Electric Conductivity of Metals with Account of Phonon Drag

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Low temperature electric conductivity of pure metals with open Fermi surfaces is considered for the case when the only cause of the electric resistance are Umklapp processes occurring in collisions between electrons and phonons. It is shown that at sufficiently low temperatures, when the phonon thermal pulse is small compared with the characteristic Fermi surface dimensions, the problem reduces to the solution of a single integro-differential equation describing electron diffusion on the Fermi surface. Umklapp processes are taken into account in the periodic boundary conditions for the equation. A solution of the diffusion equation is obtained for metals whose Fermi surfaces consist of large electron (or hole) groups arbitrarily connected by narrow necks (case when phonon drag is most important). Simple equations are obtained for the electric conductivity which is determined by the neck resistances, topology of the Fermi surface, and difference between the electron and hole group volumes. In the presence of bridges of a certain type, the electric conductivity of the metal is proportional to the fourth power of temperature. An exact solution of the diffusion equation is found and the electric conductivity of metals described by the weak pseudopotential model is found.

THE modern theory of the electric conductivity of metals was founded in the early thirties principally by the work of Bloch and Peierls.

Starting with an analysis of the kinetic equation, Bloch has shown that at low temperatures the metal resistance due to electron-phonon collisions is proportional to the fifth power of the temperature: $\rho \sim T^5$, $T \ll \Theta$ (Θ is the Debye temperature). This result was obtained for the simplest model of isotropic dispersion laws for the electrons and phonons, and was essentially based on the assumption of an equilibrium phonon distribution. In other words, it is assumed that there exists a certain sufficiently effective deceleration mechanism preventing the phonons from being dragged by the electrons. As shown by Peierls, in pure metals this mechanism is provided by phonon-phonon collisions with Umklapp. With decreasing temperature, however, the probability of these U-processes decreases, as is well known, exponentially: the corresponding collision frequency is $\nu_U^{pp} \sim \exp(-\gamma\Theta/T)$. It is difficult to estimate the value of the numerical coefficient γ, since it is determined by the properties of the phonon spectrum at large values of the quasimomentum ($2\gamma\Theta$ is equal to the smallest value of the sum of energies of all the three phonons participating in the collision, with allowance for the corresponding energy and quasimomentum conservation laws). In any case, it is obvious that for each metal there exists a certain characteristic temperature, below which the U-processes can no longer ensure equilibrium of the phonons. A comparison with the experimental results on the thermal conductivity of dielectrics (see, for example[1]) shows that such a situation should obtain in a sufficiently wide range of low temperatures, say at $T/\Theta \lesssim 1/10$.

The degree of coupling between the phonons and the electrons is determined by the frequency of the phonon-electron collisions: $\nu^{pe} \sim T$. The inequality $\nu^{pe} \gg \nu_U^{pp}$ therefore holds at low temperatures. Under such conditions the momentum transferred to the electron returns with overwhelming probability to the electron system before it relaxes in the phonon system. This means that the dragging of the phonons by the electrons is appreciable and the phonons cannot be regarded as being in equilibrium when the electric conductivity is calculated.

If the metal has a closed Fermi surface and the number of electrons is not equal to the number of holes, then at sufficiently low temperatures its electric conductivity should increase exponentially with decreasing temperature. This result can be easily understood. The normal electron-phonon collisions, under conditions of total dragging of the phonons by electrons (i.e., neglecting phonon-phonon Umklapp) can obviously not lead to a finite resistance. On the other hand, to realize electron-phonon collisions with Umklapp it is necessary to have a phonon momentum not less than the minimum distance Δp in p-space between the closed electron or hole groups. If the thermal momentum of the phonons is much smaller than this distance, then the number of such phonons is proportional to $\exp(-\Delta ps/T)$, i.e., it is exponentially small[1)] (s is the speed of sound).

According to Peierls, the situation is different in metals with open Fermi surfaces. In this case Bloch's law $\rho \sim T^5$ should be valid at arbitrary low temperatures, owing to the fact that the Umklapp processes in collisions between electrons and thermal phonons are possible no matter how small the momenta of these phonons may be.

It is known that electron-phonon collisions can be regarded with a high degree of accuracy as elastic,

[1)]It should be noted that no exponential decrease of the resistance of metals with decreasing temperature has been observed experimentally to date. This is possibly connected with the fact that in real metals with closed Fermi surfaces and unequal numbers of electrons and holes the distances Δp are quite small, and therefore the electron-phonon U-processes have a noticeable probability down to very low temperatures. We note that in sodium and potassium at helium temperatures one observes a dependence $\rho \sim T^6$ [2,3]. It is possible that this dependence is connected with the contraction, with decreasing temperature, of that part of the Fermi surface from which Umklapp processes are possible, and thus precedes the exponential decrease of the resistance.

i.e., when an electron absorbs (or emits) a phonon, it undergoes transitions within the limits of the equal-energy surface. One can therefore expect at sufficiently low temperatures, when the thermal momentum of the phonon is $q \sim T/s \ll p_F$ (p_F is the minimum characteristic dimension of the Fermi surface), the problem of the electric conductivity can be formulated in terms of the diffusion of the electrons in momentum space on the Fermi surface[2)].

1. DERIVATION OF DIFFUSION EQUATION

We start from a system of kinetic equations in which account is taken of the connection between the electrons and a constant homogeneous electric field and collisions between the electrons and the phonons. The collisions between phonons at low temperatures, as already noted, are much less probable than collisions with electrons, and are therefore disregarded.

In the linear approximation, the kinetic equations can be written in the form

$$I^e\{\chi_p, \Phi_q\} = e\mathbf{E}\frac{\partial n_p}{\partial \mathbf{p}}, \tag{1}$$

$$I^p\{\Phi_q, \chi_p\} = 0, \tag{2}$$

$$I^e = \sum_{k,q}(\Gamma^+_{pkq} - \Gamma^-_{pkq}), \quad I^p = \sum_{k,p}\Gamma^-_{pkq},$$

$$\Gamma^\pm_{pkq} = \frac{2\pi}{\hbar}|B_{pkq}|^2\frac{dN_q}{d\Omega_q}(n_p - n_k)(\chi_p - \chi_k - \Phi_{\mp q})\delta(\varepsilon_{p,k} \pm \Omega_q),$$

$$B_{pkq} = b_{pkq}\sum_g \delta_{p,\,k+q+g}, \quad \varepsilon_{p,k} = \varepsilon_p - \varepsilon_k. \tag{3}$$

Here B_{pkq} is the matrix element of the electron-phonon interaction (the interaction Hamiltonian is $H_{int} = \Sigma B_{pkq}a^+_p a_k (c_q + c^+_{-q})$). The electron and phonon distribution functions f_p and F_q are represented in the form

$$f_p = n_p - \chi_p \partial n_p / \partial \varepsilon_p, \qquad F_q = N_q - \Phi_q \partial N_q / \partial \Omega_q,$$

where n_p and N_q are the equilibrium distribution functions of the electrons and phonons, and ϵ_p and Ω_q are their respective energies. We assume that the indices p and q determine not only the quasimomentum but also the number of the branch of the energy spectrum of the electrons and phonons.

We note that Eq. (2) can be solved with respect to Φ_q:

$$\Phi_q = \frac{1}{\nu^{pe}}\frac{2\pi}{\hbar}\sum_{p,k}|B_{pkq}|^2(n_p - n_k)(\chi_p - \chi_k)\delta(\varepsilon_{p,k} - \Omega_q),$$

$$\nu_q{}^{pe} = \frac{2\pi}{\hbar}\sum_{p,k}|B_{pkq}|^2(n_p - n_k)\delta(\varepsilon_{p,k} - \Omega_q), \tag{4}$$

where ν^{pe}_q has the meaning of the frequencies of the collisions between phonons and equilibrium electrons.

Substituting (4) in (1) we arrive at a rather complicated integral equation for the electron function χ_p, an analysis of which is impossible in the general case. The problem becomes much simpler at sufficiently low temperatures, when the phonon momentum $q \sim T/s$ is small in comparison with all the characteristic dimensions of the Fermi surface (Bethe and Sommerfeld[5], Supek[6]). It can be shown that in this case the sought function χ_p is independent of the energy with a high degree of accuracy (in the region where the Fermi distribution is smeared out), and varies significantly within the limits of the equal-energy surface only over distances on the order of the dimensions of this surface. Therefore χ_{p-q}, as well as other smooth functions of p contained in (1) and (4), can be expanded in powers of q, and it turns out a nonzero result occurs only in the approximation quadratic in q. (This circumstance is closely connected with the low efficiency of each individual collision.) It is clear that such an expansion can lead to an integro-differential equation for the function χ_p on the Fermi surface, and the integral term in this equation is connected with the phonon dragging. The corresponding calculations, however, are quite cumbersome, and their result cannot be written down in a lucid form (see the paper by Gurzhi[7]).

We consider it more convenient to obtain the diffusion equation by another method, which leads directly to a compact expression for the collision integral I^e.

We sum the kinetic equation (1) over an arbitrary region V in p-space. Replacing p and q by k and $-q$ under the summation sign in the expression for Γ^-_{pkq} and recognizing that $B_{p,k,q} = B^*_{k,p,-q}$ because the interaction Hamiltonian is Hermitian, we are left as a result only with terms corresponding to transitions of the electrons through the boundary of the region V:

$$\sum_{p\subset V} I^e = \Big(\sum_{p\subset V,\, k\not\subset V,\, q} - \sum_{p\not\subset V,\, k\subset V,\, q}\Big)\Gamma^+_{pkq}. \tag{5}$$

This equality expresses the conservation of the number of particles in p-space in the case of electron-phonon collisions.

We note that when expression (5) is expanded in terms the temperature momentum of the phonons $q \sim T/s$, a nonzero result is obtained already in the linear approximation, whereas in the expansion of the quantity I^e itself, as stated above, it is necessary to take into account second-order terms. (There is no contradiction here, since the expression (5) contains an extra power of q because of the smallness of the summation region, namely, the electron transitions can be realized only from a narrow layer near the boundary of the region V.) This is precisely the advantage of our method of deriving the diffusion equation.

For convenience in calculation, we break up the collision integral into two parts:

$$I^e = I^{ep} + I^{epe},$$

where I^{ep} is the integral of the collisions between the electrons and the equilibrium phonons i.e., without $\Phi_{\pm q}$ in the expression for $\Gamma^\pm_{pkq}$(3)), and I^{epe} describes collisions between electrons via phonons.

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2)Such an approach was used by Klemens and Jackson[4], who, starting from purely physical considerations, wrote down the diffusion equation for the simplest model in which the electron and phonon dispersion laws were assumed to be isotropic, and the phonons were assumed to be in equilibrium. In Sec. 4 below we shall return to a discussion of their results.

We calculate first ΣI^{ep}. We note that in the first order in q the difference $\chi_p - \chi_k$, where $\mathbf{k} = \mathbf{p} - \mathbf{q} - \mathbf{g}$, can be written in the form

$$\chi_p - \chi_k = \mathbf{q}\nabla\chi_p$$

for any vector g. (It should be recognized that when the principal region in p-space is suitably chosen the transition between fixed states p and k is a normal process.) For the matrix element of the interaction in (5) we can therefore confine ourselves to the first non-vanishing approximation: $|b_{pkq}|^2 = qM_p(e)$, where $\mathbf{e} = \mathbf{q}/q$, and, since H_{int} is Hermitian, $M_p(-e) = M_p(e)$.

Simple calculations lead to the following result:

$$\sum_{p\subset V} I^{ep} = \frac{2}{\hbar^3}\oint (\hat{D}_p\nabla\chi_p)\,dl. \tag{6}$$

The integration is carried out here along the line of intersection of the boundary of volume V with the Fermi surface, the vector dl is directed along the outward normal to this line, lying in plane tangent to the Fermi surface, and $\hat{D}_p$ has obviously the meaning of a diffusion tensor in an inhomogeneous anisotropic medium,

$$D_p^{ik} = T^5\frac{30\zeta(5)}{\pi^2\hbar^4 v_p^2}\int_0^{2\pi}\frac{M_p(e)}{s^5(e)}e^i e^k\,d\varphi. \tag{7}$$

The unit vector $\mathbf{e}(\varphi)$ lies here in the plane tangent to the Fermi surface, the angle φ is measured in this plane, s(e) is the velocity of sound:

$$\Omega_q = qs(e), \qquad \zeta(5) = 1.037.$$

Applying to (6) the two-dimensional analog of the Gauss divergence theorem, we obtain[3)]

$$\sum_{p\subset V} I^{ep} = \frac{2}{\hbar^3}\int_V \operatorname{div}(\hat{D}_p\nabla\chi_p)\,dS. \tag{8}$$

The integration is over that part of the Fermi surface which is enclosed in the volume V.

Proceeding to the calculation of ΣI^{epe}, we separate first the low-temperature asymptotic form of the phonon distribution function (4). Calculations analogous in many respects to those carried out above yield

$$\Phi_q = qa(e), \quad a(e) = \frac{\int_F D_p(e)\,\nabla\chi_p\,\delta(\mathbf{e}\mathbf{n}_p)\,dS_p}{\int_F D_p(e)\,\delta(\mathbf{e}\mathbf{n}_p)\,dS_p}. \tag{9}$$

Here $n_p = v_p/v_p$, and $D_p(e)$ is a "partial" diffusion coefficient defined by the relations

$$\hat{D}_p = \int_0^{2\pi}\hat{D}_p(e)\,d\varphi, \quad D_p^{ik}(e) = D_p(e)e^i e^k. \tag{10}$$

The integration in (9) is over the entire Fermi surface, but the δ-function separates the line L on which this surface is parallel to the phonon momentum; using the relation $\delta(\mathbf{e}\cdot\mathbf{n}_p)\,dS = |\hat{K}_p e|^{-1}dl$ we can go over to integration directly along the line L ($\hat{K}_p$ is the curvature tensor).

Further calculations lead to a result similar to (8):

$$\sum_{p\subset V} I^{epe} = -\frac{2}{\hbar^3}\int dS\,\operatorname{div}\int_0^{2\pi}\hat{D}_p(e)\,a(e)\,d\varphi,$$

where $\hat{D}_p(e)$ is a "partial" diffusion tensor (see (10)). Finally, for the field term we obtain

$$\sum_{p\subset V} e\mathbf{E}\frac{\partial n_p}{\partial p} = -\frac{2e}{\hbar^3}\int_V \mathbf{n}_p\mathbf{E}\,dS.$$

Thus, all the terms of the kinetic equation (1) summed over the region V are represented in the form of integrals over the section of the Fermi surface contained in this region. Recognizing that the region V is arbitrary, we obtain the sought diffusion equation

$$\operatorname{div}\hat{D}_p(\nabla\chi_p - a_p) = -e\mathbf{E}n_p, \tag{11}$$

where

$$a_p = \hat{D}_p^{-1}\int_0^{2\pi} D_p(e)\,a(e)\,d\varphi = \int_F \hat{A}_{pp'}\nabla\chi_{p'}\,dS_{p'}, \tag{12}$$

$$\hat{A}_{pp'} = \frac{2\hat{D}_p^{-1}\hat{D}_p(\mu)\hat{D}_{p'}(\mu)}{\gamma(\mu)\sin(\mathbf{n}_p\mathbf{n}_{p'})}, \quad \gamma(\mu) = \int_F D_p(\mu)\,\delta(\mu\mathbf{n}_p)\,dS_p,$$

μ is the unit vector of $\mathbf{n}_{p'}\times\mathbf{n}_p$. The quantities $\hat{D}_p$, $\hat{D}_p(e)$, and $D_p(e)$ are given by formulas (7) and (10).

The electric-current density is

$$\mathbf{j} = \frac{2e}{\hbar^3}\int_F \chi_p\mathbf{n}_p\,dS_p. \tag{13}$$

2. ANALYSIS OF DIFFUSION EQUATION

Equation (11) describes the diffusion of the electrons on the Fermi surface in the presence of an electric field that determines the density of the sources and sinks. This equation is integro-differential and the integral term a_p is connected with phonon dragging. The latter can be easily understood. The emission of a phonon by a certain electron leads to two consequences: first, this electron is displaced on the Fermi surface by an amount equal to the phonon momentum and, second, a change takes place in the momentum of the other electron which absorbed the emitted phonon.

The boundary conditions for (11) follow from the periodicity of the distribution function in p-space:

$$\chi_p = \chi_{p+g}, \quad \nabla\chi_p = \nabla\chi_{p+g}, \tag{14}$$

i.e., the function χ and its first derivatives should be continuous on the equivalent edges of the band. We note that in the diffusion approximation the phonon momentum should be regarded as infinitesimally small and therefore the imposition of the boundary conditions (14) is completely equivalent to allowance for the Umklapp processes.

Let us rewrite (11) in the following form (the subscript p will be emitted wherever there is no danger of misunderstanding):

$$\nabla\chi - \mathbf{a} = \hat{D}^{-1}\psi, \tag{15}$$

where the vector ψ lies in the plane tangent to the corresponding point of the Fermi surface and $\operatorname{div}\psi = -e\mathbf{E}n$. It is clear that the latter relation does not define ψ uniquely.

[3)] In these formulas, ∇ and div must be taken to mean the corresponding two-dimensional operations carried out in the plane tangent to the Fermi surface: $\nabla\phi = (\hat{P}\nabla^3)\phi$ and $\operatorname{div}\mathbf{A} = (\hat{P}\nabla^3)\mathbf{A}$. When quadratic differential operations are performed it should be remembered that the projection operator $\hat{P}$ depends on the momentum and for example, $\operatorname{div}\nabla \neq \nabla^2$.

We note that (15) is a purely integral equation with respect to $\nabla\chi$. It is important in what follows that the corresponding homogeneous equation has, as can be easily verified, a drift solution $\Delta\chi = \nabla(\mathbf{u}\cdot\mathbf{p}) = \mathbf{u}_{||}$ ($\mathbf{u}_{||}$ is the component of the drift velocity parallel to the Fermi surface), regardless of whether the Fermi surface is closed or not.

The existence of a drift solution of the homogeneous equation corresponding to (15) has the following physical meaning: the electron flux density $-\psi$, which is the sum of the diffusion flux $-\hat{D}\nabla\chi$ and of the flux $\hat{D}\mathbf{a}$ of electrons dragged by the non-equilibrium phonons is invariant against the Galilean transformation $\chi \to \chi - \mathbf{u}\cdot\mathbf{p}$. We note that in spite of such an invariance, a metal with an open Fermi surface does have a singled-out reference frame, namely the one in which the lattice is stationary. Only in this frame are the periodic boundary conditions (14) satisfied, and in any other reference frame (14) is replaced by

$$\chi_{p+g} - \chi_p = -\mathbf{ug}, \tag{16}$$

where $\mathbf{u}$ is the translational velocity of the reference frame relative to the lattice. Thus, Eq. (11) is invariant under a Galilean transformation, but the boundary conditions of this equation is not.

It is easy to show that if $\mathbf{u}_{||}$ is a solution of a homogeneous equation with kernel (12), then the corresponding transfer equation has a solution $\nabla\chi = \hat{D}\mathbf{u}_{||} = \hat{D}\mathbf{u}$. It follows therefore that the condition under which (15) has a solution is

$$\int_F \psi\, dS = 0. \tag{17}$$

We note that in the general case this condition does not eliminate completely the leeway in the choice of ψ.

The solution of (15) as an integral equation with respect to $\nabla\chi$ can be represented in the form

$$\nabla\chi = \mathbf{C}\{\psi\} + \mathbf{u}_{||}, \tag{18}$$

where $\mathbf{u}_{||}$ is the solution of homogeneous equations and $\mathbf{C}\{\psi\}$ is the sum of the infinite iteration series:

$$\mathbf{C}_p\{\psi\} = \hat{D}_p^{-1}\psi_p + \int dS_{p'}\hat{A}_{pp'}\hat{D}_{p'}^{-1}\psi_{p'} + \ldots \tag{19}$$

The reference frame moving relative to the lattice with velocity $\mathbf{u}$ will be called co-moving. (In a number of cases considered below, the electron and phonon fluxes in this system are equal to zero.)

We note that the higher iterations in (19) (i.e., the difference $\mathbf{C}\{\psi\} - \hat{D}^{-1}\psi$) are connected with the non-equilibrium character of the phonon distribution in the co-moving reference frame, i.e., with the deviation of their distribution from the drift distribution in the laboratory frame. (We recall that the term $\mathbf{a}$ in (15) is connected with phonon dragging.) On the other hand, it will be shown in Sec. 4, with a concrete example, that the deviation of the distribution function of the phonons from the drift function is small. This means that in a qualitative consideration of the problem we can neglect in the co-moving system the term $\mathbf{a}$ of (15) and assume $\nabla\chi = \hat{D}^{-1}\psi + \mathbf{u}_{||}$.

Equation (18) is a differential equation for χ. The condition for its solvability and the boundary conditions (14) eliminate completely the leeway in the choice of ψ and determine the velocity $\mathbf{u}$ of the co-moving system.

Let us establish also certain relations which will be of use to us later and which are the consequence of the conservation of the quasi-momentum in electron transitions within a band.

We multiply the diffusion Eq. (11) by $\mathbf{p}$ and integrate over the entire Fermi surface (which in the general case can be located in several bands). As a result we have

$$\sum_n \int_{L'} \mathbf{g}\hat{D}(\nabla\chi_n - \mathbf{a}_n)\,\mathbf{dl} = \mathbf{e}\int_F \mathbf{p}(\mathbf{En})\,dS. \tag{20}$$

In the transformations we used Eqs. (15) and the solvability condition (17), which ensures conservation of the quasimomentum in interband transitions. The integration in (20) is over that part of the line of intersection between the Fermi surface and the band boundaries, which does not contain equivalent points (see Fig. 1); the vector $\mathbf{g}$ is directed from this line and generally speaking is different in different sections of the line; the summation is over the numbers of the bands in which the Fermi surface is located.

We note that Eq. (20) is valid for an arbitrary choice of the main cells in reciprocal space, and these cells can be chosen apparently in different bands. Therefore (20) can be rewritten in the form

$$\int_{L_n'} \mathbf{g}\hat{D}(\nabla\chi_n - \mathbf{a}_n)\,\mathbf{dl} = e\int_{F_n} \mathbf{p}(\mathbf{En})\,dS + \mathbf{C}_n, \quad \sum_n \mathbf{C}_n = 0, \tag{21}$$

where L_n' and F_n are those sections of the line L' and of the Fermi surface which are located in the n-th zone, and the quantities $\mathbf{C}_n$ do not depend on the choice of the cells and have the meaning of the quasimomentum received (given up) by the n-th band from (2) from the remaining bands.

Transforming the surface integral into a volume integral, we can show that

$$e\int_{F_n} \mathbf{p}(\mathbf{En})\,dS = -e_n\sum_g \mathbf{g}(\mathbf{ES}_g) + e_n\mathbf{E}V_n.$$

V_n, at our convenience, can be understood either as the volume occupied by the electrons or the "hole" volume free of electrons in the n-th cell. The charge e_n must be taken with the appropriate sign. The vector $\mathbf{S}_g$ is equal in magnitude to the area of contact between the volume V_n and the phase of the cell and is directed along the outward normal to the phase, while $\mathbf{g}$ is the reciprocal-lattice vector corresponding to this phase.

The quantities $\mathbf{C}_n$ can be easily determined in the most frequent case when only one of the bands (with number n = 0) of the Fermi surface is open. Then

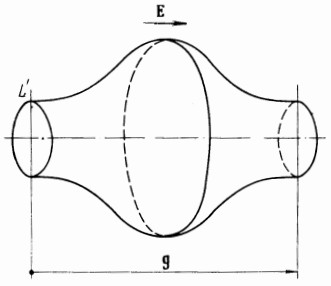

FIG. 1

$$C_{n\neq 0} = -e_n E V_n, \quad C_0 = E(\Omega - e_0 V_0),$$
$$\Omega = \sum_n e_n V_n. \tag{22}$$

To determine the character of the solution of the diffusion equation (11), it is useful to consider a simple model of the electron spectrum, in which the Fermi surfaces in all the bands are surfaces of revolution and all the quantities depend on one coordinate measured along the axis of revolution (see Fig. 1). The integration along the line L′ in (21) then reduces simply to multiplication by $2\pi r$, where r is the radius of the intersection of the Fermi surface by the face of the band. From (21) and (22) we obtain

$$|\nabla\chi| - a = E\frac{\Omega - e_0 Sg}{2\pi g r D}, \qquad n = 0.$$
$$|\nabla\chi| - a = -Ee_n\frac{\pi r}{2D} \qquad n \neq 0. \tag{23}$$

As already noted, the integral term a, which takes into account the nonequilibrium character of the phonons in the co-moving reference frame, is of little significance. If we omit this term in (23), then the solution can be readily completed.

3. FERMI SURFACES WITH NARROW NECKS

In this section we consider cases when a Fermi surface consists of large electron (or hole) groups interconnected arbitrarily by relatively narrow necks (see Fig. 2). The Fermi surface, generally speaking, lies in several bands, and some of the groups can be isolated. This introduces into the problem a small parameter[4] r_0/p_f (r_0 is the radius of the neck and p_F is the characteristic dimension of the large group), and the solution can be carried through to conclusion. It is clear that it is precisely in such a model that the phonon dragging effects are most appreciable, for when the widths of the necks tend to zero the electric conductivity becomes infinite. Fermi surfaces with narrow necks are possessed, for example, by noble and many polyvalent metals.

Proceeding to the calculations, we note first that, as seen from (23), an electron flux of high density, on the order of $E\Omega/gr$, flows through the neck. For this reason, in the co-moving reference frame, the integral term a can be neglected in comparison with $\nabla\chi$. (It is easy to verify that the higher iterations in (19) are small, since the $1/r$ singularity vanishes upon integration.) The action of the field on the neck can also be neglected, since the corresponding change of the flux is proportional to the area of the neck. It follows therefore from (11) that in the co-moving reference frame the following equation is satisfied on the neck

$$\operatorname{div}\hat{D}\nabla\chi = 0. \tag{24}$$

In the analysis that follows it is useful to employ the analogy between this problem and the flow of stationary currents through a branched network. The necks correspond to the conductors of the network and the large group to nodes. The current flowing through the neck is

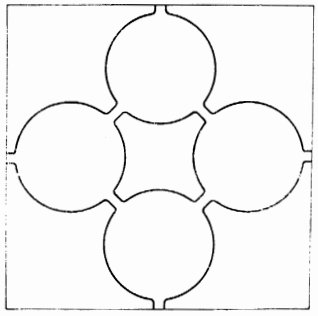

FIG. 2

$$J = \oint \hat{D}\nabla\chi\,\mathbf{dl},$$

where the integration is carried out over any closed line enclosing the neck.

The analog of the potential in this problem is the nonequilibrium increment χ. The "potential" drop occurs mainly on the narrow necks (where $\nabla\chi \sim 1/r$), and the potential can be regarded as constant within the limits of the large groups.

By virtue of the linearity of (24), the current J flowing through the neck satisfies "Ohm's law":

$$\chi_2 - \chi_1 = JR, \tag{25}$$

where χ_1 and χ_2 are the potentials on the large groups joined by the neck, and the "resistance" R is determined by the properties of only the neck itself, and can be obtained from (24).

Let us show now that the currents J obey Kirchof's law. We integrate the diffusion equation (11) over the surface of a certain large group with the necks that are connected to it. The integral of the right-hand side of this equation can be neglected, since it is proportional to the cross section area of the necks. ($\int \mathbf{E}\cdot\mathbf{n}\,ds = 0$ over the closed surface.) On the other hand, the integral of the left-hand side, in accordance with the Gauss divergence theorem, is equal to the sum of the currents flowing through the neck. Thus, for each node we have

$$\sum J = 0. \tag{26}$$

By virtue of the uniqueness of χ and Ohm's law (25) for any "internal" circuit not intersecting the band boundaries, we have

$$\sum JR = 0. \tag{27}$$

If the circuit intersects the band boundary, then the potential χ experiences a jump equal to $-\mathbf{u}\cdot\mathbf{g}$ (see (16)), where $\mathbf{u}$ is the velocity of the co-moving reference frame (in which our analysis is carried out). Therefore for the "external" circuits

$$\sum JR = \mathbf{ug}, \tag{28}$$

where g is the Umklapp vector closing the circuit, and its sign is determined by the direction of flow in the circuit. Thus, the potential-difference sources are included in the external circuits.

[4] Strictly speaking, it is necessary that the quantity rD on the neck be much smaller than on the large group, and the small parameter is the ratio $r_0 D_0/p_F D_F$ (see (23), and particularly the expression (31) obtained below for the resistance of the neck). If the diffusion coefficient (10) has singularities at $r \sim r_0$, then the neck can be characterized by an effective width $\sim rD_0/D_F$.

In addition, the quasimomentum balance equation (20) imposes the following condition:

$$\sum J_g = \Omega \mathbf{E}. \tag{29}$$

The foregoing equations suffice to determine all the currents and the velocity u of the co-moving system. In the model considered here, the electric conductivity of the metal is determined only by the velocity u. This follows from the fact that in a reference frame connected with the lattice the electron distribution within the limits of the large group is of the drift type, $\chi = \mathbf{u} \cdot \mathbf{p} + \text{const}$.

If we write the solution of (26)—(29) in the form $\mathbf{u} = \Omega \hat{S} \mathbf{E}$, then the electric conductivity tensor $\hat{\sigma}$ of the metal (see (13)) takes the form

$$\hat{\sigma} = \frac{2}{\hbar^3} \Omega^2 \hat{S}. \tag{30}$$

The electric conductivity, naturally, is proportional to the resistance of the necks. For the simplest case, when all the necks are intersected by the boundaries of the band, we obtain from (28) and (29)

$$(\hat{S}^{-1})^{ik} = \sum g^i g^k / R,$$

The summation is over all the necks.

Let us proceed now to calculate the resistance of an individual neck. For an arbitrary neck this cannot be done because of the complexity of (24). It is possible, however, to determine the dependence of the resistance on the neck parameters by using as an example the one-dimensional model considered at the end of Sec. 2. In this case we obtain from (24) and (25)

$$R = \frac{1}{2\pi} \int d\tau / rD, \tag{31}$$

where $d\tau$ is the element of length of the generatrix; the integration should be carried out over the "entire" neck, i.e., over the region that makes an appreciable contribution to this integral. The quantity D can be taken outside the integral sign if, as noted above, r is taken to mean the effective width of the neck.

The neck resistance R is significantly different in two limiting cases, when the characteristic width of the neck r_0 is of the order of the radius ρ of the neck generatrix (see Fig. 3) and when $r_0 \ll \rho$. In the former case the main contribution to the resistance (31) is made by relatively large distances, $r_0 \ll \tau \ll p_F$,

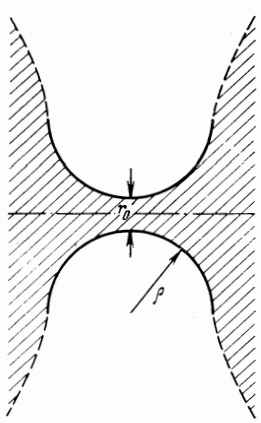

FIG. 3

where an increase of r with increasing τ follows the law characteristic of the large group. Without limiting the generality, we can assume $r = \alpha\tau$ ($\alpha < 1$) and then

$$R = \frac{1}{\pi D \alpha} \ln \frac{p_F}{r_0},$$

p_F is the characteristic dimension of the large group. In the second case we can assume in (31) $r = r_0 + \tau^2/\rho$, and then

$$R = \frac{1}{2D} \sqrt{\rho / r_0}, \tag{32}$$

and the characteristic length of the neck is $\sqrt{r_0 \rho}$.

It has been assumed so far that the thermal momentum of the phonon is much smaller than the characteristic distances on the Fermi surface. In the presence of long necks (case 2), interest attaches to the region of intermediate temperatures, in which the thermal momentum of the phonon $q \sim T/s$ satisfies the inequalities

$$r_0 \ll q \ll \sqrt{r_0 \rho}. \tag{33}$$

Under such conditions, the diffusion approximation remains in force, since the non-equilibrium increment χ on the neck depends only on the variable τ with a characteristic scale of variation $\sqrt{r_0 \rho}$, and the length of the Brownian step q is much smaller than this distance. However, the diffusion tensor $\hat{D}$ changes its form appreciably. Calculations analogous to those performed in Sec. 1 lead to the result

$$D = Ar, \quad A = \frac{4\pi^3}{15\hbar^4} (T/s(\mathbf{e}))^4 M_p(\mathbf{e}) / v_p^2. \tag{34}$$

Here D is the diagonal component of the diffusion tensor along the neck axis and e is the unit vector along this axis.

Using (34), we obtain

$$R = \frac{1}{4A} (\rho / r_0^3)^{1/2}.$$

Thus, under the conditions of (33), the dependence of the neck resistance on this thickness and on the temperature is significantly altered, namely, $R \sim r_0^{-3/2} T^{-4}$, whereas in the case of sufficiently low temperatures, at $q \ll r_0$, Eq. (32) yields $R \sim r_0^{-1/2} T^{-5}$. The change of the temperature dependence is connected with the one-dimensional character of the diffusion: only phonons whose momenta are almost parallel to the neck axis can interact with the electrons. The number of such phonons is proportional to T, whereas in the case of two-dimensional diffusion the number of phonons is proportional to T^2. Thus, for metals with long necks in the region of intermediate temperatures (33) the electric resistance turns out to be proportional to T^4. This result possibly explained the T^4 law observed experimentally for the resistivity of aluminum. Another explanation of this law was proposed by Pytte[8]. We note that the results will be valid also for closed Fermi surfaces, provided the gap between these surfaces is $\Delta p \lesssim q$.

4. WEAK-COUPLING APPROXIMATION

We begin with consideration of a very simple model, for which the electric conductivity problem can be solved exactly. Let a spherical Fermi surface be intersected by only one pair of Bragg planes and be thus

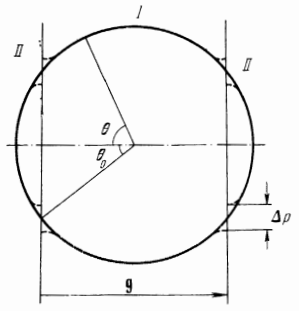

FIG. 4

located in two energy bands. The distortion of the electron dispersion law in the vicinity of the intersection lines will not be taken into account. (The corresponding distortions of the Fermi surface are shown dashed in Fig. 4.) It will also be assumed that all the characteristics of the metal are isotropic, and in particular that the diffusion tensor reduces to a constant scalar D. The electric field, naturally, is perpendicular to the Bragg planes.

In the model under consideration, the kernel of the diffusion equation (12) takes the form

$$A^{ik}_{pp'} = \frac{\mu^i \mu^k}{\pi^2 p_F^2 \sin(\widehat{\mathbf{nn}'})}$$

Using this expression, we can easily verify that

$$\operatorname{div}\int_F \hat{A}_{pp'} \nabla\chi_{p'} dS_{p'} = \frac{1}{\pi^2}\int \operatorname{ctg}(\widehat{\mathbf{nn}'}) \operatorname{div}\nabla\chi_{p'} d\mathbf{n}',$$

where $d\mathbf{n}' = dS_{p'}/p_F^2$ is the solid-angle element, and the operator div ∇ is the angular part of the Laplacian. In this connection, it is convenient to choose as the sought function $\eta = \operatorname{div}\nabla\chi$, which, as follows from the diffusion equation (11), satisfies the equation

$$\eta(\theta) = \frac{1}{\pi^2}\int \eta(\theta') \operatorname{ctg}(\widehat{\mathbf{nn}'}) d\mathbf{n}' - \frac{eE}{D}\cos\theta + \frac{G}{D}[\delta(\theta-\theta_0)-\delta(\theta-\theta_0')]. \quad (35)$$

Here θ is the angle between the vector $\mathbf{n}$ and the direction of the opening, $0 \le \theta \le \pi$, $\cos\theta_0 = g/2p_F$, and $\theta_0' = \pi - \theta_0$ (see Fig. 4). The last term in the right-hand side of (35) describes sources and sinks having a power G and located on the line of intersection between the Fermi surface and the Bragg planes. The point is that Eq. (11) is valid in the interior of each individual band, but on the boundary between two bands the function χ and its derivatives may, generally speaking, experience discontinuities. Discontinuities of the function χ itself are eliminated by the symmetry of the problem. Indeed, it follows from the fact that χ is odd as a function of p (because the field term in (11) is odd), from the periodicity of the boundary conditions (14) (these conditions pertain to each band separately), and from the one-dimensional character of the problem, that

$$\chi^{I}(\theta_0) = \chi^{I}(\theta_0') = \chi^{II}(\theta_0) = \chi^{II}(\theta_0') = 0, \quad (36)$$

I and II are the numbers of the energy bands.

Thus, the last term in the right-side of (35) specifies the value of the jump $\Delta\chi$ on the boundary of two bands. The constant G can be obtained from the condition for the solvability of Eq. (35). We have

$$G\int \cos\theta[\delta(\theta-\theta_0)-\delta(\theta-\theta_0')]d\mathbf{n} = eE\int\cos^2\theta d\mathbf{n},$$
$$G = 2eE/3\sin 2\theta_0.$$

It is clear that it is convenient to represent the solution of the integral equation (35) in the form of a series in Legendre polynomials $P_n(\theta)$. The eigenvalues λ_{nn} corresponding to the kernel $\cot\langle \mathbf{nn}'\rangle$ are equal to

$$\lambda_n = \frac{2}{n(n+1)}\left[\frac{n!!}{(n-1)!!}\right]^2$$

for odd n, and $\lambda_n = 0$ for even n; when $n \gg 1$ we have $\lambda_n \approx 4/\pi n$.

The solution of (35) in the co-moving reference frame can be written in the form

$$\eta = \eta_1 + \eta_2,$$
$$\eta_1 = -\frac{eE}{D}\left\{\cos\theta - \frac{2}{3\sin 2\theta_0}[\delta(\theta-\theta_0)-\delta(\theta-\theta_0')]\right\},$$
$$\eta_2 = \frac{2eEp_F}{Dg}\sum_{n=3}^{\infty}\frac{2n+1}{1-\lambda_n}\lambda_n P_n(\theta_0)P_n(\theta).$$

Here η_1 is the zeroth order of iteration with respect to the integral term. The term η_2, as shown in Sec. 2, is connected with the non-equilibrium character of the phonons in the co-moving reference frame.

Now the function χ in the co-moving reference frame can be easily obtained by solving the equation $\operatorname{div}\nabla\chi = \eta$, since the Legendre polynomials are eigenfunctions of the operator div∇ with eigenvalues $-n(n+1)/p_F^2$. To save space, we do not present the solution here. We note only that this solution, like $\eta(\theta)$, is orthgonal to $P_1(\theta) = \cos\theta$, and consequently makes no contribution to the electric current $j \sim \int \cos\theta\, d\mathbf{n}$. Thus, for the model in question, the electron current in the co-moving reference frame is equal to zero; it can also be shown that the phonon current vanishes. The electric-current density is determined therefore by the velocity u of the co-moving reference frame

$$j = \frac{8\pi}{3}\left(\frac{p_F}{h}\right)^3 eu.$$

The velocity u can be determined with the aid of the condition (16). The result takes the form

$$u = u_1 + u_2,$$
$$u_1 = u_0[\beta(\theta_0)-1], \quad u_2 = \frac{2}{3\cos^2\theta_0}u_0\sum_{n=3}^{\infty}\frac{2n+1}{n(n+1)}\frac{\lambda_n}{1-\lambda_n}[P_n(\theta_0)]^2,$$
$$u_0 = \frac{eEp_F}{2D}, \quad \beta(\theta_0) = \frac{1}{3\cos^2\theta_0}\ln\frac{1+\cos\theta_0}{1-\cos\theta_0}. \quad (37)$$

The series for u_2 converges, since $|P_n(\theta)| \le 1$ and at $n \gg 1$ the coefficients decrease in proportion to n^{-2}.

To clarify the physical meaning of the results, we rewrite (37) in the form

$$u = u_0 - u_0\beta^{-1} + u_0(\beta^{1/2} - \beta^{-1/2})^2 + u_2.$$

The first two terms in this formula correspond to the results of the already mentioned paper at Klemens and Jackson[4], in which no account was taken of the phonon dragging[5]. It is easy to show that u_0 is the electron drift velocity under conditions when the phonons are in equilibrium and there are no Umklapp processes. The second term $(-u_0\beta^{-1})$ is connected with Umklapp processes. The third term is due to the phonon drift.

[5]Some difference between the formulas is connected with the fact that Klemens and Jackson considered only one energy band.

Finally, the term u_2 is connected with the deviation of the phonon distribution from the drift distribution. An analysis of (37) shows that the contribution from this term is relatively small. For example, for trivalent fcc metals $g/2p_F = 0.89$ and calculations yield $u_2/u \approx 0.22$.

So far we have considered a one-dimensional model, in which the Fermi surface is intersected only by one pair of Bragg planes and therefore there is only one opening direction. For a more realistic model with many opening directions, the calculations can be carried through to conclusion only if the radii of all the sections are small: $\theta_0 \ll 1$. We present the final result for this case, which obviously is the most realistic, when all the opening directions are equivalent

$$u = u_1 + u_2,$$

$$u_1 = u_0(B-1), \quad B = \left(\sum_k \cos^2 \alpha_k\right)^{-1} \sum_k \cos \alpha_k \cdot \beta(\alpha_k),$$

$$u_2 = \frac{2}{3} u_0 \left(\sum_k \cos^2 \alpha_k\right)^{-1} \sum_{n=3}^{\infty} \frac{2n+1}{n(n+1)} \frac{\lambda_n}{1-\lambda_n} \sum_k \cos \alpha_k [P_n(\alpha_k)]^2.$$

Here k is the number of the opening axis, α_k is the angle between this axis and an arbitrarily chosen reference axis, and $\alpha_0 = \theta_0$.

We note that if $\ln(1/\theta_0) \gg 1$ these formulas go over, as can be easily verified, into the corresponding formulas of Sec. 3 for short necks.

Another circumstance, not taken into account so far, is that in the weak-coupling approximation the electron dispersion law is not isotropic near the Bragg planes. The distortion of a small part of the Fermi surface is in itself of little importance for our problem and leads to increments on the order of V_g/ϵ_F, where V_g is the Fourier component of the pseudopotential. However, the presence in p-space of a discontinuity $\Delta p \sim V_g/v_F$ between the energy bands (see Fig. 4) should be suitably taken into account in the boundary conditions.

At sufficiently low temperatures, when $q \sim T/s \ll \Delta p$ and interband transitions are therefore impossible, we have for each pair of Bragg planes

$$\chi^{I}(\theta_0) = \chi^{I}(\theta_0'), \quad \chi^{II}(\theta_0) = \chi^{II}(\theta_0'),$$

$$\nabla_\perp \chi^{I}(\theta_0) + \nabla_\perp \chi^{I}(\theta_0') = \nabla_\perp \chi^{II}(\theta_0) + \nabla \chi^{II}(\theta_0') = 0, \qquad (38)$$

where $\nabla_\perp \chi$ is the projection of $\nabla \chi$ on the outward normal to the band boundary.

At higher temperatures, when $q \gg \Delta p$, the boundary conditions take the form

$$\chi^{I}(\theta_0) = \chi^{I}(\theta_0') = \chi^{II}(\theta_0) = \chi^{II}(\theta_0'),$$

$$D^{I}(\nabla_\perp \chi^{I}(\theta_0) + \nabla_\perp \chi^{I}(\theta_0')] + D^{II}[\nabla_\perp \chi^{II}(\theta_0) + \nabla_\perp \chi^{II}(\theta_0')] = 0. \qquad (39)$$

For the one-dimensional model with one direction of opening, the conditions (38) and (39) coincide, by virtue of the symmetry of the problem, and reduce to (36). This means that the proportionality coefficient in Bloch's law $\rho \sim T^5$ does not change on going from temperatures $T \ll \Delta p/s$ to temperatures $T \gg \Delta p/s$. The situation is the same also in the model considered above, with several narrow openings ($\theta_0 \sim 1$). On the other hand, if the openings are large ($\theta_0 \sim 1$), then the conditions (38) and (39) are not equivalent. A particularly large coefficient in the $\rho \sim T^5$ law should be expected. In those cases when narrow necks exist in the absence of interband transitions, and at higher temperatures the electron flux can get around these necks and propagate through a neighboring band. If the situation considered at the end of Sec. 3 obtains in this case, then a transition from $\rho \sim T^4$ to $\rho \sim T^5$ is possible.

Note added in proof (21 October 1971). In connection with the interpretation of the $\rho \sim T^4$ for aluminum (see the last paragraph of Sec. 3), we wish to note that Pytte's calculations [8] were performed on the basis of a variational principle using a drift trial function $\chi_p = \mathbf{u} \cdot \mathbf{p}$ which was not periodic in reciprocal space. It is easy to show, however, that such a method of analysis does not apply to metals at low temperatures, where the Fermi surface crosses the boundaries of the Brillouin zone (or passes close to them). The contribution of the Unklapp processes to the electric resistance turns out to be appreciably overestimated and proportional to T^4, as was indeed found by Pytte. The use of any periodic and sufficiently smooth trial function would have led to the result $\rho \sim T^5$ (if phonon dragging is disregarded).

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