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THEORY OF THE CLASSICAL SIZE EFFECT IN THE ELECTRIC CONDUCTIVITY OF SEMIMETALS

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A general theory of the size effect in the electric conductivity of semimetals is developed in the relaxation time approximation which takes into account the various mechanisms of carrier relaxation on the surface and within the sample. The kinetic equations are reduced to a set of integral equations determining the spatial distribution of the concentrations of carriers belonging to different valleys and also of the transverse electric field. A general analysis shows that intervalley scattering at the surface leads to a specific result, viz. in the quasineutral region the transverse electric field and all concentration gradients become nonuniform and increase logarithmically with approach to the surface at distances of the order of the usual mean free path l. In plates with a thickness $2b \gtrsim l$ the coefficient before the logarithmic term is of the order of the applied longitudinal field. The bend in the band near the surface V should be of decisive importance for the electric conductivity of thin plates ($2b < l$); the bend makes access of the surface difficult for carriers of one sign or another (electrons or holes) and creates conditions for specular reflection for a certain part of the carriers. The behavior of the conductivity consequently changes for $2b \ll l$; thus it tends to saturation if V at both surfaces is of the same sign, in distinction to the usual monotonous decrease. The general course of the dependence of the conductivity on thickness (which should include three plateaus) is established. The height of the first (for $2b \approx l$) elevation is related to the degree of specularity of scattering at the surface; the height of the second elevation for large thicknesses is related to the intensity of intervalley scattering at the surface.

INTRODUCTION

GORKUN and one of the authors[1] have shown that earlier attempts[2,3] of generalizing the well known Fuchs theory[4] of the size effect in the electric conductivity of thin films to include multivalley semimetals and semiconductors were incorrectly performed, and in certain cases even lead to an incorrect qualitative picture. The reason is that the effect of the redistribution of the carriers among the valleys[5,6] is ignored in[2,3], and a non-self-consistent procedure is used to solve the equations.

The case considered in[1] is one for which a simple exact solution is obtained, namely the case when there is no intervalley scattering in the volume or on the surface. Since the experimental situation is also discussed in detail in[1], we shall not touch upon this aspect of the problem here.

We consider below a much more general model, when intervalley scattering in the volume and on the surface is taken into account (but it is assumed, as before, that the ordinary mean free path l is much smaller than the diffusion displacement length L with respect to intervalley scattering), and a wide range of thicknesses is considered. We investigate also the role of the near-surface bending of the bands in connection with its influence on the surface scattering. Unlike metals, in which there is practically no bending, and semiconductors, where the predominant effect is modulation of the conductivity in the surface layer of the space charge, in semi-metals of the Bi type with large l the near-surface bending of the bands greatly influences the distribution function of the carriers in the quasineutral region. It must be emphasized that a unique role is played in this case by the intervalley surface scattering.

The main qualitative results of the paper are as follows: in the assumed model, the effective electric conductivity σ of plates, as a function of the thickness 2b, should exhibit three plateaus (Fig. 1). The first plateau ($2b \ll l$) is due to the transport of current exclusively by a definite fraction of the carriers of that sign, for which the near-surface bending of the bands is repulsive. The second plateau ($l \ll 2b \ll L$) is due to the non-equilibrium concentration of the carriers from different valleys under the conditions of the diffusion approximation (cf. [1,5]). The third plateau ($2b \gg L$) corresponds to samples of maximum thickness. Owing to the intervalley scattering of the carriers from the surface, the transverse field produced in the interior of the plate turns out to be sharply inhomogeneous and increases logarithmically on approaching the boundary of the quasineutral region.

A plateau in the $\sigma(b)$ dependence of Bi has been observed in a number of already performed experimental investigations[7-10]. Apparently, for a unique correspondence with the plateaus obtained in our theory, it would be desirable to carry out a more detailed quantitative study and to perform the measurements in a wider range of thicknesses. It would also be of great

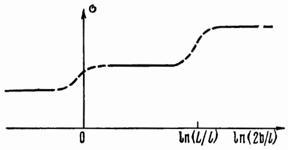

FIG. 1. Dependence of the effective electric conductivity σ on the thickness of the plate 2b in the presence of a near-surface bending of the bands.

interest to measure the transverse field, since such measurements would make it possible to estimate directly the role of the intervalley scattering on the surface. It is particularly advisable to perform all these experiments under conditions of controlled bending of the bands in field-effect experiments.

1. FUNDAMENTAL EQUATIONS AND BOUNDARY CONDITIONS

Let us consider a degenerate semimetal with several electron valleys, which we shall number by the index β, and one valley in the valence band, which we shall designate by the index v. We shall henceforth assume that all the valleys are ellipsoidal, and assume for simplicity that the intravalley scattering can be described by a scalar relaxation time (τ_c^0 in the electronic valleys and τ_v^0 in the valence band); we introduce the times T and T_v characterizing respectively the scattering between electronic valleys and scattering from electronic valleys into the valence band. We shall assume throughout that $T, T_v \gg \tau_c^0, \tau_v^0$. All the distribution functions f for all the valleys will be regarded as functions of the velocities and will be represented, as usual, in the form

$$f = f_0(\varepsilon - \zeta) + \frac{\partial f_0}{\partial \varepsilon}\varphi,$$

The chemical potentials ζ_β and ζ_v are reckoned from the edge of the corresponding band. Then the system of kinetic equations can be written in the form

$$v_z\frac{\partial \varphi_\beta}{\partial z} - e\mathbf{E}\mathbf{v} + \frac{\varphi_\beta - \overline{\varphi}_\beta}{\tau_c{}^0} + \sum_{\beta' \neq \beta}\frac{\overline{\varphi}_\beta - \overline{\varphi}_{\beta'}}{T} + \frac{\overline{\varphi}_\beta - \overline{\varphi}_v}{T_v} = 0, \quad \text{(1a)}$$

$$v_z\frac{\partial \varphi_v}{\partial z} - e\mathbf{E}\mathbf{v} + \frac{\varphi_v - \overline{\varphi}_v}{\tau_v{}^0} + \sum_\beta \frac{\overline{\varphi}_v - \overline{\varphi}_\beta}{qT_v} = 0. \quad \text{(1b)}$$

The symbol $\overline{\varphi}$ denotes here the mean values over the corresponding Fermi ellipsoids, for example $\overline{\varphi}_\beta = \langle \varphi \rangle_\beta / \langle 1 \rangle_\beta$, where the angle brackets denote integrals:

$$\langle F \rangle_\beta = -\int F_\beta(\mathbf{v})\frac{\partial f_0{}^\beta}{\partial \varepsilon}d\tau_\beta, \quad d\tau_\beta = \frac{2}{h^3}d^3p_\beta. \quad \text{(2)}$$

The quantities $\overline{\varphi}_\beta$ and $\overline{\varphi}_v$, taken with the inverse sign, have the meanings of additions to the chemical potential for the corresponding carrier groups, i.e., they are proportional to the non-equilibrium additions to their concentrations. All the intervalley relaxation terms are written in such a manner that they are cancelled out when the Fermi levels of any two valleys are raised by equal amounts (two electron valleys or one electron and one valence valley). The parameter q is determined from the detailed balancing principle and equals

$$q = \frac{\langle 1 \rangle_v}{\langle 1 \rangle_\beta} = \left(\frac{m_v{}^3\zeta_v}{m_c{}^3\zeta_\beta}\right)^{1/2}, \quad \text{(3)}$$

m_c and m_v are masses which determine the density of states (i.e., the geometric means of the three principal values).

The kinetic equations (1) should be supplemented by the Poisson equation, which reduces throughout, with the exception of the narrow layer near the surface, to the quasineutrality condition

$$\sum_\beta \overline{\varphi}_\beta + q\overline{\varphi}_v = 0. \quad \text{(4)}$$

It is necessary to formulate boundary conditions for the system (1) and (4). Since (4) does not hold in the space-charge regions near the boundaries of a semimetal, with a width of the order of several Debye lengths $l_D = (\kappa\zeta/4\pi e^2 n)^{1/2}$ (which amounts to usually 10^{-5}–10^{-6} cm, where κ is the dielectric constant), it is necessary to formulate effective boundary conditions for the boundaries of the quasineutral region. We shall consider below only plates with $2b \gg l_D$, when the thickness of the quasineutral region is practically equal to the thickness of the plate. Since in semimetals (unlike semiconductors) the carrier density in the near-surface layers is of the same order of magnitude as inside the volume, the conductivity of the near-surface channels should in itself not make an appreciable contribution to the total current, and therefore the bending of the bands should influence the conductivity mainly via changes of the boundary conditions for the quasineutral region.

This latter question is considered in the Appendix. Physically, the situation reduces to the fact that if the bands at the surface are curved, say, upward (see Fig. 2), then only electrons moving to the surface inside a certain cone (attainability cone), surrounding the normal, can reach the surface. The remaining electrons are specularly reflected from the space-charge layer. This is correct in the compressed-gas approximation $nl_D^3 \gg 1$.

As a net result, the effective boundaries on the left boundary can be represented in the form

$$\varphi_\beta^>(-b, \mathbf{v}^*) = \varphi_\beta^<(-b, \mathbf{v}), \quad \text{outside the cone} \quad \text{(5a)}$$

$$\varphi_\beta^>(-b, \mathbf{v}^*) = p_c^-\,\varphi_\beta^<(-b, \mathbf{v}) + B_\beta^-, \quad \text{inside the cone} \quad \text{(5b)}$$

$$\varphi_v^>(-b, \mathbf{v}^*) = p_v^-\,\varphi_v^<(-b, \mathbf{v}) + B_v^-. \quad \text{(5c)}$$

Here $\varphi \gtrless$ are respectively the distribution functions for the electrons with $v_z \gtrless 0$, the velocities v and v* are connected by the conditions for elastic specular scattering for non-spherical surfaces (see [3], and also (I.12)[1)]), p_c and p_v are the effective specularity coefficients, and the constants B_β and B_v are determined from the condition of the integral flux balance on the surface[2)]. Although (5) has been formally written out for z = b, actually we have in mind the condition on the boundary of the quasineutral region. An analogous system is written for z = b. Equations (5a) and (5b) are best represented in a unified form (5b), regarding p_c and B_β as functions of v_z, which change jumpwise on the surface of the cone.

Using (4), we can partly decouple the system (1):

$$v_z\frac{\partial \varphi_\beta}{\partial z} + \frac{\varphi_\beta}{\tau_c} - e\mathbf{E}\mathbf{v} - \frac{\overline{\varphi}_\beta - G_\beta}{\tau_c} = 0, \quad \text{(6)}$$

and analogously for φ_v, where (N is the number of electronic valleys)

[1)] Here and below, all references to the formulas of the article [1] are marked with the index I.

[2)] The role of this condition is explained in [11].

$$\frac{1}{\tau_c}=\frac{1}{\tau_c^0}+\frac{N-1}{T}+\frac{1}{T_v},\quad \frac{1}{\tau_v}=\frac{1}{\tau_v^0}+\frac{N}{qT_v},\tag{7a}$$

$$G_\beta(z)=\tau_c\left(\frac{N}{T}+\frac{1}{T_v}\right)\bar\varphi_\beta-\tau_c\left(\frac{1}{T_v}-\frac{q}{T}\right)\bar\varphi_v,\quad G_v(z)=\tau_v\frac{N+q}{qT_v}\bar\varphi_v.\tag{7b}$$

We solve formally the equations (6), assuming $\overline{\varphi}$ and E_Z to be known function of z, and we use the boundary conditions. Then

$$\varphi_\beta^{\lessgtr}(z,\mathbf{v})=\bar\varphi_\beta(z)-G_\beta(z)+\frac{1}{\Delta_c(v_z)}\Big\{\mathscr{B}_\beta^{\mp}\exp\left(-\frac{z\mp b}{v_z\tau_c}\right)+\mathscr{B}_\beta^{\pm}p_c^{\mp}$$
$$\times\exp\left(-\frac{z\pm b}{v_z\tau_c}\right)+\frac{p_c^{\mp}}{|v_z|}\int_{-b}^{b}dz'e(\mathbf{v}^*\mathbf{E}_\beta(z'))\exp\left(-\frac{z+z'}{v_z\tau_c}\right)$$
$$+\frac{1}{v_z}\int_{\mp b}^{z}dz'e(\mathbf{v}\mathbf{E}_\beta(z'))\exp\left(\frac{z'-z\pm 2b}{v_z\tau_c}\right)$$
$$+\frac{p_c^+p_c^-}{v_z}\int_{z}^{\pm b}dz'e(\mathbf{v}\mathbf{E}_\beta(z'))\exp\left(\frac{z'-z\mp 2b}{v_z\tau_c}\right)\Big\},\tag{8}$$

and analogously for $\varphi_V^{\gtrless}$. Here

$$\Delta_c(v_z)=\exp\left(\frac{2b}{|v_z|\tau_c}\right)-p_c^+p_c^-\exp\left(-\frac{2b}{|v_z|\tau_c}\right),\tag{9}$$

$$E_\beta(z)=\left(E_x,E_y,E_z-\frac{1}{e}\frac{d}{dz}(\bar\varphi_\beta-G_\beta)\right),\tag{10}$$

$$\mathscr{B}_\beta^{\pm}=B_\beta^{\pm}-(1-p_c^{\pm})[\bar\varphi_\beta(\pm b)-G_\beta(\pm b)].\tag{11}$$

Outside the attainability cone in (8) it is necessary to put $p_c^{\pm}=1$ and $\mathscr{B}_\beta^{\pm}=0$.

The parameters $B^{\pm}$ should be determined in terms of the probabilities of the different types of scattering. We introduce for electrons moving inside the attainability cone, besides $p_c^{\pm}$ and $p_v^{\pm}$, the probabilities of diffuse intravalley scattering $d_c^{\pm}=d_{\beta\beta}^{\pm}$ and $d_v^{\pm}$, of the electron intervalley scattering $d_{\beta\beta'}^{\pm}$, and of scattering from the electron valleys to the hole valley, $d_{\beta v}^{\pm}$, and back, $d_{v\beta}^{\pm}$. It is obvious that

$$p_\beta^{\pm}+\sum_{\beta'}d_{\beta\beta'}^{\pm}+d_{\beta\iota}^{\pm}=1,\quad p_v^{\pm}+d_\iota^{\pm}+\sum_\beta d_{v\beta}^{\pm}=1.\tag{12}$$

According to the detailed-balancing principle

$$d_{\beta\beta'}^{-}\langle v_z^<\rangle'_\beta=d_{\beta'\beta}^{-}\langle v_z^<\rangle'_{\beta'},\quad d_{\beta v}^{-}\langle v_z^<\rangle'_\beta=d_{\iota\beta}^{-}\langle v_z^<\rangle_v,\tag{13}$$

where the < sign of v indicates that the integration is carried out only over the half-space $v_Z<0$, and the indices β and v denote the ellipsoid over which the averaging is carried out (in those cases when the angle brackets contain a function with index β or v, the averaging region is determined uniquely and therefore we shall omit the appropriate indices at the angle brackets). The primed brackets denote here (as in (15)–(17) below) that the integration is carried out only within the limits of the attainability cone. If the dispersion law of the β-th ellipsoid is represented in the form $\epsilon_\beta(\mathbf{p})=\epsilon_{ij}^{\beta}p_ip_j/2m$ (where m can be chosen to be, for example, the mass of the free electron), then (13) reduces to

$$\frac{d_{\beta\beta'}^{-}}{d_{\beta'\beta}^{-}}=\left(\frac{\varepsilon_{zz}^{\beta'}}{\varepsilon_{zz}^{\beta}}\right)^{1/2},\quad\frac{d_{\beta\iota}^{-}}{d_{v\beta}^{-}}=\frac{\zeta_\iota}{\zeta_c}\left(\frac{m_v^3\,\varepsilon_{zz}^{v}}{m_c^3\,\varepsilon_{zz}^{\beta}}\right)^{1/2}.\tag{14}$$

The conservation condition for the number of electrons of the valley β at the boundary z = −b is of the form

$$\langle v_z\varphi_\beta^>\rangle'+p_c\langle v_z\varphi_\beta^<\rangle'+\sum_{\beta'}d_{\beta'\beta}\langle v_z\varphi_{\beta'}^<\rangle'+d_{v\beta}\langle v_z\varphi_v^<\rangle=0.\tag{15}$$

Substituting here $\varphi_\beta^{\gtrless}$ from (5) and using (13), we get

$$B_\beta^-=\sum_{\beta'}d_{\beta\beta'}^-\frac{\langle v_z\varphi_{\beta'}^<\rangle'}{\langle v_z^<\rangle'_{\beta'}}+d_{\beta v}^-\frac{\langle v_z\varphi_v^<\rangle}{\langle v_z^<\rangle_\iota},\tag{16}$$

$$B_v^-=d_\iota^-\frac{\langle v_z\varphi_\iota^<\rangle}{\langle v_z^<\rangle_v}+\sum_\beta d_{v\beta}^-\frac{\langle v_z\varphi_\beta^<\rangle'}{\langle v_z^<\rangle'_\beta}.\tag{17}$$

In (15)–(17) all the mean values are taken at z = −b; similar equations can be easily written for z = b. Equations (16) and (17), in which, according to (8), the right-hand sides themselves depend linearly on $B^{\pm}$ form a linear system from which it is possible to determine in principle all the parameters $B^{\pm}$.

2. INTEGRAL EQUATIONS FOR THE CONCENTRATIONS AND FOR THE FIELD

In solving (6), $\overline{\varphi}_\beta$ and $\overline{\varphi}_V$ were assumed to be known functions of z. It is now necessary to reconcile the solution, stipulating that all the mean values of φ, defined by formula (8), actually be equal to $\overline{\varphi}$. Averaging of the terms of the type $(\mathbf{E}_\beta\mathbf{v})$ in (8) is best carried out by using the transformations (I.6), which transform ellipsoids into spheres, and the half-space $v_Z<0$ into $u_Z<0$:

$$\mathbf{v}=\hat{A}^\beta\mathbf{u},\qquad A_{zi}^\beta=\delta_{zi}A_{zz}^\beta.$$

we obtain

$$\langle v_iF_\beta(v_z)\rangle=a_{iz}^\beta\langle v_zF_\beta(v_z)\rangle,$$

where $\hat{a}^\beta=\hat{A}^\beta/A_{ZZ}^\beta$, since $\langle u_{x,y}F(v_Z)\rangle=0$.

By laborious but elementary manipulations we can transform the equations for $\overline{\varphi}_\beta$ into

$$\left\langle\frac{\mathscr{B}_\beta^+}{\Delta_c}\left[\exp\left(\frac{z+b}{v_z\tau_c}\right)+p_c^-\exp\left(-\frac{z+b}{v_z\tau_c}\right)\right]\right\rangle^>+\left\langle\frac{\mathscr{B}_\beta^-}{\Delta_c}\left[\exp\left(\frac{b-z}{v_z\tau_c}\right)\right.\right.$$
$$\left.\left.+p_c^+\exp\left(\frac{z-b}{v_z\tau_c}\right)\right]\right\rangle^>+\int_{-b}^{b}dz'e\mathscr{E}_\beta(z')\left\{\left\langle\frac{p_c^+}{\Delta_c}\exp\left(\frac{z+z'}{v_z\tau_c}\right)\right\rangle_\beta^>\right.$$
$$-\left\langle\frac{p_c^-}{\Delta_c}\exp\left(-\frac{z+z'}{v_z\tau_c}\right)\right\rangle_\beta^>-\operatorname{sign}(z'-z)\left[\left\langle\frac{1}{\Delta_c}\exp\left(\frac{2b-|z'-z|}{v_z\tau_c}\right)\right\rangle_\beta^>\right.$$
$$\left.\left.-\left\langle\frac{p_c^+p_c^-}{\Delta_c}\exp\left(\frac{|z'-z|-2b}{v_z\tau_c}\right)\right\rangle_\beta^>\right]\right\}=\langle 1\rangle_cG_\beta(z).\tag{18}$$

The symbol > at the angle brackets indicates here that the averaging is carried out over the half-surface of the ellipsoid β with $v_Z>0$, and

$$\mathscr{E}_\beta(z)=(E_\beta(z)\hat{a}_\beta)_z.\tag{10a}$$

Since the $\mathscr{B}^{\pm}$ cancel out outside the attainability cones, only the region inside the cones contributes to the first two terms of (18) when the bands are curved upward.

In conjunction with (4), Eqs. (18) form a system of integral equations, which makes it possible in principle to determine $\overline{\varphi}$ and $E_Z(z)$.

Naturally, the solution of the system in general form is impossible, and we shall analyze in Secs. 2 and 3 below the limiting cases. However, one interesting general regularity can be revealed by differentiating with respect to z and transforming Eq. (18) into a second-order equation

$$\tau_z\langle 1\rangle_ce\mathscr{E}_\beta(z)+\int_{-b}^{b}dz'\,e\mathscr{E}_\beta(z')\left\langle\frac{1}{v_z\Delta_c}\left[p_c^+\exp\left(-\frac{z+z'}{v_z\tau_c}\right)\right.\right.$$
$$\left.\left.+p_c^-\exp\left(-\frac{z+z'}{v_z\tau_c}\right)-\exp\left(\frac{2b-|z-z'|}{v_z\tau_c}\right)-p_c^+p_c^-\exp\left(\frac{|z-z'|-2b}{v_z\tau_c}\right)\right]\right\rangle_\beta^>$$
$$+\left\langle\frac{\mathscr{B}_\beta^+}{v_z\Delta_c}\left[\exp\left(\frac{z+b}{v_z\tau_c}\right)-p_c^-\exp\left(-\frac{z+b}{v_z\tau_c}\right)\right]\right\rangle^>$$
$$-\left\langle\frac{\mathscr{B}_\beta^-}{v_z\Delta_c}\left[\exp\left(\frac{b-z}{v_z\tau_c}\right)-p_c^+\exp\left(\frac{z-b}{v_z\tau_c}\right)\right]\right\rangle^>=\tau_c\langle 1\rangle_c\frac{\partial G_\beta}{\partial z}.\tag{19}$$

The free terms of (19), which contain the parameters

$\mathscr{B}^{\pm}$, diverge logarithmically at the points $z = \pm b$ in the absence of a bending of the bands for all the carriers, owing to the appearance of v_z in the denominator; in the presence of a bend, they diverge for those groups, which are attracted to the surface (the region of integration in the angle brackets retains for these groups the singular point $v_z = 0$). As a net result, in these $\mathscr{E}_\beta$, and consequently also in the concentration gradients of all the groups of carriers and in the field E_z, there arise logarithmic singularities at the boundaries. This is a direct consequence of the finite intervalley scattering on the surface, for in its absence all the gradients in E_z, as shown in[1], are constant at the boundaries.

We now establish a general relation for the main measured quantity—the total current flowing through the plate. It is required to calculate the partial densities of the currents, the expressions for which reduce, using the variables u_i, to the form:

$$j_i^\beta = e\langle v_i\varphi_\beta^>(\mathbf{v}) + v_i^*\varphi_\beta^<(\mathbf{v}^*)\rangle^> = e\sum_{\lambda=x,y} A_{i\lambda}^\beta \langle u_\lambda[\varphi_\beta^>(\mathbf{v}) + \varphi_\beta^<(\mathbf{v}^*)]\rangle^> + a_{iz}^\beta j_z^\beta. \tag{20}$$

Thus, the longitudinal current includes as a component part the transverse current multiplied by a_{iz}^β:

$$\begin{aligned} j_z^\beta = e\Big\{&\Big\langle\frac{\mathscr{B}_\beta^- v_z}{\Delta_c}\Big[\exp\Big(\frac{b-z}{v_z\tau_c}\Big) - p_c^+\exp\Big(\frac{z-b}{v_z\tau_c}\Big)\Big]\Big\rangle^> \\ &-\Big\langle\frac{\mathscr{B}_\beta^+ v_z}{\Delta_c}\Big[\exp\Big(\frac{z+b}{v_z\tau_c}\Big) - p_c^-\exp\Big(-\frac{z+b}{v_z\tau_c}\Big)\Big]\Big\rangle^> \\ &+\int_{-b}^{b} dz'\, e\mathscr{E}_\beta(z')\Big\langle\frac{v_z}{\Delta_c}\Big[\exp\Big(\frac{2b-|z-z'|}{v_z\tau_c}\Big) + p_c^+p_c^-\exp\Big(\frac{|z-z'|-2b}{v_z\tau_c}\Big) \\ &- p_c^+\exp\Big(\frac{z+z'}{v_z\tau_c}\Big) - p_c^-\exp\Big(-\frac{z+z'}{v_z\tau_c}\Big)\Big]\Big\rangle_\beta^>\Big\}. \end{aligned} \tag{21}$$

To determine j_z it is necessary to solve the system (4) and (18) and to obtain the parameters B by means of formulas (11), (16), and (17). The first term of the right side of (20) does not contain the quantities B and $\overline{\varphi}$, and can be explicitly calculated. Integration of (20) over the thickness yields

$$\begin{aligned} J_i^\beta = \int_{-b}^{b} dz\, j_i^\beta(z) = 2be^2\tau_c \sum_{\lambda,\mu=x,y} E_\mu A_{\mu\lambda}^\beta A_{i\lambda}^\beta\Big\{2\langle u_\lambda^2\rangle^> \\ -\Big\langle\frac{v_z\tau_c}{2b\Delta_c}u_\lambda^2\Big[(1-p_c^+)\Big(\exp\Big(\frac{b}{v_z\tau_c}\Big) + p_c^-\exp\Big(-\frac{b}{v_z\tau_c}\Big)\Big) \\ +(1-p_c^-)\Big(\exp\Big(\frac{b}{v_z\tau_c}\Big) + p_c^+\exp\Big(-\frac{b}{v_z\tau_c}\Big)\Big)\Big] \\ \times\Big(\exp\Big(\frac{b}{v_z\tau_c}\Big) - \exp\Big(-\frac{b}{v_z\tau_c}\Big)\Big)\Big\rangle_\beta^>\Big\} + a_{iz}^\beta J_z^\beta. \end{aligned} \tag{22}$$

The total current in the plate is obtained by summing the partial currents J_i^β and J_i^v (the formulas for the latter are analogous to expressions (20)–(22).

3. THIN PLATE

If the thickness of the plate is small compared with the length L of the intervalley diffusion displacement, then the right sides of Eqs. (18) and (19) can be omitted[3)]. In this case Eqs. (18) or (19) can be decoupled and be used to determine the functions $E_\beta(z)$. In terms of these functions, $d\overline{\varphi}/dz$ and E_z can be expressed with the aid of (4) and (10):

$$E_z(z) = \frac{1}{N+q}\Big\{\sum_\beta[\mathscr{E}_\beta(z) - (\mathbf{E}^{\parallel}\hat{\mathbf{a}}_\beta)_z] + q[\mathscr{E}_v(z) - (\mathbf{E}^{\parallel}\hat{\mathbf{a}}_v)_z]\Big\}, \tag{23}$$

$$\overline{d\overline{\varphi}_\beta / dz} = e(\mathbf{E}(z)\hat{\mathbf{a}}^\beta)_z - e\mathscr{E}_\beta(z), \tag{24}$$

where $\mathbf{E}^{\parallel} = (E_x, E_y, 0)$.

When $b \ll l$ we can omit from (19) the integral term[4)]

$$\begin{aligned} e\mathscr{E}_\beta(z) = \frac{1}{\tau_c\langle 1\rangle_c}\Big\{&\Big\langle\frac{\mathscr{B}_\beta^-}{v_z\Delta_c}\Big[\exp\Big(\frac{b-z}{v_z\tau_c}\Big) - p_c^+\exp\Big(\frac{z-b}{v_z\tau_c}\Big)\Big]\Big\rangle^> \\ &-\Big\langle\frac{\mathscr{B}_\beta^+}{v_z\Delta_c}\Big[\exp\Big(\frac{b+z}{v_z\tau_c}\Big) - p_c^-\exp\Big(-\frac{b+z}{v_z\tau_c}\Big)\Big]\Big\rangle^>\Big\}. \end{aligned} \tag{25}$$

Simultaneously with (19), it is necessary to satisfy for all values of z also the equation (18) from which (19) was obtained by differentiation. When $b \ll l$ it is also possible, approximately, to omit the integral term in (18), and all the exponentials can be replaced by unity. Then

$$\Big\langle\mathscr{B}_\beta^+\frac{1+p_c^-}{1-p_c^+p_c^-}\Big\rangle^> + \Big\langle\mathscr{B}_\beta^-\frac{1+p_c^+}{1-p_c^+p_c^-}\Big\rangle^> = 0,$$

$$\mathscr{B}_v^+(1+p_v^-) + \mathscr{B}_v^-(1+p_v^+) = 0. \tag{26}$$

Thus, for a complete solution of the problem and for a determination of the parameters $\overline{\varphi}(\pm b)$ and $\mathscr{B}^{\pm}$, we have Eqs. (16), (17), (and analogous equations with $z = b$), (24), and (26). Since there is a single linear connection between the conservation equations on two surfaces (owing to the identical conservation of the total transverse current), we must use Eqs. (4) for absolute calibration of $\overline{\varphi}$ (which in the weaker form—in the form of a derivative—was already used in the derivation of (23)).

Let us consider the particular case of a symmetrical plate, when all the p and d on both sides are the same. It then follows from (23)–(26) that

$$\mathscr{B}_\beta^- = -\mathscr{B}_\beta^+ \equiv \mathscr{B}_\beta, \quad \varphi_\beta(-z) = -\varphi_\beta(z), \quad \mathbf{E}(-z) = \mathbf{E}(z),$$

$$\mathscr{E}_\beta(-z) = \mathscr{E}_\beta(z). \tag{27}$$

Eq. (25) simplifies to

$$e\mathscr{E}_\beta(z) = \frac{\mathscr{B}_\beta}{2l_\beta}F\Big(\frac{z}{l_\beta}, \frac{b}{l_\beta}, p_c, \theta_c\Big);$$

$$F(\xi,\eta,p,\theta) = \int_{\cos\theta}^{1}\frac{du}{u}\,\frac{e^{\xi/u}+e^{-\xi/u}}{e^{\eta/u}+pe^{-\eta/u}} \qquad l_\beta = \tau_c\sqrt{2\varepsilon_{zz}^\beta\zeta_c/m}; \tag{28}$$

The formula for $\mathscr{E}_v$ is established from (28) by means of the substitutions $\beta \to v$, $p_c \to p_v$, and $\theta_c \to \pi/2$ (θ_c is the apex angle of the attainability cone). If θ_c is not too close to $\pi/2$, namely when $b \ll l\cos\theta_c$, all the exponentials under the integral sign in (28) can be replaced by unity, and

$$e\mathscr{E}_\beta(z) \approx [\mathscr{B}_\beta / l_\beta(1+p_c)]\,|\ln\cos\theta_c|, \tag{29}$$

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3)It is obvious that this approximation suffices to determine the spatial dependences of all the quantities. At the same time, in the case of weak intervalley scattering on the surface, when the rates of the intervalley transitions in the volume and on the surface become comparable, it is necessary to introduce certain modifications in the foregoing procedure, and the absolute values $\overline{\varphi}$ must be determined from the conditions of the integral balancing (see, for example, [12]). Since we shall consider here mainly the symmetrical case, when all the $\overline{\varphi}(0) = 0$, we shall not have to resort to this condition. In addition, the case of a weak intervalley scattering on the surface is of no interest to us here, since it is considered in [1].

4)The error introduced in this case is easiest to estimate in the symmetrical case. The correction to $\mathscr{E}_\beta$ turns out to be of the order of $(b/l)\ln(l/b)\,\overline{\mathscr{E}}_\beta$, where $\overline{\mathscr{E}}_\beta$ is the mean value of $\mathscr{E}_\beta$. The relative error introduced by all the succeeding approximations is of the same order, or approximately equal to b/l.

i.e., it is constant. At the same time $\mathscr{E}_v(z)$ near $z = \pm b$ diverges logarithmically:

$$e\mathscr{E}_v(z) \approx \frac{\mathscr{B}_v}{2l_v} \ln \frac{l_v^2}{b^2 - z^2}. \tag{30}$$

As a result of (23) and (24), analogous singularities appear also in E_z and in all the $d\overline{\varphi}/dz$. In the case of a small bending of the bands ($b \gtrsim l_\beta \cos\theta_c$), all the $\mathscr{E}_\beta$ begin to depend on z, and when $V(0) \to 0$, singularities similar to (30) appear in them. The singularities vanish only when $V(0) > \zeta_c$, when the intervalley scattering on the surface vanishes completely.

Let us proceed to determine the quantities $\mathscr{B}$. When (8) is substituted in (16) and (17), the main contribution comes again from the integral terms in (8):

$$\mathscr{B}_\beta + \frac{1}{1+p_c}\sum_{\beta'} d_{\beta\beta'}\mathscr{B}_{\beta'} + \frac{d_{\beta v}}{1+p_c}\mathscr{B}_v = \sum_{\beta'} d_{\beta\beta'}(\overline{\varphi}_{\beta'} - \overline{\varphi}_\beta) + d_{\beta v}(\overline{\varphi}_v - \overline{\varphi}_\beta), \tag{31}$$

$$\left(1 + \frac{d_v}{1+p_v}\right)\mathscr{B}_v + \sum_\beta \frac{d_{v\beta}}{1+p_\beta}\mathscr{B}_\beta = \sum_\beta d_{v\beta}(\overline{\varphi}_\beta - \overline{\varphi}_v), \tag{32}$$

where $\overline{\varphi} \equiv \overline{\varphi}(-b)$. Let us now determine these $\overline{\varphi}$, integrating (24). According to (28) $\mathscr{E}_\beta \sim \mathscr{B}_\beta$, and integrals of all the terms of (24) containing $\mathscr{E}_\beta$ do not exceed in order of magnitude $\mathscr{B}_\beta\,(b/l)\ln(l/b)$ and can be discarded as small compared with the left sides of (31) and (32). The right sides of (31) and (32) are then determined by the formulas

$$\begin{aligned} \overline{\varphi}_\beta - \overline{\varphi}_{\beta'} &= eb\,[(\mathbf{E}^{\parallel}\hat{\mathbf{a}}_{\beta'})_z - (\mathbf{E}^{\parallel}\hat{\mathbf{a}}_\beta)_z], \\ \overline{\varphi}_\beta - \overline{\varphi}_v &= eb\,[(\mathbf{E}^{\parallel}\hat{\mathbf{a}}_v)_z - (\mathbf{E}^{\parallel}\hat{\mathbf{a}}_\beta)_z]. \end{aligned} \tag{33}$$

It is interesting to note that they do not depend on the intensity of the surface intervalley scattering (unlike the thick plates[5], where they are cancelled in the case of strong scattering). The system (31)—(33) defines $\mathscr{B}$, in terms of which all the remaining quantities are expressed. It is seen directly that in order of magnitude $\mathscr{B} \sim ebdE^{\parallel}$, where d characterizes the probabilities of the intervalley transitions. Consequently, the singular part is

$$E_z \sim \left(d\frac{b}{l}\ln\frac{l^2}{b^2 - z^2}\right)E^{\parallel} \tag{34}$$

(the constant part of E_z, according to (23) is of the order of $E^{\parallel}$).

In the current j_z^β in (21) non-integral terms predominate, which, in accordance with the estimate obtained for $\mathscr{B}$, are of the order of $\sigma_0 d(b/l)E^{\parallel}$, where σ_0 is the electric conductivity of the bulky sample; consequently, the role of the effective free path is played here by db. At the same time, in the first term in (22), as can be readily understood in analogy with[4], the effective free path may vary, depending on the surface conditions, from l to $b\ln(l/b)$, making it possible to neglect in a thin plate ($b \ll l$) the last term of (22).

Let us proceed to analyze the principal term in (22) in a symmetrical plate; in the absence of bending of the bands, it coincides with (I.16). It must be emphasized first of all that it depends exclusively on the fraction of the specular scattering p_c, and does not depend on the fraction of the intervalley scattering in the overall diffuse scattering. In the limit of "thick" plates ($L \gg 2b \gg l$), the second mean value in (22) is smaller than $\langle u_\lambda^2\rangle^{>}$ by a factor l_β/b, and can be omitted. The effective conductivity is then determined by the sum of the first and third terms, and reaches saturation. However, as already noted in[1], unlike the results of[2,3,13], this value of the conductivity ("intermediate plateau") does not coincide with the conductivity of the bulky material, and goes over into the asymptotic value of the conductivity at "small" thicknesses in the diffusion size effect[5].

When $V(0) = 0$, and even when $V(0) > 0$ for the electrons of the valence band, the principal terms in the two mean values in the curly bracket of (22) cancel out, and when $b \ll l(1-p)$ the effective conductivity decreases by a factor

$$\frac{b}{l(1-p)}\ln\left(\frac{l(1-p)}{b}\right).$$

However, for electrons from the conduction bands, when $V(0) \neq 0$, the integration in the second mean value of (22) is limited to the attainability cone and therefore the effective conductivity tends to saturate as $b/l \to 0$. If $b \ll l_\beta(1-p)\cos\theta_c$, then the average saturation current, calculated from the formula (22), is equal to

$$\frac{1}{2b}J_i = \frac{e^2\tau_c n_c}{m}\sum_\beta \sum_{\lambda,\,\mu=x,\,y} E_\mu A_{\mu\lambda}{}^\beta A_{i\lambda}{}^\beta \cdot \frac{3}{2}\cos\theta_c\left(1 - \frac{1}{3}\cos^2\theta_c\right), \tag{22a}$$

where n_c is the equilibrium concentration in one of the electronic valleys. The last factor in (22a) describes the dependence of the effective electric conductivity on the near-surface bending of the bands.

It must be noted that the first to obtain a plateau at $b/l \ll 1$ was Parrot[13], who also assumed, but from other considerations (see the Appendix), that the scattering of the glancing electrons is purely specular. Unfortunately, however, his final formulas are incorrect, owing to errors in his solutions, which are similar to those in[2,3].

4. THICK PLATE

If $2b \gg l$, the diffusion approximation is valid everywhere except in surface layers of thickness $\sim l$. It is precisely these layers where the singularities of $E_z(z)$ arise. The purpose of this section is: 1) to determine the singular part of E_z and 2) to connect the phenomenological boundary conditions for the diffusion approximation, which determines the carrier distribution in the interior of the plate, with the parameters characterizing the scattering from the boundary.

To simplify the analysis, we confine ourselves to an account of the electronic valleys only, assume the scattering to be diffuse ($p = 0$), and the band bending to be equal to zero. We choose the origin on the left surface of the plate, and define the distance δ such that $l \ll \delta \ll L$, where $L \sim v_F\sqrt{\tau T}$ is the diffusion length. Then we can neglect the intervalley scattering in the kinetic equation if $z \le \delta$, and use the diffusion approximation if $z \ge \delta$. The region near the second surface is considered perfectly independently and in similar fashion.

Near the left boundary, Eq. (18) reduces to

$$\int_0^\infty dz'\, e\mathscr{E}_\beta(z')\,\mathrm{sign}(z'-z)\,E_2\left(\frac{|z-z'|}{l_\beta}\right) = \mathscr{B}_\beta E_2\left(\frac{z}{l_\beta}\right), \tag{35}$$

and the differential equation (19) that is obtained from it reduces to

$$e\mathscr{E}_\beta(z)=\frac{1}{2l_\beta}\int_0^\infty dz'\,e\mathscr{E}_\beta(z')E_1\left(\frac{|z-z'|}{l_\beta}\right)+\frac{\mathscr{B}_\beta}{2l_\beta}E_1\left(\frac{z}{l_\beta}\right),\quad (36)$$

where

$$E_n(x)=\int_0^\infty dt\,t^{-n}e^{-xt}.$$

Equation (36) is the inhomogeneous Milne equation[14], which has been well investigated, in particular, in neutron-transport problems[15]. If we denote by $M_\beta(z)$ the solution of the homogeneous Milne equation, corresponding to (36), and normalize it in such a way that $M_\beta(0)=1$, then it is possible to verify by direct substitution that the solution of (35) is

$$e\mathscr{E}_\beta(z)=\mathscr{B}_\beta\frac{dM_\beta}{dz}.\quad (37)$$

It is known[14,15] that when $z\gg l_\beta$ we have

$$M_\beta(z)\approx\sqrt{3}\left(\frac{z}{l}+q_\infty\right),\quad q_\infty\approx 0.710.\quad (38)$$

When $z\ll l_\beta$, in accordance with (36),

$$e\mathscr{E}_\beta(z)\approx\frac{\mathscr{B}}{2l}\ln\frac{l_\beta}{z}.\quad (39)$$

We proceed to determine the effective boundary conditions and to calculate $\mathscr{B}_\beta$. Using (21), (23) and (24) (see also[15], Sec. 6, 3), we can show that

$$j_z^\beta=\frac{el_\beta}{\tau_c\sqrt{3}}\langle 1\rangle_c\mathscr{B}_\beta,\quad (40)$$

$$\overline{\varphi}_\beta(z)=\overline{\varphi}_\beta(0)-\mathscr{B}_\beta(M_\beta(z)-1)+\frac{1}{N}\sum_{\beta'}\mathscr{B}_{\beta'}(M_{\beta'}(z)-1)$$
$$+e\left[(\mathbf{E}^{\|}\hat{\mathbf{a}}_\beta)_z-\frac{1}{N}\sum_{\beta'}(\mathbf{E}^{\|}\hat{\mathbf{a}}_{\beta'})_z\right]z.\quad (41)$$

From (41) and (38) it follows that when $z\gg l_\beta$ the functions $\overline{\varphi}_\beta(z)$ depend linearly on z. This is natural, since in this region the diffusion approximation is already valid and the nonequilibrium concentrations of the electrons $n_\beta(z)=-\langle 1\rangle_c\overline{\varphi}_\beta(z)$ should vary linearly with z if intervalley scattering is neglected[5]. Therefore the phenomenological boundary concentrations $n_\beta(0)$ should be obtained by extrapolating to $z=0$ the asymptotic expression for $\overline{\varphi}_\beta(z)$ from (41) in the region of large z. Thus,

$$n_\beta(0)=-\langle 1\rangle_c\left\{\overline{\varphi}_\beta(0)+(\sqrt{3}q_\infty-1)\left(\frac{1}{N}\sum_{\beta'}\mathscr{B}_{\beta'}-\mathscr{B}_\beta\right)\right\}.\quad (42)$$

It remains to write down Eqs. (16), in which the right-hand sides are calculated in analogy with (40):

$$\mathscr{B}_\beta+\sum_{\beta'}d_{\beta\beta'}\left(\frac{4}{\sqrt{3}}-1\right)\mathscr{B}_{\beta'}=\sum_{\beta'}d_{\beta\beta'}(\overline{\varphi}_{\beta'}(0)-\overline{\varphi}_\beta(0)).\quad (43)$$

Eliminating all the $\overline{\varphi}_\beta(0)$ and $\mathscr{B}_\beta$ from (40), (42), and (43), we obtain

$$\frac{1}{e}j_z^\beta+\frac{4-3q_\infty}{3q_\infty e}\sum_{\beta'}d_{\beta'\beta}j_z^{\beta'}=\frac{l_\beta}{3\tau_c q_\infty}\sum_{\beta'}d_{\beta\beta'}[n_\beta(0)-n_{\beta'}(0)].\quad (44)$$

Equations (44) solve our problem, since they relate the phenomenological fluxes j_z^β/e with the concentrations n_β. Solving these equations we can obtain the rates of surface recombination s, which, as is obvious from (44), are of the order of $v_F d$. The current through the plate is then directly determined by the formulas of[5].

Let us also estimate $\mathscr{B}_\beta$. If the values of s are not not too small, then $j_z^\beta\sim\sigma_0 E^{\|}$ [5], and as a result of (40), $\mathscr{B}_\beta\sim eE^{\|}l$, which exceeds by a factor l/b the values of $\mathscr{B}_\beta$, and consequently also of the singular part of the field in thin plates.

CONCLUSION

Without repeating the main conclusions made in the text and summarized in the Introduction, let us make a few remarks concerning the size effect under certain conditions for which the calculations were not performed, but for which the qualitative picture is perfectly clear.

If the bands are curved downward in a thin plate, then when $b\to 0$ the hole conductivity saturates, and the electron conductivity is cancelled out. Therefore, for example in bismuth, where under normal conditions the electron conductivity predominates, it is possible to change the type of conductivity by decreasing the electron effective mean free path. Since it is assumed that the electrons, unlike the holes, have a multivalley spectrum, even when $|V(0)|>\zeta_V$, when the holes are all crowded away from the surface, the logarithmic singularity in $E_z(z)$ still remains. If the bands on two surfaces are curved in opposite directions, then the plateaus in the electric conductivity at small values of b, naturally, vanish and the conductivity, as usual, tends to zero[5)].

It is clear from the foregoing that it is important to carry out investigations of the size effect when the bending of the bands is controlled, and to combine these investigations with experiments on the field effect.

The schematic dependence of the electric conductivity on the thickness, described in the Introduction, may become complicated by an additional structure connected with the difference of the electron and hole free paths, and also with the anisotropy of l_β; the anisotropy of l_β should lead to a different thickness dependence of the currents J_i^β (formula (22)) for ellipsoids having different orientations relative to the surface of the plate. It is difficult to estimate the order of magnitude of the corrections that may result from the allowance for the anisotropy of the relaxation times, deviations from the condition $k_F l_D\gg 1$, etc.

It should be noted that the singularities in $E_z(z)$ should arise also in normal metals with complicated Fermi surfaces, and not only in semimetals.

We note in conclusion one more consequence of the developed theory. Violation of the equilibrium distribution of the carriers among the valleys with large concentration gradients near the surfaces should lead, as a result of the ordinary electron-photon interaction, to the occurrence of inhomogeneous deformation. Obviously, in an alternating external electromagnetic field the same effect should cause a new mechanism of sound generation.

APPENDIX

Let us consider the region of the near-surface bending of the bands upward at the left boundary, which we assume here for convenience to be the plane $z=0$; we denote by z_0 the value of z, starting with which the

5)Disregarding the purely "optical" effect [13], the role of which is as yet unclear.

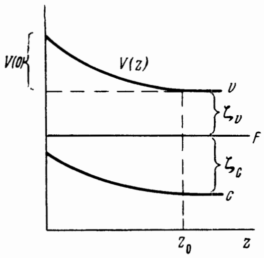

FIG. 2. Plot of the bottom of the conduction bands (c) and of the top of the valence band (v) near the surface; F – Fermi level.

near-surface field can be neglected in practice and the bending of the bands V(z) vanishes (Fig. 2). Let us assume that collisions can be neglected in the layer $(0, z_0)$, an assumption valid when $l \gg l_D$, and that the kinetic equations hold everywhere. If $\epsilon(\mathbf{p}) = \epsilon_{ij}p_ip_j/2m$ for one of the electron valleys, then it follows from the energy integral that

$$v_z(z) = \pm\left[(v_z^0)^2 - 2\frac{\varepsilon_{zz}}{m}V(z)\right]^{1/2}$$

where v^0 is the velocity on entering the space-charge layer. We see therefore that the electrons entering the attainability cone are those with $|v_z^0| > v_{cr} = \sqrt{2\epsilon_{zz}V(0)/m}$, which corresponds, in the coordinates **u**, to an attainability cone apex angle θ_c, such that $\cos^2\theta_c = V(0)/\zeta_c$. The remaining integrals of motion for the electrons entering in the layer are given by

$$v_i + \frac{\varepsilon_{iz}}{m}\int_0^V \frac{dV}{v_z(V)} = v_i^0, \tag{A.1}$$

where the integration is along the trajectories of the motion.

The distribution function in the surface layer is

$$f(z, \mathbf{v}) = f_0(\varepsilon - \mu(z)) + \varphi\partial f_0/\partial\varepsilon,$$

where $\mu(z) = \zeta - V(z)$ is the electrochemical potential $(eE_z = dV/dz)$. Neglecting collisions, we should discard E_x and E_y in the same approximation. Then the equation for φ reduces to $v_z\partial\varphi/\partial z - eE_z\partial\varphi/\partial p_z = 0$, and its solutions are arbitrary functions of the integrals of motion (A.1), i.e., they remain constant when **v** and z are connected by the relations (A.1).

For electrons outside the attainability cone, (A.1) is valid along the entire trajectory, and for V at the turning point V_{tur} we have

$$\frac{\varepsilon_{zz}}{m}\int_0^{V_{tur}} \frac{dV}{v_z(V)} = v_z^0. \tag{A.2}$$

Since v_z reverses sign when moving on the opposite branch of the trajectory, the velocities on emerging from the layer, according to (A.1), are equal to

$$(v_i^0)^* = v_i^0 - 2\frac{\varepsilon_{iz}}{\varepsilon_{zz}}v_z^0, \tag{A.3}$$

which coincides with (I.12) and confirms (5a).

For the electrons in the attainability cone, (A.1) relates the velocity $v_i(0)$ on the surface with v_i^0. A similar relation holds for the outgoing electrons. It follows directly from (A.1) that if the velocities $\mathbf{v}(0)$ and $\mathbf{v}^*(0)$ at $z = 0$ are connected by relations of the type (A.3), then these relations will also be satisfied by the corresponding velocities at $z = z_0$. Therefore, if we assume at $z = 0$ the boundary condition

$$\varphi^>(\mathbf{v}(0)) = p\varphi^<(\mathbf{v}^*(0)) + B,$$

where B is determined from the conservation of the number of particles, this automatically leads to an effective boundary condition (5b). The electrons of the valence band all reach the surface and equation (5c) is valid for them.

The next problem is to relate the effective constants $d_{\beta\beta'}$ and the other constants in (13) with the constants $d^0_{\beta\beta'}$ and the others on the true surface. For the sake of brevity, we shall only indicate the procedure and present the final results. Writing down an equation similar to (13) for the true surface $z = 0$, we can go over in all the integrals containing $\varphi_\beta(0, \mathbf{v})$, using the method indicated above, to $\varphi_\beta(z_0, \mathbf{v})$, i.e. to fluxes on the fictitious boundary z_0.

The situation is different in the case of the valence-band electrons, since those electrons that go off from the surface at glancing angles are returned to the surface by the contact field (this can be readily visualized by considering holes in the valence band). The distribution function of these "trapped" electrons, naturally, cannot be connected directly with the distribution function at z_0, but in analogy with the function of the glancing electrons from the conduction band, this function has the property $\varphi_v^>(z, \mathbf{v}) = \varphi_v^<(z, \mathbf{v}^*)$. As to the remaining electrons of the valence band, the values of $\varphi_v(0, \mathbf{v})$ and $\varphi_v(z_0, \mathbf{v})$ for these electrons are expressed directly in terms of each other. Writing now the balance equation for the "trapped" electrons at $z = 0$, we can determine from this equation their flux at $z = 0$ in terms of the different fluxes at $z = z_0$, and then eliminate it from the balance equation for the conduction electrons and for the valence electrons emerging from the space-charge layer As a result we obtain a system of equations for the fluxes through the surface z_0, similar to (15), in which

$$d_{\beta\beta'} = d^0_{\beta\beta'} + \alpha d_{\beta v}{}^0 d^0_{v\beta'}\cos^2\theta_v$$

$$d_{\beta v} = \alpha d_{\beta v}{}^0(1 - p_\beta{}^0)\sin^2\theta_v, \quad p_\beta = p_\beta{}^0,$$

$$d_{v\beta} = \alpha(1 - p_v{}^0)d_{v\beta}{}^0, \quad d_v = d_v{}^0(1 - p_v{}^0)\sin^2\theta_v, \quad p_v = p_v{}^0$$

$$\alpha = (1 - p_v{}^0 - d_v{}^0\cos^2\theta_v)^{-1}, \quad \cos^2\theta_i = \frac{V(0)}{\zeta_v + V(0)}; \tag{A.4}$$

The angle θ_v limits the region of "trapped" valence electrons in the coordinates **u**. When $V \to 0$, the angle $\theta_v \to \pi/2$ and all the $d \to d^0$. It follows directly from (A.4) that all the d depend on V(0). It should be noted in passing that the d^0 also depend on V(0), since relations of the type (12) hold for them, too, except that the right-hand sides contain the electrochemical potentials on the true surface. Therefore, for example, when $V(0) \geq \zeta_c$, the surface scattering of the holes becomes purely intravalley (in the elastic-scattering approximation).

Let us stop also to discuss the criteria for the applicability of the kinetic equation to the surface layer, and consequently, the region if validity of formulas (5) and (A.4). They are valid if $k_F l_D \gg 1$, where k_F is the Fermi momentum of the group under consideration. This is equivalent to $r_B \gg l_D$, where r_B is the effective Bohr radius, i.e., the radius in the dense-gas approximation. Since the criterion for the existence of a semi-metal (the absence of pairing of electron-hole pairs into excitons) has the same form (but with a weak inequality), the use of the quasiclassical approximation can be regarded as valid. However, in real semimetals, the satisfaction of the criterion is apparently still on the borderline; a more general theory should take into account tunneling through the space-charge layer towards a rough boundary, which is far beyond the scope of the present article.

The potential in the space-charge layer was assumed above to be dependent only on one coordinate z. This is valid either when the relief ρ on the surface has dimensions $\rho \gg l_D$, or when $\rho \ll l_D$ (i.e., macroscopic violations). In both cases, allowance for the potential V has a strong influence on the intervalley scattering, but only in the second case does it change d_c appreciably. If the criterion $k_F l_D \gg 1$ is satisfied, then the intravalley scattering on the surface will occur in any case at small angles. But since the scattering even through small angles becomes very appreciable when $2b \ll l$, the criteria for the applicability of the theory will become more and more stringent.

We note that Parrot[13] was apparently the first to consider the "cutoff" of the diffuse scattering for glancing electrons; he started from the usual optical analogy. It seems to us that the mechanism considered above is more effective, is capable of explaining a wide range of variation of the angle θ_c, and points to direct experiments, of the field-effect type, for a controlled variation of this angle. Naturally, of course, both mechanisms should be considered in parallel.

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