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QUANTUM OSCILLATIONS OF THE THERMAL CONDUCTIVITY COEFFICIENT OF AN ELECTRON GAS IN A MAGNETIC FIELD

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The quantum oscillations of the thermal conductivity coefficient of conduction electrons in a strong magnetic field H ($\omega\tau \gg 1$, $\omega = eH/mc$, τ is the relaxation time) are computed at low temperatures ($kT \ll \zeta$, ζ being the chemical potential of the electron gas) when scattering of the electrons on impurities is of decisive importance. It is shown that the oscillating part of the thermal conductivity coefficient can be expressed in a simple manner in terms of the oscillations of the specific electric conductivity.

1. The thermal conductivity of metals in a magnetic field at low temperatures exhibits a singularity similar to the Shubnikov—De Haas phenomenon: the thermal conductivity coefficient depends on the magnetic field in a non-monotonic, oscillating manner.[1] Since the presence of oscillations in a magnetic field is a common quantum property of the thermodynamic and kinetic characteristics of a degenerate electron gas, one can assume that the electronic part of the thermal conductivity of the metal is responsible for the observed effect. Therefore, theoretical consideration of the quantum oscillations of the electronic contribution to the thermal conductivity coefficient of metal is of interest.

In the present work, quantum corrections to the classical (smoothly dependent on the magnetic field) coefficient of thermal conductivity of a metal[2] are investigated within the framework of a free gas of conduction electrons. We consider the electron gas in a metal whose temperature T has a small constant gradient grad T perpendicular to an external homogeneous magnetic field H. The density of the electrons is assumed to be sufficiently great that the temperature and the magnetic field satisfy the conditions $\Theta \equiv kT \ll \zeta$ and $\hbar\omega \ll \zeta$, where ζ is the chemical potential of the electron gas and $\omega = eH/mc$. These conditions make it possible to use a quasi-classical approximation for the investigation of the behavior of an electron gas in a magnetic field.

In the calculation of kinetic coefficients, only the scattering of electrons on impurities present in metals at low temperatures is taken into account. It is assumed that the concentration of the impurities is small and the stationary state of the electron in the given magnetic field can be established in the time interval between collisions with impurities, i.e., it is assumed that if τ is the characteristic relaxation time, then $\omega\tau \gg 1$. The inequalities $\hbar\omega \ll \zeta$ and $\omega\tau \gg 1$ can easily be satisfied simultaneously in metals at low temperatures. $1/\omega t$ and $\hbar\omega/\zeta$ are small parameters, in powers of which the expansions will later be carried out.

The state of the electron gas with account of scattering of electrons on impurities is described by the single-particle statistical operator ρ, which is found from the quantum kinetic equation obtained in our previous work.[3] The "collision integral" of this equation was calculated by perturbation theory for the interaction potential of an electron with the impurity. Such an approximation suffices if we are interested only in the principal term of the expansion in powers of $1/\omega\tau$ and $\hbar\omega/\zeta$. Actually, comparison of the results of our work[3] with the calculation of Skobov,[4] carried out without perturbation theory in the case $\omega\tau \gg 1$ for point impurities, shows that the principal terms in the parameter $\hbar\omega/\zeta$ in the expansion of the smooth and oscillating parts of the conductivity of the electron gas, measured in terms of the classical characteristics of the conductivity, are correctly described by the solution of the given kinetic equation. The latter verifies the possibility of use of the quantum kinetic equation of reference 3 to find the chief terms of the expansion of other kinetic coefficients in powers of $1/\omega\tau$ and $\hbar\omega/\zeta$.

The method used in the present work makes it possible to study the thermal conductivity of an electron gas with an arbitrary dispersion law; however, for simplicity, the case of an isotropic quadratic dispersion law is considered.

2. The Hamiltonian $\mathcal{H}$ of an individual electron in an external field has the form

$$\mathcal{H} = \varepsilon(H) - e\mathbf{E}\mathbf{r}, \qquad \varepsilon(H) = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2,$$

where $\epsilon(H)$ is the Hamiltonian of the electron in a homogeneous magnetic field **H**, which is considered to be parallel to the z axis; $\mathbf{E}(E_1, E_2, 0)$ is the electric field derived from grad T. The remaining notation is standard.

If grad T is directed along the y axis, then the vector potential of the magnetic field **A** is conveniently chosen such $(A_x = -Hy,\ A_y = A_z = 0)$ that the operator $y_0 = -cp_x/eH$, which plays the role of the y coordinate of the center of the electronic charge in a stationary orbit in a magnetic field, commutes with the Hamiltonian $\epsilon(H)$.

In the stationary case, the single-particle statistical operator ρ, which describes the electron gas, is determined from the following equation $(\partial\rho/\partial t = 0)$:

$$(i/\hbar)[\mathcal{H}, \rho] + D\{\rho\} = 0, \tag{1}$$

where $[\mathcal{H}, \rho] = \mathcal{H}\rho - \rho\mathcal{H}$, and $D\{\rho\}$ is the quantum analog of the "collision integral," depending exclusively on the electric field.[3] In the case of elastic scattering by large impurities, $D\{\rho\}$ is a linear transformation of ρ.

If we limit ourselves to the quasi-classical approximation, it is natural to seek ρ (by analogy with the solution of the classical kinetic equation) in the form

$$\rho = f_0\left[\frac{\varepsilon - \zeta(y_0)}{\Theta(y_0)}\right] + F_0 + \rho_1. \tag{2}$$

Here f_0 is the Fermi distribution function, while $\zeta(y)$ and $T(y)$ are the chemical potential and the temperature, which depend on the coordinate y in classical fashion, in particular, $T(y) = T_0 + (\partial T/\partial y)y$ (T_0 is a certain mean temperature for the entire gas). By F_0 is meant a definite matrix (obtained in reference 3) which takes into account the shift in the energy levels of the electron in the field of the impurities and which leads to a small shift in the chemical potential, while ρ_1 is the small change that is sought, and is linear in $\partial T/\partial y$ and E.

Since the operator y_0 commutes with $\epsilon(H)$, the choice of the solution of (1) in the form (2) makes it possible to carry out a simplification of Eq. (1), linearizing it in the small quantities $\partial T/\partial y$ and E.

If we are not interested in the shift of the electron levels in the field of the impurities and if from the very beginning we take into account the small shift in the chemical potential, then we can neglect in (2) the matrix F_0, which makes no contribution to the current and the heat flow. Then the quantum kinetic equation, linearized in $\partial T/\partial y$ and E, takes the form[3]

$$\frac{i}{\hbar}[\varepsilon, \rho_1] + D_0\{\rho_1\} = \frac{i}{\hbar}[e\mathbf{E}\mathbf{r}, \rho_0]$$
$$- \frac{\partial T}{\partial y} T D_0\left\{y_0 \rho_0' \frac{\partial}{\partial T}\left(\frac{\varepsilon - \zeta}{\Theta}\right)_0\right\} - e\mathbf{E}\, D_0\{\mathbf{r}\, g\},$$
$$\rho_0(\varepsilon) = f_0\left(\frac{\varepsilon - \zeta_0}{\Theta_0}\right), \tag{3}$$

where ζ_0 is the chemical potential corresponding to the temperature T_0. The matrix g in the representation of the Hamiltonian $\epsilon(H)$, the eigenvalues of which $\epsilon_\mu \equiv \epsilon_n(p_z)$, $(\mu = n, p_x, p_z)$, are determined by the formula

$$g^{\mu\mu'} = (\rho^0_\mu - \rho^0_{\mu'})/(\varepsilon_\mu - \varepsilon_{\mu'}), \qquad \rho^0_\mu = \rho_0(\varepsilon_\mu),$$

and the product rg can be understood as the direct product of the operators:

$$(\mathbf{r}\, g)^{\mu\mu'} = \mathbf{r}^{\mu\mu'} g^{\mu\mu'}.$$

The linear transformation D_0 appearing in (3) no longer contains the electric field and can be expressed in terms of the classical collision integral.[3]

The meaning of the first two terms on the right hand side of (3) is evident, while the third component describes the effect of the electric field on the "collision integral." Writing down of the last component is somewhat different from the corresponding expression in reference 3, since in the given case the field is not directed along the y axis but is located at a certain angle with respect to the y axis in the xy plane.

In the classical limiting case, in which the scattering of the electron on a short-range center takes place with the conservation of the coordinate **r** at the scattering point, $D_0\{\mathbf{r}g\} \rightarrow D_{cl}\{\mathbf{r}\rho_0'(\epsilon)\} = 0$, and Eq. (3) transforms into the classical kinetic equation for the correction to the distribution function of an electron gas.

3. The solution of Eq. (3) is found in the form of an expansion in powers of $1/\omega\tau$, where use is made of the fact that D_0 is proportional to $1/\tau$. In the expansion of ρ_1, just as in reference 3, the terms of zero and first approximation in $1/\omega\tau$ remain. With the help of the matrix ρ_1 determined in such fashion, and also with the help of the expression for the density of the electric current **j** and the energy flux **q**

$$\mathbf{j} = e\,\mathrm{Sp}\{\rho\mathbf{v}\}, \qquad \mathbf{q} = \tfrac{1}{2}\mathrm{Sp}\{\rho(\varepsilon\mathbf{v} + \mathbf{v}\varepsilon)\},$$

we establish a linear connection relating **j** and **q** with **E** and grad T:

$$j_\alpha = \sigma_{\alpha\alpha'} E_{\alpha'} + s_\alpha(\partial T/\partial y), \qquad q_y = \eta_\alpha E_\alpha + \beta(\partial T/\partial y)$$
$$(\alpha, \alpha' = 1, 2).$$

In the approximation under consideration,

$$\sigma_{xx} = \sigma_{yy} = (emc/H)\,\mathrm{Sp}\,\{D_0\,(y_0\rho_0')\,v_x\},\quad \sigma_{xy} = -\sigma_{yx} = ecn_0/H,$$

$$s_x = 0,\qquad s_y = (\Theta mc/H)\,\mathrm{Sp}\left\{D_0\left[y_0\rho_0'\frac{\partial}{\partial\Theta}\left(\frac{\varepsilon-\zeta}{\Theta}\right)_0\right]v_x\right\},$$

$$\eta_x = -\tfrac{5}{3}\,\bar{\varepsilon}cn_0/H,$$

$$\eta_y = (mc/2H)\,\mathrm{Sp}\,\{D_0\,(y_0\rho_0')\,(\varepsilon v_x + v\ \varepsilon)\},$$

$$\beta = (\Theta mc/2eH)\,\mathrm{Sp}\left\{D_0\left[y_0\rho_0'\frac{\partial}{\partial\Theta}\left(\frac{\varepsilon-\zeta}{\Theta}\right)\right]_0(\varepsilon v_x + v_x\varepsilon)\right\},\qquad (4)$$

where n_0 is the electron number density corresponding to the chemical potential ζ_0, while $\bar{\epsilon}$ is the average energy of the electron.

Expressions of the type (4) for the tensors of the thermoelectric coefficients in a magnetic field are obtained in completely analogous fashion in the case of an arbitrary dispersion law. Similar to what was done for σ,[3] one can easily study its oscillating parts, expressing the latter in terms of the oscillation of the magnetic moment. However, calculation of the oscillating part of the thermal conductivity coefficient in the general case entails very great computational difficulties; therefore, the simplest case of a quadratic isotropic dispersion law is considered.

Any of the thermoelectric coefficients (4) is expressed by a formula of the type

$$\sigma = \mathrm{Sp}\,\{D_0\,(R)\,\varphi\},$$

in which R is the diagonal matrix of the form $R = \rho_0'\psi\,(y_0, \epsilon)$, while φ is a matrix which is diagonal in y_0 and p_z.

The linear transformation $D_0\,(R)$ is written in matrix form in the following way:

$$D_0\,(R)^{nm} = \sum D^{nm}_{n'm'}\,(y_0, p_z;\ y_0';\ p_z')\,R^{n'm'}\,(y_0',\ p_z')$$

$$= \sum W_{KK'}\,(\varepsilon_n, y_0, p_z;\ \varepsilon_n', y_0', p_z')\,R^K\,(\varepsilon_n', y_0', p_z')$$

(summation is carried out over all primed indices). Here $K = n - m$, $K' = n' - m'$, and for the matrix element W_{KK}, we substitute the Fourier component of the kernel of the corresponding classical collision integral (this substitution of matrix elements is discussed in the work of I. M. Lifshitz[5] and is used in reference 3).

If we make use of the form of R given above and the Hermitian character of the operator φ, then we get the following expression for the coefficient σ:

$$\sigma = \sum \rho_0'\,(\varepsilon_{n'})\,\varphi_K^*W_{K0}\psi_0,\qquad (5)$$

in which summation is carried out over all indices, and which can be represented in a form similar to Eq. (19) of reference 3:

$$\sigma = -2\sum_{\varepsilon_n}\int\frac{df_0}{d\varepsilon_n}\,\chi m\Delta\varepsilon_n\,dp_z.\qquad (6)$$

The definition of the quantity χ entering into σ is evident from (5).

Writing down of an arbitrary thermoelectric coefficient in the form (6) makes it possible, directly or with a little alteration (brought about by an account of the higher powers of the expansion in Θ/ζ) to make use of Eqs. (20) — (24) of reference 3. These formulas make it possible to separate the basic classical parts of coefficients of the type σ and the corresponding oscillatory quantum contributions, and it is found that the essential dependence on H and Θ of the oscillating parts of the thermoelectric coefficients (4) is the same as for the oscillating magnetic moment, and is always taken into account either by a factor F* (see reference 6) of the form

$$F^* = \sum_{K=1}^{\infty}\frac{(-1)^K}{K^{3/2}}\frac{K\lambda}{\sinh(K\lambda)}\cos\left(\frac{2\pi K\zeta_0}{\hbar\omega} - \frac{3\pi}{4}\right),\qquad \lambda = \frac{2\pi^2\Theta}{\hbar\omega},\qquad (7)$$

or by its derivatives with respect to H and Θ.

4. The coefficient of thermal conductivity κ is usually identified with the coefficient of proportionality (taken with reverse sign) between the component q along grad T and the gradient of the temperature at j = 0. In the case under consideration, it is composed of the coefficients (4) in the following fashion:

$$\varkappa = s_y\,(\eta_y\sigma_{xx} - \eta_x\sigma_{xy})\,/\,\Delta - \beta,\qquad \Delta = \sigma_{xx}^2 + \sigma_{xy}^2.\qquad (8)$$

Having the expressions given above for the smooth and oscillating portions of the coefficients (4) in the coefficient of thermal conductivity defined by Eq. (8), we can also separate the classical part κ_0, which is smoothly varying with the magnetic field, and a small oscillating quantum correction $\Delta\kappa$. The classical part κ_0 is connected in obvious fashion with the classical electrical conductivity in a magnetic field σ_0:

$$\varkappa_0 = (\pi^2/3)\,(k/e)^2\,T\sigma_0,$$

where k is the Boltzmann constant and the oscillating part $\Delta\kappa$ is expressed in terms of the oscillating part of the electrical conductivity $\Delta\sigma$, determined in references 3, 4, and 7.

It is convenient to write the connection of the principal term (for small parameters $\hbar\omega/\zeta$ and Θ/ζ) in $\Delta\kappa$ with $\Delta\sigma$ following from (8) and (4) in compact form, after a long series of calculations and estimates:

$$\pi^2H^2\frac{\partial^2}{\partial H^2}\left(\frac{\Delta\varkappa}{\varkappa_0}\right) = 3\,\zeta_0\,(0)^2\frac{\partial^2}{\partial\Theta^2}\left(\frac{\Delta\sigma}{\sigma_0}\right),\qquad (9)$$

where $\zeta_0\,(0)$ is the classical chemical potential at $T = 0^0$K, and the differentiation takes into account only the very strong and important dependence on H and Θ, determined by the factor F^*.

The quantity $\Delta\sigma$ entering into (9), as was emphasized above, can in turn be expressed through the oscillating part of the magnetic moment of the electron gas.[3] The latter indicates that the periods of oscillation of the thermal conductivity coefficient coincide with the periods of oscillation in the DeHaas—Van Alphen effect (this result naturally remains true even in the case of an arbitrary dispersion law). It is well known that experimental measurements of the period of oscillation of κ lead to the same conclusion.[1]

If we take into account only the fundamental dependence of $\Delta\kappa$ and $\Delta\sigma$ on H and Θ, given by a factor of the type (7), then we have a quantity of order of magnitude

$$H\frac{\partial}{\partial H}\Delta\varkappa \sim \frac{\zeta_0}{\hbar\omega}\Delta\varkappa, \qquad \zeta_0\frac{\partial}{\partial\Theta}\Delta\sigma \sim \frac{\zeta_0}{\hbar\omega}\Delta\sigma,$$

and therefore it follows from (9) that

$$\Delta\varkappa/\varkappa_0 \sim \Delta\sigma/\sigma_0.$$

For not very low temperatures, when $\hbar\omega < \Theta$, we have the equality

$$\Delta\varkappa/\varkappa_0 = 3(\Delta\sigma/\sigma_0).$$

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138