Influence of defects on phonon drag in metals

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The influence of scattering of electrons and phonons by defects in metals on the phonon drag in the electric conductivity of uncompensated metals with a closed Fermi surface is analyzed. It is shown that there are two different concepts of a "pure" and "dirty" limit for the phonon and electron subsystems respectively. In the phonon dirty limit (the momentum flow from the phonon system to the defects exceeds the momentum exchange with the electron system) the resistance has the usual value in absence of drag. In the phonon pure but electron dirty limit (the phonon resistance is less than the residual resistance) the low-temperature resistivity of a metal with an anisotropic electron spectrum has a power-law dependence on the temperature *T*. The pure and dirty electron limits do not differ for metals with a Fermi surface that is almost spherical, and the resistivity is determined by the competition between Umklapp processes in the electron and phonon subsystems, and by the scattering of phonons by the defects. At sufficiently low temperatures the latter lead to a change from an exponential to a power-law dependence on *T*.

1. INTRODUCTION

The question of the influence of the dragging effect on the electric conductivity of metals and the assessment of the feasibility in principle of experimentally observing manifestations of this effect in real metals remains one of the most interesting problems of the physics of transport phenomena at low temperatures. In spite of the lucidity of the physical ideas, which were introduced by Peierls back in the 30's (see, e.g.,[1]), an exhaustive analysis of the phenomenon for a real situation has never been carried through to conclusion. As a result, publications appear from time to time, in which the anomalies in the electric resistivity of metals are unjustifiably ascribed to the dragging effect or where it is categorically stated that it is impossible, or conversely possible, to observe dragging under one condition or another. Perhaps the only common point of view is the inevitability of the existence of the dragging effect in alkali metals (the case most closely corresponding to the Peierls picture), but even here the fundamental question concerning the role of defects remains in fact open.

We have previously presented[2] a general analysis of the possibility of a manifestation of the dragging effect in the electric conductivity for metals with arbitrary togology of the Fermi surface in the absence of defects. It was established as a result that the exponential dependence of the resistance on the temperature, which is a characteristic of the dragging effect, should not occur in any of the compensated metals (where the number of electrons n_e is equal to the number of holes n_h)[1)], nor in metals having open Fermi surfaces. (In metals with cubic symmetry, the last statement is general. In noncubic metals, a distinction should be made between the resistivity tensory components $\rho^{\alpha\alpha}$ along the principal axes. The dragging effects will become manifest for components along those axes which are perpendicular to the normals to all the boundaries of the Brillouin zone that are intersected by the open Fermi surface.) In a metal with a closed Fermi surface ($n_e \neq n_h$), the dragging effect should exist in principle at any arbitrary topology of the latter, and particularly in the case of a multiply-connected Fermi surface when individual pieces of the surface are localized on faces of the Brillouin zone. However, an analysis of the existing experimental data have shown (see, e.g.,[3]) that apart from the alkali metals one can this group includes at the present time only aluminum and indium, and possibly thallium (for the resistivity-tensor component along the c axis). The overwhelming majority of polyvalent metals have either open Fermi surfaces or equal numbers of electrons and holes.

In those cases when a manifestation of the dragging effect is still possible, it is more natural to raise the question of the role of defects, which inevitably produce a channel for the outflow of momentum from the electron-phonon system of the metal. This is all the more interesting, since it has become clear recently that at low temperatures there exists a peculiar strong "interference" between the scattering of electrons by phonons and impurities, which leads in particular to effects which are strongly nonlinear in the impurity concentration (see[4] and also[5]) and which manifest themselves extensively in experiments (see, e.g., the review[6]). On the other hand, the question of how the resistivity is influenced by the irreversible outflow of the momentum as a result of phonon scattering by defects is no less interesting. The present article is devoted to the corresponding analysis.

2. INFLUENCE OF THE SCATTERING OF ELECTRONS AND PHONONS BY DEFECTS

To analyze the resistance at low temperatures, we used the usual linearized system of Boltzmann kinetic equations for the electron-phonon system of the metal, which can be represented in the following symbolic form:

$$\begin{aligned} N &= \hat{P}^{e,\,ph}(\varphi,\ \chi)+\hat{R}(\varphi), \\ 0 &= \hat{P}^{ph,\,e}(\chi;\ \varphi)+\hat{L}(\chi)+\hat{L}^{d}(\chi). \end{aligned} \qquad (2.1)$$

Here $\hat{P}$, $\hat{L}$, and $\hat{R}$ are linear collision operators, which describe respectively the interaction of the electrons with phonons and with impurities in the first equations, and of the phonons with electrons and with one another as a result of the anharmonicity, and also with the defects ($\hat{L}^d$) in the second equation; N is the standard field term; the functions φ and χ are connected with the corrections to the electron and phonon distribution functions by the relations

$$f^{(1)}(k)=-\frac{\partial f^{(0)}(k)}{\partial \varepsilon(k)}\varphi(k), \qquad g^{(1)}(q)=-\frac{\partial g^{(0)}(q)}{\partial \omega(q)}\chi(q),$$

where k stands for the aggregate of the electron quasimomentum **k** and the number of the energy band n, while q combines the phonon quasimomentum **q** and the number of the branch α.

In (2.1) we take the operator for collisions with the defects to mean the summary operator, which includes scattering by impurities, by the crystal boundaries, etc. Thus, we neglect in (2.1) only the electron-electron interaction, which is apparently always small in practice, at least in nontransition metals.

We expand the functions φ and χ in the complete systems of the functions $\{\varphi_s\}$ and $\{\chi_\alpha\}$, and the first of these functions we choose in both systems linear functions of the quasimomenta

$$\varphi_1(k)=\mathbf{ku}, \quad \chi_1(q)=\mathbf{qu}, \tag{2.2}$$

where **u** is a unit vector in the direction of the electric field. In the case when pieces of the Fermi surface lie on the boundary of the Brillouin zone, it is necessary to choose the corresponding piecewise-linear quasimomentum function k, which conserves periodicity in the reciprocal-lattice space, for details see[2].) With respect to the remaining functions we shall assume that they are orthogonal to N. This choice is always possible since the scalar product is

$$\langle\varphi_1|N\rangle \sim n_e - n_h \neq 0.$$

Substituting the expansions of the functions $\varphi(k)$ and $\chi(q)$ in (2.1), multiplying the first equation by $\varphi_s(k)$ and the second by $\chi_\alpha(q)$, and integrating respectively with respect to the variables k and q, we arrive at the system of equations of the method of moments, which corresponds to the usual variational principle. Solving the homogeneous subsystem that corresponds to the second equation with respect to the expansion coefficients of the phonon distribution function and substituting the resultant values in the first subsystem, we arrive at the following system of equations for the expansion coefficients a_s of the function $\varphi(k)$:

$$j_1\delta_{1s} = \sum_{s'} \tilde{P}_{ss'} a_{s'}, \tag{2.3}$$

$$\tilde{P}_{ss'} = T_{ss'} - \sum_{\alpha\alpha'} P'_{s'\alpha}(Q^{-1})_{\alpha\alpha'} P'_{\alpha's}, \qquad j_1 = \langle\varphi_1|N\rangle. \tag{2.4}$$

Here $T_{ss'}$ is the matrix element of the collision operator in the equation for the electrons in the absence of the dragging effect ($\chi = 0$). In this case

$$T_{ss'} = P_{ss'} + R_{ss'}, \tag{2.5}$$

where $P_{ss'}$ is the matrix element of the electron-phonon collision operator

$$P_{ss'} = \frac{1}{T}\iiint W(k,q;k')\,(\varphi_s(k)-\varphi_s(k'))\,(\varphi_{s'}(k)-\varphi_{s'}(k'))\,dk'\,dk\,dq. \tag{2.6}$$

The matrix elements $Q_{\alpha\alpha'}$, which result from the equations for the phonons, are given by

$$Q_{\alpha\alpha'} = P''_{\alpha\alpha'} + L_{\alpha\alpha'} + L^d_{\alpha\alpha'}, \tag{2.7}$$

where $P''_{\alpha\alpha'}$ is obtained from $P_{ss'}$ (2.5) by simply replacing each function difference $\varphi_s(k) - \varphi_s(k')$ by $\chi_\alpha(q)$. In turn, $P'_{s\alpha} = P'_{\alpha s}$ is obtained from (2.6) by replacing one of these differences by $\chi_\alpha(q)$.

Solving the system (2.2) with respect to a_1 and recognizing that the resistivity is given by

$$\rho = (a_1 j_1)^{-1},$$

we obtain (see the analogous derivation in[5])

$$\rho = \frac{1}{j_1^2}\Big[\tilde{P}_{11} - \sum_{s,s'\neq 1} \tilde{P}_{1s}(\tilde{\tilde{P}}^{-1})_{ss'}\tilde{P}_{s'1}\Big]. \tag{2.8}$$

The matrix $\tilde{\tilde{P}}$ is obtained from the matrix $\hat{\tilde{P}}$ by crossing out the first row and the first column.

It is important that in a metal without defects, neglecting umklapp processes, i.e., under conditions of total dragging, the right-hand side of (2.8) vanishes both for the exact solution and when the approximation of the limited number of moments is used. Indeed, the conservation of the momentum in the collision of the electrons with the phonons leads to the relations

$$P_{1s}{}^N = -P_{1s}{}'^N; \quad P''^N_{1\alpha} = -P_{1\alpha}{}'^N, \quad P_{11}{}^N = P''^N_{11}. \tag{2.9}$$

(the index N will denote from now on the matrix elements of that part of the collision operator which corresponds to the normal processes.) Substituting this result in (2.4) we obtain directly (at arbitrary s)

$$\tilde{P}_{s1}{}^N = \tilde{P}_{1s}{}^N = 0. \tag{2.10}$$

We note that when umklapp processes are taken into account all the matrix elements $\tilde{P}_{1s}$ have the usual exponential smallness. Consequently, at extremely low temperatures the second term of (2.8) is negligibly small in comparison with the first, and the resistivity is determined completely by the matrix element $\tilde{P}_{11}$.

In the case of polyvalent metals, when pieces of the Fermi surface cross the boundary of the Brillouin zone, the separation of the normal processes from the umklapp processes calls for a definite accuracy. However, as shown in[2], when the first function is chosen for the electrons in a suitable piecewise-linear form, it is always possible to resolve the scattering probability W into components W^N and W^U such that relations (2.9) are valid for the normal part, and W^U causes the appearance of exponentially small values of the matrix elements $\tilde{P}^N_{1s}$. It should be noted in this connection that the statement contained for example in[7, 8], namely that in polyvalent metals it is impossible for an exponentially small resistivity to exist as a result of the dragging effects, is incorrect. In indirect form, the same statement is contained also in a paper by Holstein[9].

Let us analyze the problem in the presence of defects, confining ourselves to the two-moment approximation of the electron distribution function and to the one-moment approximation of the phonon function, and using functions of the type (2.2) for the phonon trial function and the first of the electron trial functions. As seen in[4] (see also[5]), a most basic step in the analysis of electric conductivity at low temperatures is to go outside the framework of the single-moment approximation, so as to be able to take the crystalline anisotropy of the electron distribution function into account. It is only in this case that a strong interference between the inelastic scattering by phonons and elastic scattering by impurities can be revealed. To obtain the complete qualitative picture it suffices to have two moments in the expansion of the electron function, and inclusion of a larger number of moments yields only quantitative corrections. On the other hand, as shown by direct analysis, going outside the framework of the one-moment approximation for the phonon function in the problem of the electric conductivity leads likewise only at quantitative corrections.

We separate in explicit form the scattering of the electrons by the defects. Then, introducing the notation (see (2.4))

$$\tilde{P}_{ss'}=R_{ss'}+\tilde{P}_{ss'}^{(0)}, \tag{2.11}$$

we obtain for the resistivity in the approximation formulated above

$$\rho=\frac{1}{j_1^2}\left(R_{11}+\tilde{P}_{11}^{(0)}-\frac{\tilde{P}_{12}^{(0)2}+2R_{12}\tilde{P}_{12}^{(0)}}{R_{22}+\tilde{P}_{22}^{(0)}}-\frac{R_{12}^2}{R_{22}+\tilde{P}_{22}^{(0)}}\right). \tag{2.12}$$

Let us consider the region of sufficiently low temperatures, when the terms quadratic in the umklapp process and the terms of the type P_{1s}^U can be neglected in comparison with P_{1s}^N. Then, using (2.4), (2.6), (2.7), and (2.9) we obtain

$$\tilde{P}_{11}^{(0)}\approx\frac{P_{11}^N}{P_{11}^N+L_{11}^d}(Z_{11}^U+L_{11}^U+L_{11}^d),$$

$$\tilde{P}_{12}^{(0)}=\frac{P_{11}^N}{P_{11}^N+L_{11}^d}(P_{12}^U+P_{12}'^U)+\frac{P_{12}^N}{P_{11}^N+L_{11}^d}(P_{11}''^U+P_{11}'^U+L_{11}^U+L_{11}^d), \tag{2.13}$$

$$Z_{1t}^U=P_{1t}^U+P_{11}'^U+P_{12}'^U+P_{11}''^U \qquad (t=1,2). \tag{2.14}$$

We note that expression (2.14) reduces directly to (2.6) at s = 1 and s′ = t, if the difference $\varphi_s(k)-\varphi_s(k')$ is replaced by $\varphi_s(k)-\varphi_s(k')+\chi_1(q)$, confining ourselves in this case to integration only over the umklapp processes.

The matrix element $P_{22}^{(0)}$ does not vanish when account is taken of only the normal processes, and has the same power-law temperature dependence as in the absence of the dragging effect. From the form of (2.12), and (2.13) it follows that in the case of the dragging effect there are two different conceptions of the so-called "clean" and "dirty" limits for the electrons and phonons, respectively.

Thus, the relation between the quantities L_{11}^d and P_{11}^N that enter in the denominator of (2.13) (in fact, with $P_{11}''^N$ equal to P_{11}^N), actually determines the ratio of the momentum outflow from the phonon system as a result of the interaction with the defects to the momentum transfer to the electron system. The dirty limit with respect to phonons corresponds to the condition

$$L_{11}^d\gg P_{11}^N, \tag{2.15}$$

which leads directly to the result

$$\tilde{P}_{1t}^{(0)}\approx P_{1t}^N \qquad (t=1,2).$$

Under the condition (2.15), the resistivity therefore assumes the same value as in the absence of the dragging effect.

In the opposite clean limit

$$L_{11}^d\ll P_{11}^N \tag{2.16}$$

the phonon system turns out to be nonequilibrium as a result of the electron-phonon interaction, and the expression for the resistance takes the form

$$\rho-\rho_0=\frac{1}{j_1^2}\left[Z_{11}^U+L_{11}^U+L_{11}^d-\frac{2R_{12}}{R_{22}+\tilde{P}_{22}^{(0)}}(Z_{12}^U+L_{11}^U+L_{11}^d)+\frac{R_{12}^2\tilde{P}_{22}^{(0)}}{R_{22}(R_{22}+\tilde{P}_{22}^{(0)})}\right], \tag{2.17}$$

where

$$\rho_0=\frac{1}{j_1^2}\left(R_{11}-\frac{R_{12}^2}{R_{22}}\right) \tag{2.18}$$

is the usual residual resistivity.

Direct estimates show that in the region of low temperatures, where $P_{1t}^U \ll P_{1t}^N$ (several degrees K), the condition (2.16) is well satisfied in ordinary pure crystals when account is taken of scattering by defects ($L_{11}^d \sim T^8$ in the case of point defects). The scattering of the phonons by the boundaries can violate the inequality (2.16) only in very thin samples or at appreciably lower temperatures.

Thus, (2.17) yields in fact a general expression for the resistivity under the conditions of the dragging effect. Let us consider first the clean electron limit, i.e., the case when

$$R_{22}\ll\tilde{P}_{22}^{(0)}. \tag{2.19}$$

Then the last term in (2.17) leads to a renormalization of the residual resistivity and

$$\rho-\tilde{\rho}_0\approx\frac{1}{j_1^2}(Z_{11}^U+L_{11}^U+L_{11}^d)-\frac{1}{j_1^2}\frac{R_{12}^2}{\tilde{P}_{22}^{(0)}}, \tag{2.20}$$

$$\tilde{\rho}_0=R_{11}/j_1^2. \tag{2.21}$$

The reason for the change of the residual resistivity is that in the clean limit the nonequilibrium part of the distribution function of the electrons is formed as a result of scattering by phonons, and under dragging conditions it loses the crystalline anisotropy. This is precisely the cause of the transition from (2.18) to (2.21).

In the real situation it is very difficult to ensure satisfaction of the condition (2.19) for the clean limit in the temperature interval typical of the manifestation of the dragging effect. As a rule, to the contrary, in this interval of temperatures we have a condition inverse to (2.19), i.e., we shall operate in the dirty limits with respect to electrons. In this case the last term of (2.17) becomes equal to

$$j_1^{-2}(R_{12}/R_{22})^2\tilde{P}_{22}^{(0)} \tag{2.17'}$$

and in the case of anisotropy of the electron spectrum (in this case $R_{12} \neq 0$) the temperature dependence of the resistivity is determined precisely by the term which no longer contains the exponential dependence and causes the appearance of the usual Bloch temperature dependence ($\tilde{P}_{22}^{(0)} \sim T^5$). A similar result was first obtained by Gurzhi[10]. Physically, this nontrivial result is connected with the "nondrift" part of the distribution function, which appears when the electron are anisotropically scattered by the impurities, and has the symmetry of the crystal and causes the same temperature dependence of the resistance as in the absence of dragging processes.

A recent analysis has shown[5] that, for example in aluminum, the parameter R_{12}/R_{22} is far from small. It appears that in polyvalent metals in the low-temperature limit, corresponding to the "dirty" limit, the exponential dependence of the resistance will always be masked by the T^5 law. The only possibility of revealing the dragging effect is the use of samples of so high purity that the region of the clean limit would become compatible with the region of the exponential dependence of the matrix elements of the collision operator.

In the case of alkali metals, whose Fermi surface is close to spherical, the role of the anisotropy of the scattering by impurities is small, and $R_{12} \approx 0$. There is then no difference between the dirty and clean limits with respect to electrons, and the resistivity is determined by (2.20), from which the last term has been omitted, and which is now valid in the general case. It is interesting that the influence of the defects on the temperature-dependent part of the resistivity becomes manifest in this case only via the finite damping of the phonons.

As seen from (2.20), the temperature dependence of the resistivity in the considered region is determined by the competition between the umklapp processes and phonon scattering by the defects. With the latter playing a rather small role with decreasing temperature, the exponential dependence of the resistivity should give way to a power-law dependence, the character of which is determined by the leading mechanism of phonon scattering. We note that in the temperature region where L_{11}^{d} is relatively small, the resistivity can be determined not by umklapp processes in electron-phonon interactions, but by umklapp processes in the system of the phonons themselves, owing to the anharmonicity.

Recent measurements of the resistivity of alkali metals[11, 12] have established that at $T < 4°K$ the exponent of the temperature dependence increases continuously with decreasing T, reaches values 7.5 to 9, and then begins to decrease. In samples with larger residual resistivity, the exponent at the maximum was smaller. This behavior can be directly understood on the basis of (2.20). Indeed, the presence of the term L_{11}^{d} should inevitably lead to a power-law dependence of ρ at sufficiently low temperatures. If scattering by point defects plays the decisive role, then a T^8 dependence should be observed. If dislocations or crystallite boundaries are decisive, the exponent becomes smaller. On the other hand, the presence of even slight nonsphericity of the Fermi surface, or in the more general case anisotropy of the elastic scattering of the electrons by the defects ($R_{12} \neq 0$), leads at sufficiently low temperature to the T^5 dependence, in accord with (2.17′). We note that at quite low temperatures the Knudsen regime of momentum transfer by the phonons to the boundary can become decisive. This creates a condition corresponding to the dirty limit (2.15) with respect to phonons, and the exponent should again be $n = 5$.

[1)] It is interesting that in compensated metals the dragging effect becomes manifest in strong magnetic fields, which should lead to an exponential temperature dependence of the transverse magnetoresistance. This case will be considered separately.

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