\epsilon_{ik})_I$, since we are essentially interested in the frequency region where the main role is played by interband transitions. But such a calculation can be made if necessary, since the quantities contained in (8) can be determined from the electronic spectrum [5]. The order of magnitude of this part of ϵ_{ik} is obviously

$$(\epsilon_{ik})_I \sim - \frac{4\pi e^2}{\omega^2} \frac{v^2 \rho_0^2}{v\pi^2} \sim - \frac{\epsilon_F^2}{\omega^2},$$

where ϵ_F is the Fermi energy, on the order of several hundredths of an electron volt.

3. DIRECT TRANSITIONS BETWEEN LEVELS WITH OPEN EQUAL-ENERGY SURFACES

In the region of not too high frequencies (an exact criterion will be established later) expression (8), together with the analogous expression for electrons, determines the entire dielectric constant. When the frequency increases, transitions between bands come into play. A special role will be assumed, of course, by transitions between levels corresponding to open equal-energy surfaces. We therefore first concentrate on such transitions [we denote the corresponding contribution to ϵ_{ik} by $(\epsilon_{ik})_{II}$]. We again assume that an account of the spatial dispersion is not essential. Therefore the absorption of a quantum should obey the conservation law

$$\epsilon_3(\mathbf{k}) - \epsilon_2(\mathbf{k}) = \omega. \quad (10)$$

It was not by accident that we have written ϵ_2 and ϵ_3 here, for only in the second and third bands are there open equal-energy surfaces.

Let us determine the threshold values of the frequencies; in other words, let us find the frequencies for which (10) is first satisfied as $\mathbf{k} \rightarrow \infty$. This is easiest to do for the vicinity of $\mathbf{k} = 0$. Since, in accord with [5], we have in this vicinity

$$f - \epsilon_2^{(0)}(\mathbf{k}) = \epsilon_3^{(0)}(\mathbf{k}) - f, \quad (11)$$

we get

$$\epsilon_3(\mathbf{k}) - \epsilon_2(\mathbf{k}) = 2[f - \epsilon_2(\mathbf{k})].$$

And since the equation $\epsilon_2(\mathbf{k}) = \text{const}$ has solutions with $\mathbf{k} \rightarrow \infty$ for $\epsilon_2(\mathbf{k}) < f - |\gamma|$, we obtain for the first threshold value

$$\omega^{(0)} = 2|\gamma|. \quad (12)$$

We note that for this value of ω Eq. (10) has a solution for infinite \mathbf{k} along the directions that fill the entire conical surface.

For the vicinity of $\mathbf{k} = \mathbf{k}_i$ the situation is somewhat more complicated. According to formula (15) of [5], at large momenta there holds for this vicinity the relation

$$\beta q_y - \left(\frac{1}{3} f + \epsilon_2^{(1)}(\mathbf{k}) \right) p = \left(\frac{1}{3} f + \epsilon_3^{(1)}(\mathbf{k}) \right) p - \beta q_y. \quad (13)$$

It follows therefore that

²Actually each band is doubly degenerate so that the result should be multiplied by 2.

$$\varepsilon_3^{(1)}(\mathbf{k}) - \varepsilon_2^{(1)}(\mathbf{k}) = 2 \left[\left(\frac{1}{3} f + \varepsilon_3^{(1)}(\mathbf{k}) \right) - \beta s \right],$$

$$s = q_y / p, \quad q_y = b(k_y - k_y^i), \quad p = a(k_z - k_z^i), \quad (14)$$

where the directions of y and z are taken in the proper frame for the vicinity of \mathbf{k}_i (see [5]). Using the earlier analysis [1,5], we obtain for the threshold value

$$\omega^{(1)} = 2 \left(\frac{1}{3} |\gamma| - |\delta| \right). \quad (15)$$

The openness occurs only in one direction. When ω increases beyond $\omega^{(1)}$, Eq. (10) already has a solution for the open surfaces in the entire interval of directions. Finally, when

$$\omega^{(1)'} = 2 \left(\frac{1}{3} |\gamma| + |\delta| \right) \quad (16)$$

these open directions again fill the conical surface for the first time. Here, too, there are grounds for expecting some singularity in ε_{ik} .

We now proceed to calculate ε_{ik} . We put $\kappa = 0$ in (6) and take the trace over the eigenfunctions of the matrix $\hat{D}(\mathbf{k})$. Recognizing that the open surfaces are encountered in the second and third bands and taking into consideration the fact that the Fermi energy enters in the middle between openness thresholds for the second and third bands, we obtain for the trace in (6)

$$\begin{aligned} & \left[\varepsilon + \frac{1}{2} \omega - \varepsilon_2(\mathbf{k}) - i\delta \right]^{-1} \left[\varepsilon - \frac{1}{2} \omega - \varepsilon_3(\mathbf{k}) + i\delta \right]^{-1} \\ & \times v_{23}^i(\mathbf{k}) v_{32}^k(\mathbf{k}) + \left[\varepsilon + \frac{1}{2} \omega - \varepsilon_3(\mathbf{k}) \right. \\ & \left. + i\delta \right]^{-1} \left[\varepsilon - \frac{1}{2} \omega - \varepsilon_2(\mathbf{k}) - i\delta \right]^{-1} v_{32}^i(\mathbf{k}) v_{23}^k(\mathbf{k}). \end{aligned}$$

Substituting this in (6) and integrating with respect to ε we get

$$\begin{aligned} Q_{ik}(0, \omega) = & \frac{2e^2}{c} \int \frac{d\mathbf{k}}{(2\pi)^3} \left\{ \frac{v_{32}^i(\mathbf{k}) v_{23}^k(\mathbf{k})}{\varepsilon_3(\mathbf{k}) - \varepsilon_2(\mathbf{k}) - \omega - i\delta} \right. \\ & \left. + \frac{v_{23}^i(\mathbf{k}) v_{32}^k(\mathbf{k})}{\varepsilon_3(\mathbf{k}) - \varepsilon_2(\mathbf{k}) - \omega + i\delta} \right\}, \quad (17) \end{aligned}$$

where the factor 2 is due to the account of the double degeneracy of the levels. It will be shown below that $v_{23}^i(\mathbf{k}) = v_{32}^i(\mathbf{k})$.

In order to obtain from among the Q_{ik} the correct value Q_{ik}^R , it is sufficient to reverse the sign of $i\delta$ in the second term of (17). Combining then the two terms in (17) and substituting in (8), we get

$$\begin{aligned} (\varepsilon_{ik})_{II} = & 8\pi e^2 \int \left[\frac{dZ}{d(\varepsilon_3(\mathbf{k}) - \varepsilon_2(\mathbf{k}))} \right]_{\varepsilon_3(\mathbf{k}) - \varepsilon_2(\mathbf{k}) = v} v_{32}^i(\mathbf{k}) v_{23}^k(\mathbf{k}) \\ & \times \frac{dv}{v[v^2 - (\omega + i\delta)^2]}, \\ dZ = & 2(2\pi)^{-3} d\mathbf{k}. \quad (18) \end{aligned}$$

For further calculation it is necessary to find the density of the states and the matrix element of the velocity. We start with the latter. In [5] we used a not too suitable form of the matrix $\hat{D}(\mathbf{k})$. As was shown by Fal'kovskii [6], it can be reduced to two four-row matrices. One has the form

$$\hat{D}(\mathbf{k}) = \begin{pmatrix} f+p+\Delta & q_+-\beta & \gamma & -\delta \\ q_--\beta & f+p-\Delta & -\delta & \gamma \\ \gamma & -\delta & f-p+\Delta & -q_+-\beta \\ -\delta & \gamma & -q_--\beta & f-p-\Delta \end{pmatrix}, \quad (19)$$

while the other differs in the sign of Δ . Both have identical eigenvalues. These matrices become interconnected only if the effect of the magnetic field on the electron spin is taken into account. If we are not interested in this small effect, we can use the four-row matrices $\hat{D}(\mathbf{k})$, as will be done from now on.

According to (7), the matrix \hat{v}^i has in this representation the form

$$\hat{v}^i = \begin{pmatrix} an_z & bn_+ & 0 & 0 \\ bn_- & an_z & 0 & 0 \\ 0 & 0 & -an_z & -bn_+ \\ 0 & 0 & -bn_- & -an_z \end{pmatrix}, \quad (20)$$

where \mathbf{n} is a unit vector in the i -direction. If

$$\Psi_n = \sum_{i=1}^4 c_i^{(n)} \psi_i$$

are the eigenvalues of the matrix (19), then according to (20)

$$\begin{aligned} \hat{v}_{23}^i(\mathbf{k}) = & an_z (c_1^{(2)*} c_1^{(3)} + c_2^{(2)*} c_2^{(3)} - c_3^{(2)*} c_3^{(3)} - c_4^{(2)*} c_4^{(3)}) \\ & + bn_+ (c_2^{(2)*} c_2^{(3)} - c_3^{(2)*} c_3^{(3)}) + bn_- (c_2^{(2)*} c_1^{(3)} - c_4^{(2)*} c_3^{(3)}). \quad (21) \end{aligned}$$

The coefficients $c_i^{(\mathbf{n})}$ are determined by solving the linear system with the matrix $D(\mathbf{k})$ (19) and the normalization condition

$$\sum_{i=1}^4 |c_i^{(n)}|^2 = 1.$$

It greatly facilitates the derivation to recognize that we are interested henceforth in large momenta, and according to Eq. (15) of [5] and Eq. (14) of the present paper we have

$$q_x^2 \approx p^2 - q_y^2 \pm \sqrt{p^2 v^2 - 4(\delta q_y + \gamma p)^2} \quad (22)$$

(for the vicinity of $\mathbf{k} = \mathbf{k}_i$ we have $\gamma^{(1)} = -\gamma/3$).

As a result of all the derivations we obtain

$$v_{23}^i(\mathbf{k}) = v_{32}^i(\mathbf{k}) = \frac{2|\delta q_y + \gamma p|}{vp} \left[an_z - \frac{b}{p} (n_x q_x + n_y q_y) \right]. \quad (23)$$

For holes, after averaging over the momentum directions in a plane perpendicular to the z axis,

we get

$$[\nu_{23}^i(\mathbf{k}) \nu_{32}^k(\mathbf{k})]_{(0)} = 4\gamma^2 \nu^{-2} \left[a^2 n_z m_z + \frac{1}{2} b^2 (n_x m_x + n_y m_y) \right], \quad (24)$$

where n and m correspond to the i -th and k -th directions.

For the electrons we average over only two signs of q_x . We then obtain

$$[\nu_{23}^i(\mathbf{k}) \nu_{32}^k(\mathbf{k})]_{(1)} = 4 (\delta s - \gamma/3)^2 \nu^{-2} \{ (an_z - bn_y s) \times (am_z - bm_y s) + b^2 n_x m_x (1 - s^2) \}, \quad (25)$$

where $s = q_y/p$.

It is further necessary to take account of the fact that there are three $\mathbf{k} = \mathbf{k}_i$ points, and for each point the axes x, y , and z are defined in different fashion. From symmetry considerations it is clear that the principal axes of the tensor ϵ_{ik} will be a z axis along the trigonal axis and two mutually perpendicular axes in the basal plane. We therefore present expression (25) for each vicinity of $\mathbf{k} = \mathbf{k}_i$ in a common coordinate system, and add the contributions of all three. We then obtain in the braces of (25) the following values:

$$\begin{aligned} \text{a) } \epsilon_{zz} &: \frac{1}{3} (a - 2\sqrt{2}bs)^2, \\ \text{b) } \epsilon_{xx} = \epsilon_{yy} &: \frac{4}{3}a^2 + \frac{3}{2}b^2 + (2\sqrt{2}/3)abs - \frac{4}{3}b^2s^2, \\ \text{c) } \epsilon_{ii} = 2\epsilon_{xx} + \epsilon_{zz} &: 3(a^2 + b^2). \end{aligned} \quad (26)$$

We now obtain the density of states $dZ/d[\epsilon_3 - \epsilon_2]$ for each vicinity. Near $\mathbf{k} = 0$ this calculation has already been made in [1]. Only a factor $1/2$ appears here, since $\nu = 2(f - \epsilon_2)$. Thus

$$\begin{aligned} \left[\frac{dZ^{(0)}}{d(\epsilon_3 - \epsilon_2)} \right]_{\epsilon_3 - \epsilon_2 = \nu} &= \frac{A}{2} \frac{\nu}{\sqrt{\nu^2 - 4\gamma^2}}, \quad \nu > 2|\gamma|; \\ A &= \frac{1}{\pi^2 ab^2} \int_{p>0} 2p dp. \end{aligned} \quad (27)$$

Here A is a constant on the order of E_0^2/ν^3 , $E_0 \sim 0.1-1$ eV, $\nu \sim 10^8$ cm/sec.

For the vicinity of $\mathbf{k} = \mathbf{k}_i$ using (22), we get

$$\begin{aligned} \left[\frac{dZ^{(1)}}{d(\epsilon_3 - \epsilon_2)} \right]_{\epsilon_3 - \epsilon_2 = \nu} &= \frac{2}{(2\pi)^3 ab^3} \int \frac{dq_x}{dv} dq_y dp \\ &= \frac{A\nu}{2\pi} \int \frac{ds}{\sqrt{1 - s^2} \sqrt{\nu^2 - 4(\gamma/3 - \delta s)^2}}, \end{aligned} \quad (28)$$

where $\nu > 2(|\gamma|/3 - |\delta|)$. The limits of the integral over s are

- a) $\frac{|\gamma|}{3|\delta|} - \frac{\nu}{2|\delta|} - 1$ for $\nu < 2\left(\frac{|\gamma|}{3} + |\delta|\right)$, $\gamma\delta > 0$;
- b) $-1 - \frac{\nu}{2|\delta|} - \frac{|\gamma|}{3|\delta|}$ for $\nu < 2\left(\frac{|\gamma|}{3} + |\delta|\right)$, $\gamma\delta < 0$;
- c) $-1 - 1$ for $\nu > 2\left(\frac{|\gamma|}{3} + |\delta|\right)$.

Thus, all the expressions contained in the integral (18) are defined. For the vicinity of $\mathbf{k} = 0$ it is necessary to integrate with respect to ν , and for the vicinities of $\mathbf{k} = \mathbf{k}_i$ it is necessary to take the double integral with respect to s and ν . The order of integration can be reversed in this integral, so that it has the form

$$\int_{-1}^1 ds \int_{|2\gamma/3 - 2\delta s|}^{\infty} d\nu.$$

The integral with respect to ν then assumes exactly the same form as for the vicinity of $\mathbf{k} = 0$. This integral is easy to calculate:

$$\int_{\alpha}^{\infty} \frac{d\nu}{\nu [\nu^2 - (\omega + i\delta)^2] \sqrt{\nu^2 - \alpha^2}} = \begin{cases} -\frac{1}{\alpha^2 \omega^2} + \frac{1}{\omega^3 \sqrt{\alpha^2 - \omega^2}} \operatorname{arctg} \frac{\omega}{\sqrt{\alpha^2 - \omega^2}}, & \alpha > |\omega|, \\ -\frac{1}{\alpha^2 \omega^2} - \frac{1}{2\omega^3 \sqrt{\omega^2 - \alpha^2}} \ln \frac{\omega + \sqrt{\omega^2 - \alpha^2}}{\omega - \sqrt{\omega^2 - \alpha^2}} + \frac{i\pi}{2\omega^3 \sqrt{\omega^2 - \alpha^2}}, & \alpha < |\omega|. \end{cases} \quad (29)^*$$

4. LIMITING FORMULAS

The contribution of the vicinity of $\mathbf{k} = 0$ to $(\epsilon_{ik})_{II}$ is thus completely determined by (we assume here that $\omega = 0$)

$$(\epsilon_{zz}^{(0)})_{II} = 4\pi e^2 a^2 A \begin{cases} -\frac{1}{\omega^2} + \frac{4\gamma^2}{\omega^3 \sqrt{4\gamma^2 - \omega^2}} \operatorname{arctg} \frac{\omega}{\sqrt{4\gamma^2 - \omega^2}}, & \omega < 2|\gamma|, \\ -\frac{1}{\omega^2} - \frac{2\gamma^2}{\omega^3 \sqrt{\omega^2 - 4\gamma^2}} \ln \frac{\omega + \sqrt{\omega^2 - 4\gamma^2}}{\omega - \sqrt{\omega^2 - 4\gamma^2}} + \frac{2\pi i \gamma^2}{\omega^3 \sqrt{\omega^2 - 4\gamma^2}}, & \omega > 2|\gamma|. \end{cases} \quad (30)$$

The other components $(\epsilon_{xx}^{(0)})_{II} = (\epsilon_{yy}^{(0)})_{II}$ differ from $(\epsilon_{zz}^{(0)})_{II}$ in that a^2 is replaced by $b^2/2$.

When $\omega \ll 2|\gamma|$ we obtain from this

$$(\epsilon_{zz}^{(0)})_{II} = 2\pi e^2 a^2 A / 3\gamma^2. \quad (31)$$

When $\omega \gg 2|\gamma|$ we have

$$(\epsilon_{zz}^{(0)})_{II} = \frac{4\pi e^2 a^2 A}{\omega^2} \left(-1 + \frac{2\pi i \gamma^2}{\omega^2} \right). \quad (32)$$

* $\operatorname{arctg} = \tan^{-1}$.

In the vicinity of $\omega \approx 2|\gamma|$ the quantity $(\epsilon_{ZZ}^{(0)})_{II}$ has the following singularity:

$$(\epsilon_{ZZ}^{(0)})_{II} \approx \begin{cases} \pi e^2 a^2 A / 2 |\gamma|^{1/2} \sqrt{2|\gamma| - \omega}, & \omega < 2|\gamma| \\ i\pi e^2 a^2 A / 2 |\gamma|^{1/2} \sqrt{\omega - 2|\gamma|}, & \omega > 2|\gamma| \end{cases} \quad (33)$$

We shall consider this singularity in greater detail later on.

The contribution to $\epsilon_{ik}(\omega)$ from the vicinity of $\mathbf{k} = \mathbf{k}_i$ cannot be obtained in analytic form for arbitrary frequencies. We therefore confine ourselves only to limiting cases. We first consider the case of low frequencies $\omega \ll |\gamma|$. According to (18), (25), (26), and (29) we get

$$(\epsilon_{ZZ}^{(1)})_{II} = \frac{2e^2}{3} \int_{-1}^1 \frac{1/3 (a - 2\sqrt{2}bs)^2 ds}{(\gamma/3 - \delta s)^2 \sqrt{1 - s^2}}.$$

Taking the integral with respect to s and adding (31), we obtain the total value

$$(\epsilon_{ZZ})_{II} = \frac{2\pi e^2}{3\delta^2} A \left\{ \left(-\frac{4\sqrt{2}}{3} ab - \frac{8}{3} b^2 \left| \frac{\gamma}{3\delta} \right|^3 + \frac{a^2}{3} \left| \frac{\gamma}{3\delta} \right| + \frac{16}{3} \left| \frac{\gamma}{3\delta} \right| b^2 \right) / \left(\frac{\gamma^2}{9\delta^2} - 1 \right)^{1/2} + \frac{8}{3} b^2 + a^2 \frac{\delta^2}{\gamma^2} \right\}. \quad (34)$$

Analogously we get

$$(\epsilon_{xx})_{II} = (\epsilon_{yy})_{II} = \frac{2\pi e^2}{3\delta^2} A \left\{ \left(\frac{2\sqrt{2}}{3} ab + \frac{4}{3} b^2 \left| \frac{\gamma}{3\delta} \right|^3 + \frac{4}{3} a^2 \left| \frac{\gamma}{3\delta} \right| - \frac{7}{6} b^2 \left| \frac{\gamma}{3\delta} \right| \right) / \left(\frac{\gamma^2}{9\delta^2} - 1 \right)^{1/2} - \frac{4}{3} b^2 + b^2 \frac{\delta^2}{2\gamma^2} \right\}. \quad (35)$$

It is easy to verify that for all ratios of the parameters all principal values of $(\epsilon_{ik})_{II}$ are greater than zero. The trace of the tensor ϵ is, in accord with (34) and (35),

$$(\epsilon_{ii})_{II} = \frac{2}{3} \pi e^2 \frac{a^2 + b^2}{\gamma^2} A \left\{ 1 + \frac{27}{[1 - (3\delta/\gamma)^2]^{3/2}} \right\}. \quad (36)$$

We now consider the opposite limiting case $\omega \gg |\gamma|$. By simple derivations and by taking (32) into account we obtain³⁾

$$\begin{aligned} \epsilon_{zz} &= \frac{4\pi e^2 A}{3\omega^2} \left[-4(a^2 + b^2) + \frac{2\pi i}{\omega^2} \left(\frac{28}{9} a^2 \gamma^2 + \frac{4}{9} \gamma^2 b^2 + \frac{1}{2} a^2 \delta^2 + 3b^2 \delta^2 + \frac{4\sqrt{2}}{3} ab\gamma\delta \right) \right], \\ \epsilon_{xx} = \epsilon_{yy} &= \frac{4\pi e^2 A}{3\omega^2} \left[-4(a^2 + b^2) + \frac{2\pi i}{\omega^2} \left(\frac{4}{9} a^2 \gamma^2 + \frac{16}{9} \gamma^2 b^2 + 2\delta^2 a^2 + \frac{3}{4} \delta^2 b^2 - \frac{2\sqrt{2}}{3} ab\gamma\delta \right) \right]. \end{aligned} \quad (37)$$

We note that when $\omega \rightarrow \infty$ we get $\epsilon_{xx} \approx \epsilon_{yy} \approx \epsilon_{zz}$. This is natural, in view of the fact that at such frequencies the difference between the lattice under

consideration and a cubic one is already insignificant.

The electronic contribution to ϵ_{ik} also yields singularities, although weaker ones than the holes near the threshold (33). The imaginary part of $\epsilon_{ik}^{(1)}$ appears, according to (29), when $\omega > \alpha_{\min}^{(1)}$, i.e., when $\omega > \omega^{(1)}$ [see (15)]. Since $\omega^{(1)} < \omega^{(0)}$ [see (12)], this is the lower threshold of the imaginary part of the direct transitions between levels with open equal-energy surfaces. Near the top side of the threshold we have

$$\begin{aligned} \text{Im } \epsilon_{zz} &= \frac{2\pi e^2 A}{[\omega^{(1)}]^3} \int_{s_0}^1 \frac{ds 4(\delta s - \gamma/3)^{2 \cdot 1/3} (a - 2\sqrt{2}bs)^2}{\sqrt{1 - s^2} \sqrt{\omega^2 - 4(\delta s - \gamma/3)^2}} \\ &\approx \frac{2\pi e^2 A}{[\omega^{(1)}]^3} \int_{s_0}^1 \frac{ds [\omega^{(1)}]^{1/3} \cdot 1/3 (a - 2\sqrt{2}b \text{sign } \delta\gamma)^2}{2\sqrt{2}|\delta| \sqrt{1 - s} \sqrt{s - s_0}} \\ &= \frac{\pi^2 e^2 A}{12(\rho - 1)^{3/2} \delta^2} (a - 2\sqrt{2}b \text{sign } (\delta\gamma))^2. \end{aligned}$$

We have introduced the notation:

$$s_0 = |\gamma|/3|\delta| - \omega/2|\delta|, \quad \rho = |\gamma/3\delta|. \quad (38)$$

Analogously

$$\text{Im } \epsilon_{xx} = \text{Im } \epsilon_{yy} = \frac{\pi^2 e^2 A}{12\delta^2(\rho - 1)^{3/2}} \left(2a + \frac{1}{\sqrt{2}} b \text{sign } (\delta\gamma) \right)^2. \quad (39)$$

Thus, the imaginary part of ϵ_{ik} assumes the final value in jumps. Accordingly, the real part of ϵ_{ik} has a logarithmic singularity. Simple calculation yields

$$\begin{aligned} \text{Re } \epsilon_{zz} &\approx \frac{\pi e^2 A}{12\delta^2(\rho - 1)^{3/2}} (a - 2\sqrt{2}b \text{sign } (\delta\gamma))^2 \\ &\quad \times \ln \frac{2|\delta|}{|^{2/3}|\gamma| - 2|\delta| - \omega|}, \\ \text{Re } \epsilon_{xx} = \text{Re } \epsilon_{yy} &\approx \frac{\pi e^2 A}{12\delta^2(\rho - 1)^{3/2}} \left(2a + \frac{1}{\sqrt{2}} b \text{sign } (\delta\gamma) \right)^2 \\ &\quad \times \ln \frac{2|\delta|}{|^{2/3}|\gamma| - 2|\delta| - \omega|}. \end{aligned} \quad (40)$$

At the point $\omega = 2/3|\gamma| + 2|\delta|$ where the cone of the open surfaces closes for the $\mathbf{k} = \mathbf{k}_i$ vicinity, the imaginary part of the ϵ_{ik} has a logarithmic singularity

$$\begin{aligned} \text{Im } \epsilon_{zz} &\approx \frac{\pi e^2 A}{12\delta^2(\rho + 1)^{3/2}} (a + 2\sqrt{2}b \text{sign } (\delta\gamma))^2 \\ &\quad \times \ln \frac{2|\delta|}{|^{2/3}|\gamma| + 2|\delta| - \omega|}, \\ \text{Im } \epsilon_{xx} = \text{Im } \epsilon_{yy} &\approx \frac{\pi e^2 A}{12\delta^2(\rho + 1)^{3/2}} \left(2a - \frac{1}{\sqrt{2}} \text{sign } (\delta\gamma) \right)^2 \\ &\quad \times \ln \frac{2|\delta|}{|^{2/3}|\gamma| + 2|\delta| - \omega|}. \end{aligned} \quad (41)$$

The real part has in this vicinity a jump:

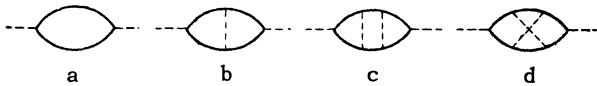
³⁾In this region $(\epsilon_{ik})_I \ll (\epsilon_{ik})_{II}$, so that $\epsilon_{ik} \approx (\epsilon_{ik})_{II}$.

$$\begin{aligned}
& \text{Re } \epsilon_{zz} (\omega = 2/3|\gamma| + 2|\delta| - 0) \\
& - \text{Re } \epsilon_{zz} (\omega = 2/3|\gamma| + 2|\delta| + 0) \\
& = \pi^2 e^2 (a + 2\sqrt{2}b \text{ sign}(\delta\gamma))^2 / 12\delta^2 (\rho + 1)^{3/2}, \\
& \text{Re } \epsilon_{xx} (\omega = 2/3|\gamma| + 2|\delta| - 0) \\
& - \text{Re } \epsilon_{xx} (\omega = 2/3|\gamma| + 2|\delta| + 0) \\
& = \pi^2 e^2 (2a - 2^{-1/2} b \text{ sign } \delta\gamma) / 12\delta^2 (\rho + 1)^{3/2}. \quad (42)
\end{aligned}$$

5. BEHAVIOR OF ϵ_{ik} IN THE VICINITY OF THE THRESHOLDS

The singularities of ϵ_{ik} found in the preceding section are the results of certain approximations. In order to study the true situation, it is necessary to carry out a more accurate analysis.

Let us estimate the role of different effects not taken into account in our calculation. First there are corrections connected with the increase in the degree of singularity, owing to the electron interaction. If we assume a Coulomb electron interaction then the corrections to ϵ_{ik} are expressed by the diagrams shown in the figure, where the dashed lines correspond to $4\pi e^2/qj\mathbf{q}\mathbf{k}\epsilon_{ik}(\omega, \mathbf{q})$.



Simple analysis shows that the momenta and frequencies of these lines are of the order of $|\gamma|/v$ and $|\gamma|$, so that we get in the denominator $\epsilon_{ik}(\omega, \mathbf{q}) \sim E_0^2/\gamma^2 \sim 100$. It is easy to see that only in diagrams of the type a, b, and c does the degree of the singularity increase with the order of the diagram. When summed, these diagrams lead to the following substitution near $\omega = 2|\gamma|$

$$\frac{1}{\sqrt{2|\gamma| - \omega}} \rightarrow \frac{1}{\sqrt{2|\gamma| - \omega + \xi\sqrt{|\gamma|}}},$$

where $\xi \sim \gamma^2/E_0^2$. Thus, this correction is significant when $\omega - 2|\gamma| \sim \xi^2|\gamma| \sim 10^{-4}|\gamma|$. In the case of a logarithmic singularity, the analogous criterion has the form $\ln(|\gamma|/|\omega_C - \omega|) \sim \xi$, i.e., $\omega - \omega_C \sim e^{-\xi}|\gamma|$. As will be shown presently, there exist many other effects which begin to come into play at much larger distances from the singularity.

Let us consider the role of the finite electron free path. We first note that at the energies of the order $|\gamma|$ in which we are interested and which exceed the Fermi energy, the mean free path in not too contaminated specimens will be determined by electron-electron scattering processes and by the phonon radiation.⁴⁾ In Sec. 8 of the present

paper we estimate these effects. The result shows that both processes lead to a lifetime on the order of $\tau \sim E_0^2\gamma^{-2}|\gamma|^{-1} \sim 10^2|\gamma|^{-1}$. This corresponds to mean free paths on the order of $l \sim 10^{-3}$ cm. In the vicinity of the singularities the finite nature of τ will obviously be manifest at distances on the order of $\omega - \omega_C \sim 1/\tau \sim 10^{-2}|\gamma|$. To obtain a qualitative idea of the changes produced thereby, let us consider the singularity at $\omega = 2|\gamma|$ and replace ω in (33) by $\omega + i/\tau$.

As a result we obtain the following limiting relations:

$$\begin{aligned}
\epsilon_{zz} &= \frac{\pi^2 e^2 a^2 A}{2\sqrt{2}\gamma^2} \left(\frac{1}{\sqrt{1 - \omega/2|\gamma|}} + \frac{i}{4|\gamma|\tau(1 - \omega/2|\gamma|)^{3/2}} \right), \\
1 &\gg 1 - \omega/2|\gamma| \gg 1/2|\gamma|\tau; \\
\epsilon_{zz} &= \frac{\pi^2 e^2 a^2 A \tau^{1/2}}{2\sqrt{2}|\gamma|^{3/2}} \left\{ \left[1 + \left(1 - \frac{\omega}{2|\gamma|} \right) |\gamma|\tau \right] \right. \\
&\quad \left. + i \left[1 - \left(1 - \frac{\omega}{2|\gamma|} \right) |\gamma|\tau \right] \right\}, \\
1 &\gg 1/2|\gamma|\tau \gg |1 - \omega/2|\gamma||; \\
\epsilon_{zz} &= \frac{\pi^2 e^2 a^2 A}{2\sqrt{2}\gamma^2} \left(\frac{1}{4|\gamma|\tau(\omega/2|\gamma| - 1)^{3/2}} + \frac{i}{\sqrt{\omega/2|\gamma| - 1}} \right), \\
\omega/2|\gamma| - 1 &\gg 1/2|\gamma|\tau. \quad (43)
\end{aligned}$$

It follows therefore that the imaginary part of ϵ_{zz} does not vanish with decreasing frequency when $\omega = 2|\gamma|$, but decreases gradually. When $\omega = 2|\gamma|$ the real and imaginary parts are finite and equal to each other. $\text{Im } \epsilon_{zz}$ reaches its maximum value when $\omega/2|\gamma| - 1 = 1/2\sqrt{3}|\gamma|$, whereas $\text{Re } \epsilon_{zz}$ has a maximum at $1 - \omega/2|\gamma| = 1/2\sqrt{3}|\gamma|$. Both maxima have an absolute value $3^{3/4}\pi^2 e^2 a^2 A \tau^{1/4} / 4\sqrt{2}|\gamma|^{3/2}$.

The next effect that must be considered is the spatial dispersion. Let us consider again the singularity at $\omega = 2|\gamma|$. Account of the finite κ modifies the conservation law (10), which must be replaced by

$$\epsilon_3(\mathbf{k} + \boldsymbol{\kappa}/2) - \epsilon_2(\mathbf{k} - \boldsymbol{\kappa}/2) = \omega.$$

Recognizing that we are interested in large momenta, we obtain with the aid of formula (11) of [5]

$$\begin{aligned}
& [\gamma^2 + (p^2 - q^2 + a\kappa_z p - b\kappa_y q)/4p^2]^{1/2} \\
& + [\gamma^2 + (p^2 - q^2 - a\kappa_z p + b\kappa_y q)/4p^2]^{1/2} = \omega.
\end{aligned}$$

It follows from this equation that the lowest value corresponds, as before, to $p^2 = q^2$. If κ lies in the y, z plane, then when $a|\kappa_z| > b|\kappa_y|$ the smallest value of ω is

$$\omega_{\min} = 2\sqrt{\gamma^2 + (a|\kappa_z| - b|\kappa_y|)^2}. \quad (44)$$

When $a|\kappa_z| < b|\kappa_y|$ Eq. (12) is satisfied, as before. It must be taken into account here, however, that in the first case ω_{\min} occurs when $q_y = p$ and $q_x = 0$, while in the latter it occurs when q_y

⁴⁾The author is grateful to V. P. Silin, who called his attention to this circumstance.

$= p a \kappa_z / b \kappa_y$, $q_x = p \sqrt{1 - (a \kappa_z / b \kappa_y)^2}$, i.e., it first appears along a definite direction, and not along the entire conical surface. An exception is the case when the vector κ is directed along the z axis. Then

$$\omega_{min} = 2\sqrt{\gamma^2 + a^2 \kappa^2}, \quad (45)$$

and the open surfaces again appear along the cone.

In view of the fact that the system of eigenfunctions of the matrix $\hat{D}(\mathbf{k})$ depends on \mathbf{k} , we must calculate Q_{ik} using the exact formula (6) and the matrices (19) and (20). Since the singularity under consideration comes from the vicinity of $\mathbf{k} = 0$, we can put $\beta = \delta = 0$ in (19). We shall not present here all the details of this calculation. The result can be written in the following form. If we introduce a quantity $\epsilon_{ijk}(\kappa, \omega)$, related with $Q_{ik}(\kappa, \omega)$ by formula (8), then

$$\begin{aligned} \epsilon_{ik}(\kappa, \omega) = & \frac{\pi e^2 A}{16 |\gamma|^{3/2}} \int \left\{ 2a^2 n_z m_z + b^2 (n_x m_x + n_y m_y) \right. \\ & - 2ab \left(n_z \frac{qm}{q} + m_z \frac{qn}{q} \right) + b^2 \frac{q_y^2 - q_x^2}{q^2} (m_y n_y - m_x n_x) \\ & \left. + \frac{2b^2 q_x q_y}{q^2} (n_x m_y + n_y m_x) \right\} F(\omega, \xi) d\Omega, \end{aligned} \quad (46)$$

where

$$\begin{aligned} F(\omega, \xi) = & \begin{cases} (2|\gamma| + \xi - \omega)^{-1/2}, & 2|\gamma| + \xi > \omega \\ i(\omega - 2|\gamma| - \xi)^{-1/2}, & 2|\gamma| + \xi < \omega. \end{cases} \\ \xi = & (a\kappa_z p - b\kappa q)^2 / 4p^2 |\gamma|, \end{aligned} \quad (47)$$

\mathbf{n} and \mathbf{m} are unit vectors in the directions of \mathbf{i} and \mathbf{k} . Account is taken here of the fact that we are considering the vicinity of $\omega = 2|\gamma|$ and put $\xi \ll \gamma$ (this will be confirmed below).

We shall not consider all the possible cases. By way of an example we confine ourselves only to the simplest case, namely when the radiation is normally incident on the plane of the specimen, and this plane is perpendicular to the trigonal axis. Formula (46) simplifies in this case and assumes the form

$$\epsilon_{xx}(\omega, \kappa) = \frac{\pi^2 e^2 b^2 A}{4 |\gamma|^{3/2}} F\left(\omega, \frac{(a\kappa)^2}{4 |\gamma|}\right). \quad (48)$$

Substitution of this value in Maxwell's equations leads to the following result in the case of specular reflection of the electrons from the surface (see, for example, [7]):

$$\frac{A(0)}{H(0)} = \frac{2}{\pi} \int_0^\infty \frac{d\kappa}{\kappa^2 - \epsilon_{xx}(\omega, \kappa) \omega^2 / c^2 - i\delta}. \quad (49)$$

The impedance is equal to

$$Z = -\frac{4\pi i \omega}{c} \frac{A(0)}{H(0)}. \quad (50)$$

We introduce the following quantities

$$S = 2\pi^2 e^2 b^2 |\gamma| A / ac^2, \quad \alpha = 4|\gamma| (2|\gamma| - \omega) / a^2.$$

We then have

$$\frac{A(0)}{H(0)} = \frac{2}{\pi} \int_0^\infty \frac{d\kappa}{\kappa^2 - S / \sqrt{\kappa^2 + \alpha} - i\delta}$$

(if $\alpha + \kappa^2 < 0$, then $\sqrt{\kappa^2 + \alpha} \rightarrow -i\sqrt{-\alpha - \kappa^2}$). According to this formula, the spatial dispersion becomes appreciable when $\alpha^{1/2} \sim S^{1/3}$ or

$$\omega - \omega_c \sim (v^2 E_0^2 / c^2 \gamma^2)^{1/3} |\gamma| \sim 0.01 |\gamma|.$$

Consequently, this effect is no less important than the finite nature of τ .

We present the limiting formulas for the impedance.

1) Case $S^{1/3} \gg |\alpha|^{1/2}$; the impedance is

$$\begin{aligned} Z = & \frac{16\pi |\gamma|}{3 \sqrt{3} c^2 S^{1/3}} \left[\sqrt{3} \left(1 + \frac{1}{2} \frac{\alpha}{S^{1/3}} - \frac{3}{4} \frac{\alpha}{S^{2/3}} \theta(-\alpha) \right) \right. \\ & \left. - i \left(1 - \frac{3 \sqrt{3}}{4\pi} \frac{\alpha}{S^{1/3}} \ln \frac{S^{1/3}}{|\alpha|} \right) \right], \end{aligned} \quad (51)$$

where $\theta(x) = 1$ when $x > 0$ and $\theta(x) = 0$ when $x < 0$. We see from this formula that the real part of the impedance has a minimum (with a kink) at the point $\omega = 2|\gamma|$, but does not vanish, as would follow from the formula $Z = 4\pi/c\sqrt{\epsilon}$ with ϵ determined from formula (33). The imaginary part of Z has for $\omega = 2|\gamma|$ an infinite derivative. If we introduce the concept of the effective dielectric constant $\epsilon_{eff} = (4\pi/cZ)^2$, then from (51)

$$\epsilon_{eff} \sim (cE_0^2 / v\gamma^2)^{1/3} (1 + i\sqrt{3}), \quad (52)$$

where $E_0 \sim 0.1-1$ eV and $v \sim 10^8$ cm/sec. Thus $\epsilon_{eff} \sim 10^3$. This means that when $\omega = 2|\gamma|$, ϵ_{eff} has time to grow tenfold compared with the value of ϵ far from this point.

2) Case $S^{1/3} \ll |\alpha|^{1/2}$; then

$$\begin{aligned} Z = & \frac{8|\gamma|}{c^2} \left(\pi \sqrt{\frac{\alpha}{S}} - \frac{2}{3} i \frac{S}{\alpha^2} \right), \quad \alpha > 0, \\ Z = & \frac{8|\gamma|}{\sqrt{2} c^2} \pi \sqrt{\frac{|\alpha|}{S}} (1 - i), \quad \alpha < 0. \end{aligned} \quad (53)$$

Thus, the imaginary part of Z does not vanish with decreasing frequency when $\omega = 2|\gamma|$, but decreases continuously toward the lower frequencies.

In addition to the effects considered, there is still another, yielding corrections of the same order of magnitude. We calculated the state density (28) inaccurately, since we effectively assumed that the surface $\nu = \epsilon_3 - \epsilon_2 = \text{const}$ changes abruptly from dimensions $\sim |\gamma|^3$ when $\nu < \omega_c$ to dimensions $\sim E_0^2 |\gamma|$ when $\nu > \omega_c$. Actually this occurs gradually, albeit within a very small frequency interval. For example, in the vicinity of $\nu = 2|\gamma|$ we would

have to take, strictly speaking, not the integral $(\nu^2 - 4\gamma^2)^{-1/2} \int p dp$ but the integral $\int p^2 dp \times [4\gamma^2 \Delta^2 + (\nu^2 - 4\gamma^2)p^2]^{-1/2}$, obtained from formula (13b) of [5]. The limit of integration is E_0 or the number obtained from the condition that the radicand be positive.⁵⁾ As a result we obtain when $\nu \approx 2|\gamma|$

$$\frac{dZ}{d\nu} = \frac{\Delta^2 |\gamma|^{3/2}}{2ab^2\pi^2 (2|\gamma| - \nu)^{3/2}} \frac{\pi}{2}, \quad |\gamma| \gg 2|\gamma| - \nu > \frac{\Delta^2}{E_0^2} |\gamma|;$$

$$\frac{dZ}{d\nu} = \frac{\Delta^2 |\gamma|^{3/2}}{2ab^2\pi^2 (2|\gamma| - \nu)^{3/2}} \left[\arcsin \left(\frac{E_0}{\Delta} \sqrt{\frac{2|\gamma| - \nu}{|\gamma|}} \right) - \frac{E_0}{\Delta} \sqrt{\frac{2|\gamma| - \nu}{|\gamma|}} \sqrt{1 - \frac{E_0^2}{\Delta^2} \left(\frac{2|\gamma| - \nu}{|\gamma|} \right)} \right],$$

$$0 < 2|\gamma| - \nu < \Delta^2 E_0^{-2} |\gamma|;$$

$$\frac{dZ}{d\nu} = \frac{\Delta^2 |\gamma|^{3/2}}{2ab^2\pi^2 (\nu - 2|\gamma|)^{3/2}} \times \left[\frac{E_0}{\Delta} \sqrt{\frac{\nu - 2|\gamma|}{|\gamma|}} \sqrt{1 + \frac{E_0^2}{\Delta^2} \left(\frac{\nu - 2|\gamma|}{|\gamma|} \right)} - \operatorname{Arsh} \left(\frac{E_0}{\Delta} \sqrt{\frac{\nu - 2|\gamma|}{2|\gamma|}} \right) \right],$$

$$|\gamma| \gg \nu - 2|\gamma| > 0. \quad (54)^*$$

It is seen therefore that $dZ/d\nu$ "gets spoiled" when $2|\gamma| - \nu \sim \Delta^2 E_0^{-2} |\gamma| \sim (10^{-2} - 10^{-3}) |\gamma|$. As a result ϵ_{ik} no longer becomes infinite. $\operatorname{Im} \epsilon_{ik}$, which is proportional to $dZ/d\nu$ has a maximum at the point $\omega = 2|\gamma| - \Delta^2 E_0^{-2} |\gamma|$. At this point

$$\operatorname{Im} \epsilon_{zz} = \pi e^2 a E_0^3 / 4b^2 \Delta \gamma^2. \quad (55)$$

$\operatorname{Re} \epsilon_{ik}(\omega)$ is also finite.

In the vicinity of the other thresholds, where there are logarithmic singularities, the formulas are employed at distances on the order of $\delta^2 E_0^{-2} |\gamma| \sim (10^{-2} - 10^{-3}) |\gamma|$ from the threshold. The logarithmic infinity disappears.

This investigation shows that the main effects determining the behavior of ϵ_{ik} in the vicinity of the singularities are the finite nature of the free path, the spatial dispersion, and the gradual increase of the open surfaces. All these effects yield results of comparable order of magnitude. In view of the fact that we are dealing with relatively weak integrable singularities, it is hardly of importance which of the effects predominates. It is merely important that all effects lead to the vanishing of the infinities.

⁵⁾Of course, this deduction and Eqs. (54) and (55) are not rigorous, since we integrated over large momenta where the form of the spectrum obtained in [5] no longer is correct. We include these formulas to illustrate the influence of the gradual growth of the open surfaces.

*Arsh = \sinh^{-1} .

6. START OF ABSORPTION

When $\omega \ll |\gamma|$, as already explained above, the principal values of the tensor $(\epsilon_{ik})_{II}$ are positive constants on the order of 100, i.e., there exists a region of frequencies in which the metal is transparent with respect to radiation. It can be shown that an account of the spatial dispersion does not introduce any imaginary additions to ϵ_{ik} , and consequently the only source of absorption is the finite free path of the electrons. Assuming the free path equal to 0.001 cm (see Sec. 8) we arrive at the conclusion that $\epsilon^{-1} \operatorname{Im} \epsilon \sim (\omega\tau)^{-1} \sim 10^{-2}$, i.e., $\operatorname{Im} \epsilon \sim 1$, in other words, the radiation with $\omega \sim |\gamma|$ will be absorbed at distances on the order of $c\sqrt{\epsilon}/\omega \operatorname{Im}(\epsilon) \sim 0.01$ cm.

In view of such transparency, interest attaches to the absorption due not only to the direct transitions between levels with open surfaces, but also between levels with closed surfaces, beginning at lower frequencies. The start of such transitions is obviously determined by formula 10, where for electrons $\epsilon_3^{(1)}(\mathbf{k}) = \mu$ and for holes $\epsilon_2^{(0)}(\mathbf{k}) = \mu$. Inasmuch as for holes the condition (11) is exact, the threshold frequency is determined by the condition

$$\omega^{(0')} = 2(f - \mu). \quad (56)$$

According to (11), the equal-energy surfaces for $\epsilon_2^{(0)}$ and $\epsilon_3^{(0)}$ coincide, so that the transitions occur between the surfaces.

In the case of electrons, the equal-energy surfaces $\epsilon_2^{(1)}$ and $\epsilon_3^{(1)}$ are different. Since both surfaces are closed, their intersections are in general closed contours. Obviously, the extreme case is tangency of the two surfaces at one point (with the surface $\epsilon_2^{(1)} = \text{const}$ inside $\epsilon_3^{(1)} = \mu$). It is difficult to determine the threshold frequency for this case. We shall denote it by $\omega^{(1)''}$.

Let us consider now the order of magnitude of the contribution made to $\operatorname{Im} \epsilon_{ik}$ by such transitions, and the behavior of $\operatorname{Im} \epsilon_{ik}$ near threshold. With the aid of formulas (6) and (8) we obtain

$$\operatorname{Im} \epsilon_{ik} = \frac{4e^2\pi^2}{\omega^2} \int_{23}^i \int_{32}^k \left[\frac{dZ}{d(\epsilon_3 - \epsilon_2)} \right]_{\epsilon_3 - \epsilon_2 = \omega} \quad (57)$$

for $\epsilon_2^{(0)} < \mu$ or $\epsilon_3^{(1)} > \mu$. It follows from this formula that at the value $\omega^{(0)'}$, given by (56) the absorption begins with a finite value of order unity. In the vicinity of the electron threshold $\omega^{(1)'}$, where the surfaces are tangent, the interval of solid angles varies in proportion to $\omega - \omega^{(1)''}$, so that in this vicinity

$$\operatorname{Im} \epsilon_{ik} \sim (\omega - \omega^{(1)'}) / \omega^{(1)'}. \quad (58)$$

Without determining the numerical values of the parameters it is impossible to indicate which

threshold will be lower, $\omega^{(0)}$, or $\omega^{(1)}$. Above the threshold $\text{Im } \epsilon$ will be of order of unity, which leads to damping of the radiation at distances on the order of 10^{-2} cm.

7. NOTES ON THE EXPERIMENTAL RESULTS

We first summarize the results obtained. In the region of low frequencies we obtained

$$\epsilon_{ik} = \epsilon_{0ik} - \Omega_{ik}^2 \omega^{-2}, \quad (59)$$

where ϵ_{0ik} is due to direct transitions between the bands, and the second term is connected with transitions inside the band. The value of ϵ_0 is of the order of $(E_0/\gamma)^2$ where according to theory $E_0 \sim 0.1-1$ eV and $|\gamma| \sim 0.01 = 0.1$ eV. The order of magnitude of Ω_{ik} is $|\gamma|$. The second term prevails over the first at frequencies

$$\omega \ll \gamma^2/E_0 \ll |\gamma|.$$

We note that in this case

$$\kappa \sim \omega c^{-1} \sqrt{|\epsilon|} \sim \Omega/c \sim \gamma/c.$$

In order for our calculation to be correct, it is required that $\omega \gg v\kappa \sim v c^{-1} |\gamma|$. Thus, $\epsilon_{ik} \approx -\Omega_{ik}^2 \omega^{-2}$ in the interval

$$\frac{|\gamma|}{E_0} |\gamma| \gg \omega \gg \frac{v}{c} |\gamma|. \quad (60)$$

According to the experimental data $|\gamma|/E_0 \sim 0.1$, and v/c can be assumed to be of the order of $10^{-2} - 10^{-3}$. Thus, the frequency interval in which $\epsilon_{ik} = -\Omega_{ik}^2 \omega^{-2}$ actually exists.

The tensor ϵ_{ik} retains its form (59) up to $\omega \sim |\gamma|$. In this region there are several weak singularities of ϵ_{ik} and a component $\text{Im } \epsilon_{ik}$ appears, comparable in value with $\text{Re } \epsilon_{ik} \sim \epsilon_{0ik}$. At frequencies $\omega \gg |\gamma|$ we have

$$\text{Re } \epsilon_{ik} = -\Theta^2 \omega^{-2} \delta_{ik}, \quad (61)$$

where $\Theta \sim E_0$. It follows therefore that in the region $\omega \sim |\gamma|$ the value of $\text{Re } \epsilon_{ik}$ reverses sign.

As regards $\text{Im } \epsilon_{ik}$, in the region of low frequencies, where, on the other hand, $\text{Re } \epsilon_{ik}$ is already positive, we have $\text{Im } \epsilon_{ik} \sim \epsilon_{0ik}/\omega\tau \sim 10^{-2} \epsilon_{ik}^{(0)} \sim 1$ ($l \sim 10^{-3}$ cm). Starting with some threshold value, an additional term appears in $\text{Im } \epsilon_{ik}$, also of order unity, and this term can either appear abruptly, or begin in accordance with formula (58). Finally, starting with the threshold value (15), $\text{Im } \epsilon_{ik} \sim \epsilon_{ik}^{(0)} \sim 10^2$ appears abruptly. Starting with the threshold (12), the value of $\text{Im } \epsilon_{ik}$ increases further by an amount of the same order. When $\omega \gg |\gamma|$ the value of $\text{Im } \epsilon_{ik}$ drops as $\text{Im } \epsilon_{ik} \sim E_0^2 \gamma^2 / \omega^4$.

At the present time we still do not have the numerical values of all the parameters. Therefore a quantitative comparison of theory with experiment is premature. Qualitatively, however, the foregoing results are in splendid agreement with the available experimental data^[2,3]. These results were obtained for bismuth with the aid of experiments on reflection from a plane surface and after passage of the radiation through thin plates. The presence of a frequency region with positive ϵ_{ik} was established there. Moreover, formula (59) was confirmed and it was found that $\epsilon_{0ik} \sim 100$. This quantity determines the ratio $(E_0/|\gamma|)^2$, which is very important for the entire theory of bismuth-type metals. The experiments with reflection have made it possible to fix especially the frequencies for which ϵ_{xx} or ϵ_{zz} vanishes. If these frequencies are denoted respectively by ω_x and ω_z , then, from (59),

$$\omega_x = \frac{\Omega_{xx}}{\sqrt{\epsilon_{0xx}}}, \quad \omega_z = \frac{\Omega_{zz}}{\sqrt{\epsilon_{0zz}}}, \quad \frac{\omega_z}{\omega_x} = \frac{\Omega_{zz}}{\Omega_{xx}} \frac{\sqrt{\epsilon_{0xx}}}{\sqrt{\epsilon_{0zz}}}. \quad (62)$$

We note that ω_z/ω_x depends only on the constants of the spectrum, while ϵ_{0ik} contains one new constant A in the form of a proportionality coefficient. Thus, knowledge of the frequencies ω_x and ω_z makes it possible once more to check qualitatively the theory and find the constant A which determines the processes in which the open surfaces participate. Of course, this can be done only after the constants of the spectrum are determined in an independent manner.

Finally, noticeable absorption was observed, starting with frequencies 0.06 eV, in experiments on the passage of radiation. According to Markov and Khaikin^[3], $\text{Re } \epsilon$ begins to decrease noticeably at high frequencies. This shows that we are dealing here with the beginning of transitions between open surfaces, i.e., the value of $\omega^{(1)}$ as determined by (15) is approximately 0.06 eV.

8. APPLICABILITY OF THE GAS MODEL

In all the calculations we used the model of non-interacting quasiparticles with a definite energy spectrum. As is well known, according to the Landau theory of the Fermi liquid (see^[8], Sec. 2), this is valid in an ordinary metal only in the vicinity of the Fermi surface. Even in this case, "Fermi-liquid" effects, due to the interaction between quasiparticles, appear in many phenomena. This pertains in particular to the dielectric constant in the infrared region [see^[9], formula (8)]. We shall show that in metals of the bismuth type

the f -function is small, and moreover, the quasi-particle concept is applicable away from the Fermi surface.

We shall find it useful, to this end, to determine the order of magnitude of the dielectric constant $\epsilon_{jk}(\omega, \kappa)$ for different ω and κ . We have established that when $\omega \gg v\kappa$ the order of magnitude of ϵ is determined by the formula $\epsilon = \epsilon_0 - \Omega^2/\omega^2$, where $\epsilon_0 \sim 100$ and $\Omega \sim |\gamma|$.

In the opposite limiting case $v\kappa \gg \omega$, the contribution of the intra-band transitions is well known. It is equal to $1/r_D^2 \kappa^2$, where r_D is the Debye radius and is of order $r_D \sim v/|\gamma|$. The interband transitions yield in this case $\epsilon \sim \epsilon_0$ for $\kappa \lesssim |\gamma|/v$ and $\epsilon \sim \epsilon_0 \gamma^2 / (v\kappa)^2$ for $\kappa \gg |\gamma|/v$.

We now consider the function f . As shown in the papers of Silin^[10] and Luttinger^[11], it is necessary to include in the function f only the "non-Coulomb" terms. They are expressed by diagrams which contain no Coulomb lines, over which the main momentum transfer takes place. These diagrams always contain integration over the momenta of the Coulomb lines. Examples are the diagrams for ϵ_{jk} shown in the figure. If the external momentum κ and the frequency ω are not large compared with $|\gamma|/v$ and $|\gamma|$, then the momentum of the Coulomb line is of order $|\gamma|/v$, and the frequency transmitted over it is of the order of the external frequency, or $v\kappa$. Thus, this line corresponds to $4\pi e^2/q^2 \epsilon_0$. An estimate shows that the diagram of type a has a relative order of magnitude $1/\epsilon_0$, while the remaining ones are accordingly even smaller. An exception is the vicinity of the singularity, but, as has been explained in Sec. 5, even there the interaction does not play an important role. An analogous estimate can be used to explain the role of the function f in other effects, too (for example, the connection between the true velocity v and the bare velocity). The result is the same.

The electrons interact not only with one another, but also with the phonons. This interaction is also of Coulomb origin. It represents the interaction between the electron charge and the polarized charge due to the lattice vibrations. Consequently, the dielectric constant plays a role here, too. If we repeat the usual derivation (see^[8], Secs. 7 and 9), then it turns out that to each phonon vertex there corresponds not the interaction constant $g \sim \sqrt{a/m}$, but $g \sim (a^{3/2} m^{1/2} \epsilon(\omega, q) q^2)^{-1}$, where a is the period of the lattice, m the mass of the free electron, and ω and q the frequency and momentum of the phonon. Putting $a \sim v/E_0$ and $m \sim E_0/v^2$ and recognizing that the momenta q of

order $|\gamma|/v$ are of importance, we arrive at the conclusion that all the effects into which g^2 enters are attenuated by a factor $1/\epsilon_0$. This pertains, in particular, to the correction to the quasi-particle velocity (see^[8], Sec. 21).

Let us consider now the question of closeness to the Fermi surface. The criterion for the applicability of the concept of quasiparticles is, as is well known, the smallness of their damping $1/\tau$ compared with the energy (reckoned from μ). The damping at $T = 0$ is determined by two processes, electron-electron scattering and phonon emission. In an ordinary metal the first of these processes yields

$$\begin{aligned} 1/\tau &\sim [\epsilon(k) - \mu]^2/\mu \quad \text{for } |\epsilon(k) - \mu| \ll \mu, \\ 1/\tau &\sim \epsilon_F \quad \text{for } \epsilon \gtrsim \mu. \end{aligned}$$

The second yields

$$\begin{aligned} 1/\tau &\sim [\epsilon(k) - \mu]^3/\omega_D^2 \quad \text{for } |\epsilon(k) - \mu| \ll \omega_D, \\ 1/\tau &\sim \omega_D \quad \text{for } |\epsilon(k) - \mu| \gtrsim \omega_D. \end{aligned}$$

It follows therefore that when $|\epsilon(k) - \mu| \sim \mu$ and $|\epsilon(k) - \mu| \sim \omega_D$ we have

$$1/\tau \sim |\epsilon(k) - \mu|.$$

Let us examine the situation in our case for electrons with energy of order $|\gamma|$. For electron-electron collisions we have in order of magnitude

$$\begin{aligned} \frac{1}{\tau} &\sim (4\pi e^2)^2 \\ &\times \int \frac{dk_2 dk'_1}{(2\pi)^3} \frac{\delta(\epsilon(k_1) + \epsilon(k_2) - \epsilon(k'_1) - \epsilon(k'_2))}{\{\epsilon_{ik} [\epsilon(k_1) - \epsilon(k'_1), k_1 - k'_1] (k_{1i} - k'_{1i}) (k_{1k} - k'_{1k})\}^2} \\ &\approx \frac{e^4}{\epsilon_0^2} \frac{1}{|\gamma|} \frac{E_0^2}{v^2} \sim \frac{|\gamma|^3}{E_0^3} \sim \frac{|\gamma|}{\epsilon_0} \ll |\gamma| \end{aligned}$$

(the factor E_0^2/v^2 is due to integration over the large momenta k_2 ; the significant transfers are $|k_1 - k'_1| \sim |\gamma|/v$). As to the damping connected with the possibility of phonon emission, it is essentially different for electrons at levels with closed and open equal-energy surfaces. In the former case the directions of the possible phonon momenta are limited by the energy conservation requirements. A simple calculation using the interaction constant obtained above yields $1/\tau \sim |\gamma|/\epsilon_0 \ll |\gamma|$. For levels with open surfaces there is no such limitation. As a result we obtain $1/\tau \sim \omega_D$ as in an ordinary metal. As is well known, in bismuth $\omega_D \approx 10^{-2}$ eV and most likely $|\gamma|$ is closer to 0.1 eV. This makes it possible to assume in the latter case that $1/\tau \ll |\gamma|$. In the vicinity of the thresholds for the appearance of open surfaces, the phase-space region accessible,

to phonons is limited by the volumes in the surfaces. Analysis shows that it is possible to use here in practice the same estimate of $1/\tau$ as for closed surfaces.

The estimates made prove the applicability of the gas model used in the present calculations. It must be borne in mind, however, that when the energy increases to an order of 1 eV the dielectric constant decreases and the interaction becomes strong. At these energies, the quasi-particle model cannot be employed, as is the case with an ordinary metal.

In conclusion I thank I. M. Lifshitz and L. P. Pitaevskii for a discussion of the work.

¹A. A. Abrikosov, JETP **44**, 1632 (1963), Soviet Phys. JETP **17**, 1099 (1963).

²W. S. Boyle and A. D. Brailsford, Phys. Rev. **120**, 1943 (1960).

³M. N. Markov and A. S. Khaikin, Opt. i spektr. **9**, 487 (1960).

⁴A. A. Abrikosov, JETP **43**, 1083 (1962), Soviet Phys. JETP **16**, 765 (1963).

⁵A. A. Abrikosov and L. A. Fal'kovskii, JETP **43**, 1089 (1962), Soviet Phys. JETP **16**, 769 (1963).

⁶L. A. Fal'kovskii, JETP **44**, 1935 (1963), this issue p. 1302.

⁷A. A. Abrikosov and I. M. Khalatnikov, Appendix to the collection Fizika nizkikh temperatur (Low-Temperature Physics), IIL, 1959, pp. 101 and 912.

⁸Abrikosov, Gor'kov, and Dzyaloshinskii, Metody kvantovoi teorii polya v statisticheskoi fizike (Methods of Quantum Field Theory in Statistical Physics), Fizmatgiz, 1962.

⁹V. P. Silin, JETP **34**, 707 (1958), Soviet Phys. JETP **7**, 486 (1958).

¹⁰V. P. Silin, JETP **33**, 495 (1957), Soviet Phys. JETP **6**, 387 (1958).

¹¹P. Nozieres and J. M. Luttinger, Phys. Rev. **127**, 1423 and 1431 (1962).

Translated by J. G. Adashko
321