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Quantum-interference contribution to the thermoelectric coefficient of degenerate and nondegenerate electron gases

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We discuss a quantum-interference (Cooper propagator) contribution to the thermoelectric coefficient of a two-dimensional electron gas. We are particularly interested in such a contribution for pure conductors (with no structural disorder) where it is a high-temperature effect due to quasielastic electron-phonon collisions. The magnetic field dependence is considered, and the case of Boltzmann statistics is discussed in some detail.

The purpose of the present paper is to discuss the interference (Cooper propagator) contribution $\Delta\eta$ to the thermoelectric coefficient η of two-dimensional conductors. We shall consider the maximally crossed diagrams whose special role has been discovered by Gor'kov, Larkin, and Khmel'nitskii[1] and by Abrahams and Ramakrishnan.[2] The influence of magnetic field H will also be considered. We suppose the electron-electron interaction to be negligibly small (see below).

The transport coefficients σ and η are determined by the relation for the current density **j**:

$$\mathbf{j}=\sigma\mathbf{E}-\eta\nabla T \quad , \tag{1}$$

where E is the electric field and T is the temperature. The coefficient $\Delta\eta$ has been calculated by Ting, Houghton, and Senna[3] for degenerate electrons. They came to the conclusion that the relative quantum-interference contribution $\Delta\eta/\eta$ is equal to the one for the conductivity, $\Delta\sigma/\sigma$. In such a case there would be no contribution to the Seebeck coefficient $S=\eta/\sigma$ and thus measurements of $\Delta\eta$ would give no new information.

The results of our calculation do not, in general, confirm this conclusion. On the contrary, we believe that experimental investigation of thermoelectric coefficient $\Delta\eta$, especially its magnetic field dependence, can provide an independent way to determine, for example, such an important parameter as the phase relaxation time, τ_φ. Indeed, for the case of Fermi statistics which we have considered recently[4,5] we have come to the conclusion that the functions $\Delta\eta(H)$ and $\Delta\sigma(H)$ have entirely different forms.

Here we wish to emphasize that it might be interesting to measure the contribution $\Delta\eta$ for nondegenerate electron gas in semiconductors. As is shown by Al'tshuler and Aronov,[6] in degenerate gas one-particle interference contribution to $\Delta\sigma$ manifests itself along with the contribution of electron-electron interaction. The expression for the last contribution contains neither the electron concentration n_0 nor the electron charge e. This is a sequence of the condition $T \ll 4\pi\sigma$. For the nondegenerate electrons the inequality can be reversed provided n_0 is small enough. In this case the electron-electron contribution has a factor n_0 and can be discarded. Thus the interference effects are present in a pure form.

Another point especially important for nondegenerate electron gas is that no structural disorder is necessary in this case for quantum contribution to be present. As is well known, the electron-acoustical phonon collisions may be almost elastic. Each collisional event results in essential change of electron momentum while the change of its energy ω is small. Thus the electron can perform its motion in almost static chaotic phonon field during relatively big time without destruction of the phase coherence. Indeed, the variation q of the electron quasimomentum due to an electron-acoustical phonon collision is for the nondegenerate electron gas of the order of $\bar{p}=(mT)^{1/2}$. The corresponding variation of the electron energy ε is of the order of $\omega \simeq wq \simeq w(mT)^{1/2}$, where w is the sound velocity. Thus, $\omega/T \simeq (mw^2/T)^{1/2}$. This ratio is small at all temperatures of interest.

Therefore one may expect that at least in some cases the almost stationary random phonon field can be considered in the zeroth approximation as a pure stationary one. In this approximation our problem is equivalent to that of impurity scattering. As is well known (see Refs. 1 and 2) the latter can bring about the quantum-interference effects.

In the next approximation one should take into account the phonon-field nonstationarity. This leads to the electron phase relaxation; it determines the time τ_φ during which an electron state remains coherent with the time-reversed one.

If this time is sufficiently big so that $\tau_\varphi/\tau_{\rm ph} \gg 1$, and

$$\bar{p}l \gg 1, \quad (\bar{p}l)^{-1}\ln(\tau_\varphi/\tau_{\rm ph}) \ll 1 \quad ,$$

one can take into account only one set of maximally crossed diagrams with the phonon lines instead of the impurity ones (see Ref. 9).

There are two distinct temperature intervals where the quantum-interference effects may be observed. At low temperatures they are due to the impurity scattering while at high temperatures they are due to the quasielastic electron-phonon scattering. At intermediate temperatures no such effects exist.

Now, the higher is the temperature and the smaller is the relative contribution of the phonon drag (which we do not take into account). Moreover, the coefficient η itself is much bigger for nondegenerate than for degenerate electrons. Thus, although observation of the effect discussed here, in fact, is possible at low temperatures for degenerate electrons, the conditions for its observation may be more favorable at relatively high temperatures.

Let us consider a semiconductor sample, its thickness d being much larger than the de Broglie wavelength $\hbar/p$ and, at the same time, much smaller than the diffusion length

$(D\tau_\varphi)^{1/2}$. (D is the diffusion coefficient.) Our calculations give for this case (cf. Refs. 3–5),

$$\Delta\eta = (2e/\pi\hbar T)\int_0^\infty d\varepsilon(\partial n/\partial\varepsilon)(\varepsilon-\zeta)D(\varepsilon)C(\varepsilon) \quad . \quad (2)$$

This equation differs from that for $\Delta\sigma$ (cf. Ref. 1) by the factor $(\varepsilon-\zeta)/eT$ in the integrand. Here n is the equilibrium electron distribution function and ζ is the chemical potential. The Cooper propagator C is the sum of maximally crossed diagrams which is usually written in the form

$$C(\varepsilon) = \int d^2q(2\pi)^{-2}[D(\varepsilon)q^2 + 1/\tau_\varphi]^{-1} \quad . \quad (3)$$

We shall give the result of our calculation of this function for quasielastic electron scattering. The corresponding condition for the case of Boltzmann statistics has the form $\hbar\omega \ll T$.

The result of our calculation depends on the relation between ω and τ_{ph}, the characteristic time of quasielastic collisions with phonons. One can discriminate between the two cases:

(i) The case of phase jumps takes place provided $\omega\tau_{ph} \gg 1$. In this case the Cooper propagator can exist only if elastic impurity scattering is present along with the quasielastic phonon scattering, the characteristic time of impurity scattering τ being much smaller than τ_{ph}. It means that the Cooper propagator is formed by elastic scattering, and the only role of quasielastic phonon scattering is to destroy coherence. Our calculations for this case give $\tau_\varphi \approx \tau_{ph}$ (which confirms the result pointed out by Al'tshuler, Aronov, Larkin, and Khmel'nitskii[7]) while time τ determines the diffusivity $D(\varepsilon)$.

(ii) The case of phase wandering takes place provided $\omega\tau_{ph} \ll 1$, irrespective of whether the Cooper propagator is formed by quasielastic collisions alone or the elastic impurity scattering is also essential.

Let us begin with visualizing the phonon random potential U as a pure static one. In this approximation the phase φ of the electron wave function would be a linear function of time t, so that $\varphi^2 = E^2t^2$, E being the electron energy. A slow variation of the potential U will bring about a mechanism of the phase wandering so that the difference $\langle\varphi^2\rangle - \langle\varphi^2\rangle$ will not vanish (the $\langle\ \rangle$'s denote the phonon ensemble averaging). For small values of t the difference can be expanded in powers of t. It is natural to suppose that the expansion begins with t^3:

$$\langle\varphi^2\rangle - \langle\varphi\rangle^2 = \alpha t^3 \quad .$$

The coefficient α should be proportional to the square of the time derivative $\dot U \simeq \omega U$ of the random potential U: $\alpha \propto \omega^2 U^2$. As a measure of the random potential intensity one can take $1/\tau_{ph} \propto U^2$, and as a result, one can get the following order-of-magnitude estimate:

$$\alpha \simeq \omega^2/\tau_{ph} \quad .$$

Hence, the characteristic time of phase destruction,

$$1/\tau_\varphi \simeq \omega^{2/3}/\tau_{ph}^{1/3} \quad . \quad (4)$$

The interference is possible provided $\tau_\varphi \gg \tau_{ph}$. For what follows, it is extremely important that this condition is equivalent to the inequality $\omega\tau_{ph} \ll 1$. The physical meaning of the last inequality is very simple: The variation of the phase of the electron wave function during the electron-phonon mean free time τ_{ph} is small. This is the so-called regime of phase wandering.

To give the analytical solution of the problem we have summed the sequence of the maximally crossed diagrams (see Ref. 9) with the phonon lines instead of the impurity ones. For this sum we have obtained an integral equation which can be solved. As a result we have

$$C(\varepsilon) = \int d^2q/(2\pi)^2 \int_0^\infty dt \exp(-Dq^2t - t^3/\tau_\varphi^3) \quad , \quad (5)$$

where τ_φ is determined by Eq. (4). One can see that this equation corresponds to the described physical picture.

Expression (4) coincides with the estimate given in Ref. 8 on the basis of physical arguments for the case where $\omega\tau_{ph} \ll 1$, and elastic scattering is predominant while the quasielastic one is taken into account as the mechanism of destruction of the phase coherence. Further discussion of these arguments is given by the authors in Ref. 9.

Let us now analyze the magnetic field dependence. For the case where $H=0$ [Eq. (3)] is valid we should insert at $H\neq 0$ in (2) the following expression obtained by Al'tshuler, Khmel'nitskii, Larkin, and Lee.[10]

$$C(\varepsilon,H) = (2b/\pi)\sum[4Db(k+\tfrac{1}{2}) + \tau_\varphi^{-1}]^{-1} \quad .$$

Here $b = eH/ch$, c is the velocity of light, and summation is taken over non-negative integers up to the value of the order of $1/2bl^2$, l being the electron mean free path. One can rewrite this equation as

$$C(\varepsilon,H) = \phi_1(\varepsilon,H)/2\pi D(\varepsilon) \quad , \quad (6)$$

$$\phi_k(\varepsilon,H) = (H/H_c)\int_{\tau/\tau_\varphi}^\infty dx \exp(-x^k)[2\sinh(Hx/2H_c)]^{-1} \quad , \quad (7)$$

$$H_c = \hbar c/4|e|D(\varepsilon)\tau_\varphi(\varepsilon) \quad . \quad (8)$$

Equation (7) is valid in the main order in the large parameter $\log(\tau_\varphi/\tau)$. If $H \ll H_c$ $\phi_k \to \ln(\tau_\varphi/\tau)$; if $H \gg H_c \phi_k \to \ln(H_c/H) - \ln(\tau/\tau_\varphi)$.

For the case where at $H=0$ we have Eq. (5) we get at $H\neq 0$, using the same methods as in Ref. 10, Eq. (6) with $k=3$ instead of $k=1$. ϕ_1 and ϕ_3 depend on H in a different way. In particular, if $H \ll H_c$ both functions have the form

$$\phi_k = \ln(\tau_\varphi/\tau) - \alpha_k(H/H_c)^2 \quad , \quad (9)$$

but the factors α_k are different: $\alpha_1 = 0.042$, while $\alpha_3 = 0.019$.

Now we shall give the result of the calculation of $\Delta\eta$ for nondegenerate electrons. Inserting (3) or (5) in (2) we get

$$\Delta\eta = e^{-1}[\ln(2\bar\nu T/n_0) + 1]\Delta\sigma \quad , \quad (10)$$

where

$$\Delta\sigma = -(en_0/4\pi^2\bar\nu\hbar T)\ln[\tau_\varphi(T)/\tau(T)] \quad , \quad (11)$$

$\bar\nu$ is the electron density of states averaged over the Boltzmann distribution. Thus Eq. (10), within the accepted accuracy, is insensitive to the exact form of the Cooper propagator.

The first term in the brackets in (10) is equal to $|\zeta|/T \gg 1$. Taking into account this term only we get $\Delta\eta/\eta = \Delta\sigma/\sigma$ which means that in this approximation there is no contribution to the Seebeck coefficient S (such a result was given by Ting *et al.*,[3] but for the Fermi statistics rather than for the Boltzmann one). In the next approximation in

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$T/|\zeta|$ such a contribution appears, and we get

$$\Delta S/S = \beta\hbar(2mT)^{-1/2}[l(T)]^{-1}\ln[\tau_\varphi(T)/\tau(T)] \ , \quad (12)$$

the dimensionless numerical factor β being dependent on the mechanism of the momentum relaxation.

For $H \neq 0$ we have

$$\Delta\eta = -en_0(4\pi^2\hbar\bar{v}T)^{-1}\int_0^\infty dx\, e^{-x}\phi_k(Tx,H)(Tx-\zeta) \ . \quad (13)$$

Again $\Delta\eta$ differs from the corresponding equation for $\Delta\sigma$ by the factor $(\varepsilon-\zeta)/eT$ in the integrand.

Let us give estimates of the range of applicability of these results for the case where only quasielastic scattering of the electrons by acoustical phonons is present. The small parameter $1/pl$ of the perturbation theory can be written for this case as $\hbar/T\tau(T)$. The quantum interference can take place if $\tau_\varphi >> \tau$ which, as we have seen, is possible only if $\omega\tau_{\rm ph} << 1$. Thus we come to the following chain of inequalities

$$(T_c m w^2)^{1/2} << T << T_c \ , \quad (14)$$

where the characteristic temperature T_c is determined by the equation $T_c\tau(T_c) = \hbar$.

A further condition emerges from the fact that we have taken into account only one set of maximally crossed diagrams. It amounts to the requirement of smallness of the quantum contribution as compared to the classical value, or

$$(T/T_c)^{1/2}\ln T(mw^2T_c)^{-1/2} << 1 \ . \quad (15)$$

Thus it is seen that in this case the quantum contribution increases with the temperature.

However, if the temperature is high enough one should take into account the optical-phonon scattering. If $T << \hbar\omega_0$, ω_0 being the optical-phonon frequency, this scattering leads to phase jumps only. At higher temperatures ($T >> \hbar\omega_0$) the scattering may become a quasielastic one. In this temperature region $T\tau \propto T^{1/2}$, and inequality (15) is satisfied provided the electron-phonon coupling is small.

It might be very interesting to investigate experimentally if the quantum contribution still exists at even higher temperatures, i.e., above the melting point, both in semiconducting and in metallic state. Atoms in a liquid acquire additional modes of motion (as compared to a solid) which interacting with electrons should contribute to the phase destruction time τ_φ. However, the conditions in some liquids may still prove favorable for existence of the Cooper propagator.

Let us now discuss when it is possible to observe the dependence on magnetic field H. Along with H-dependent quantum contribution there exists a classical one caused by distortion of electron trajectories in magnetic field. For a weak field it is proportional to $(H/H_\mu)^2$, where $H_\mu = c/\mu = cT/eD$ (μ being the mobility). The quantum contribution is of the order of $\hbar/(2mT)^{1/2}l$ as compared to the classical one. Thus in order to observe the quantum contribution against the background of the classical effect one requires the condition

$$H_c/H_\mu = \hbar/4T\tau_\varphi << h/l^{1/2}(2mT)^{1/4} \ .$$

Finally, let us briefly discuss some aspects of the quantum contribution for Fermi statistics.[1] To make estimates of the quantum contributions in semimetals and metals let us introduce a dimensionless parameter $\xi = pa/h$, a being of the order of the lattice constant. In a typical metal $\xi \approx 1$; in a semimetal $\xi << 1$.

The characteristic phonon frequency ω is of the order of $\Theta/\hbar$ (where Θ is the Debye temperature). Thus if $T << \xi\Theta$ we have $\hbar\omega >> T$, and the phonon scattering is inelastic. In the opposite case of quasielastic scattering $T >> \xi\Theta$, the phonon scattering rate $\tau_{\rm ph}^{-1}$ is of the order of $\xi T/\hbar$. Thus the condition of phase wandering $\omega\tau_{\rm ph} << 1$ can be met at $T >> \Theta$. In this region the Cooper propagator has the form (5) with $\tau_\varphi \approx \hbar/\xi T^{1/3}\Theta^{2/3}$. In the intermediate region of temperature, $\xi\Theta << T << \Theta$, which is actual if $\xi << 1$, the phase jumps take place. Consequently, the Cooper propagator has the form (3) with $\tau_\varphi \approx \hbar/\xi T$. One can see that the quantum interference in Fermi gas can take place at $T \lesssim \Theta$ if the impurity scattering is strong enough and the inequality $\tau_{\rm im} << \tau_{\rm ph}$ holds. At $T >> \Theta$ such a contribution can exist due to phonon scattering only.[2]

Generally speaking, the case of the Fermi gas is more complicated than the case of the Boltzmann one because the conditions of whether it is possible to neglect electron-electron interaction, even considering the magnetic field dependence, should be analyzed carefully:

(1) Kaveh and Mott[11] were, as far as we know, the first to discuss the high-temperature quantum contribution to the conductivity. They considered three-dimensional metals and used for the Cooper propagator Eq. (3) with the time $\tau_{\rm ph}$ for τ_φ. We believe that in three-dimensional metals too not only the case of phase jumps but also the case of phase wandering where the Cooper propagator is described by Eqs. (4) and (5) may be of importance, especially at high temperatures ($T > \Theta$).

(2) One should keep in mind that the order-of-magnitude estimates of this sort are of approximate nature. They can be made much more accurate for any definite substance provided its parameters (effective mass of the carriers, rates of their phonon scattering, etc.) are known.

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