Thermoelectric power and topological transitions in quasi-2D electron systems

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The electron-impurity relaxation time and the thermoelectric power are calculated for a quasi-2*D* electron gas with an isotropic spectrum in the case of a neck-breaking topological electron transition. Near this transition, the thermoelectric power is greater than its background value by a large factor. This result is attributed to the joint effects of the diffusion of conduction electrons and phonon drag. The results found here agree qualitatively with experimental data on the thermoelectric power in metal-insulator–semiconductor structures.

1. INTRODUCTION

Electron topological transitions have recently attracted increased interest from both theoreticians and experimentalists. When the topological properties of the Fermi surface change, anomalies appear in the electron characteristics of a metal.[1,2] Features of the kinetics of conduction electrons near an electron topological transition in 3*D* systems were studied in Refs. 3 and 4. There is also interest in the effect of topological transformations of the Fermi surface on the electronic properties of 2*D* systems. The problem of electron topological transitions in 2*D* inversion layers has been studied theoretically and experimentally by Zavaritskiĭ, Kvon, and Suslov.[5,6]

In a metal–insulator–semiconductor (MIS) structure, the electron density can be varied quite easily in the course of an experiment, by applying a potential difference between the gate and the interior of the semiconductor. A 2*D* electron gas forms in a thin boundary layer[7] (with a thickness $d \approx 50$ Å). In order to observe electron topological transitions experimentally at comparatively low values of this potential difference, Zavaritskiĭ and Suslov[6] ingeniously used a slightly skewed face of a crystal (silicon). A superstructure of a sort arises in the skew direction in this case and gives rise to Bragg reflection in this direction with a wave vector significantly lower than the standard size of the Brillouin zone. This circumstance made it possible to observe both an electron topological transition corresponding to the tangency of the faces of the Brillouin zone, accompanied by the formation of a neck, and the formation of a second zone, i.e., electron topological transitions accompanied by the appearance of an electron cavity, at comparatively low electron densities.

In a theoretical interpretation of the results in Ref. 6, the authors distinguished the diffusion-related component of the thermoelectric power of the electron gas and the component due to phonon drag. Features of the diffusion component of the thermoelectric power were studied with the help of the Mott formula; the theory of the acoustoelectric effect[8] was used to analyze the thermoelectric power due to the phonon drag. However, the validity of the Mott formula in the case of an electron topological transition is not obvious,[9] and the expression derived for the features of the diffusion-related thermoelectric power in Ref. 6 is not valid when the system is very close to the transition point (at $\Delta \leqslant T$, where Δ is a measure of the proximity of the system to the transition point, introduced below, and T is the temperature).

In the present paper we calculate the relaxation time and thermoelectric power of a quasi-2*D* electron gas through a solution of the kinetic equation. We do this first for a gas with an isotropic spectrum, and then for one with a spectrum which allows a "neck-breaking" electron topological transition. We ignore the interelectron interaction, and we assume that the electrons are scattered by screened Coulomb centers (impurity centers). We show that the corrections to the diffusion component of the thermoelectric power for the energy dependence of the time scale of the relaxation of electrons due to impurity centers may be any of the following sizes relative to the phonon-drag thermopower: greater, comparable in order of magnitude, or smaller.

2. ELECTRON-IMPURITY RELAXATION TIME AND THERMOELECTRIC POWER IN THE CASE OF AN ISOTROPIC SPECTRUM

Following Ref. 10, we consider a thin conducting film (with an important quantum-size effect) in the region $0 \leqslant z \leqslant a$. Potential centers on the $z = 0$ surface are distributed randomly and independently with a surface density n_i. The second surface is assumed for simplicity to be a mirror surface. In the approximation of a square potential well, the electron energy spectrum is

$$E_n(p_x, p_y) = \frac{p^2}{2m} + \frac{\pi^2 n^2}{2ma^2}, \tag{1}$$

where $\mathbf{p} = (p_x, p_y)$ is the momentum in the xy plane, n is the index of the quantum-size level, and (here and below) $\hbar = 1$. We restrict the analysis to the case in which the entire electron gas is in the first quantum-size level. This is a legitimate assumption if the distance between levels is greater than the Fermi energy: $\varepsilon_F < 1/ma^2$ we then have $n = 1$. Below we omit the index specifying the quantum-size level.

To describe an actual experimental situation, we need to take account of the scattering of electrons by impurities. This scattering is important in a description of the kinetic properties of a thin film at low temperatures. Let us calculate the probability for the scattering of conduction electrons by screened Coulomb centers. Following Ref. 10, we assume that if the screening radius q_0^{-1} is much smaller than the film thickness then the screening is the same as in an unbounded sample:

$$u(r) = \frac{e^2}{\varepsilon r} \exp(-q_0 r), \tag{2}$$

where ε is the static dielectric constant. The set of conditions $\varepsilon_F < 1/ma^2$ and $q_0^{-1} \ll a$ leads to the inequality $q_0^2/m \gg \varepsilon_F$,

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which we will assume is satisfied. When the effects of the thermal spreading of the Fermi surface outweigh the effects of the electron-impurity scattering ($T\tau \gg 1$), we can use the Born formula for the scattering of an individual electron by impurities. For the scattering probability per unit time we have the expression[11]

$$W(\varepsilon)=2\pi n_i \int |u(\mathbf{p}'-\mathbf{p})|^2 \delta(\varepsilon(\mathbf{p})-\varepsilon(\mathbf{p}'))\frac{d^2\mathbf{p}}{(2\pi)^2}, \quad (3)$$

where

$$u(\mathbf{p})=\frac{8\pi^3 e^2}{\varepsilon a^3}\frac{1}{(q_0^2+p^2)(q_0^2+p^2+4\pi^2/a^2)}. \quad (4)$$

Integrating, we find the following expression for the electron-impurity relaxation time $\tau(\varepsilon) = W^{-1}(\varepsilon)$:

$$\tau(\varepsilon)=\tau_0=[2\pi^2 m n_i (4\pi e^2/\varepsilon a^3 q_0^4)^2]^{-1}. \quad (5)$$

The kinetic coefficient β_{xx} which appears in the generalized transport equations

$$j_i=\sigma_{ik}E_k+\beta_{ik}\nabla_k T \quad (6)$$

($\mathbf{E}$ is the electric field, ∇T is the temperature gradient, $\mathbf{j}$ is the current density, σ_{ik} is the conductivity tensor, and β_{ik} characterizes the thermoelectric properties of the metal), can be written[11]

$$\beta_{xx}=-\frac{e}{2T^2}\int \frac{d^2\mathbf{p}}{(2\pi)^2} v_x^2 \tau(\varepsilon)(\varepsilon-\mu)\,\mathrm{ch}^{-2}\frac{\varepsilon-\mu}{2T}, \quad (7)$$

where μ is the chemical potential, and $v_x = \partial\varepsilon/\partial p_x$. Integrating, we find

$$\beta_{xx}=\beta_0=\pi e T\tau_0/6. \quad (8)$$

3. ELECTRON-IMPURITY RELAXATION TIME AND THE THERMOELECTRIC POWER IN THE CASE OF AN ELECTRON TOPOLOGICAL TRANSITION

By analogy with the 3D case,[9] we use a neck-breaking model to describe the electron topological transition in a thin film. In this model, the electron energy spectrum is

$$E(p_x, p_y)=E_c+\frac{p_x^2}{2m_x}+\frac{p_y^2}{2m_y}+\alpha p_x^4+\frac{\pi^2}{2m_z a^2}. \quad (9)$$

The last term here is the energy of an electron in the first quantum-size level (we are again restricting the analysis to the first such level). This energy can be incorporated in E_c. When we do this, the latter becomes the critical value of the chemical potential, corresponding to an electron topological transition at $T = 0$ in the absence of impurity scattering of electrons. Figure 1 shows the Fermi surface for such a system. The parameter $\Delta = \mu - E_c$ is a measure of the proximity of the system to the electron topological transition. At $\Delta = 0$, the hyperbola degenerates into two straight lines. It is near this point that the electron topological transition occurs.[9]

To calculate the electron-impurity relaxation time, we note that under the condition $q_0 \gg p^*$ (p^* is the limiting value of the momentum p_x) the amplitude for the scattering of an electron by an impurity can be assumed independent of the momentum, and the integral in (3) becomes proportional to the density of states. In the 2D model, this density of states near the electron topological transition is calculated as in a

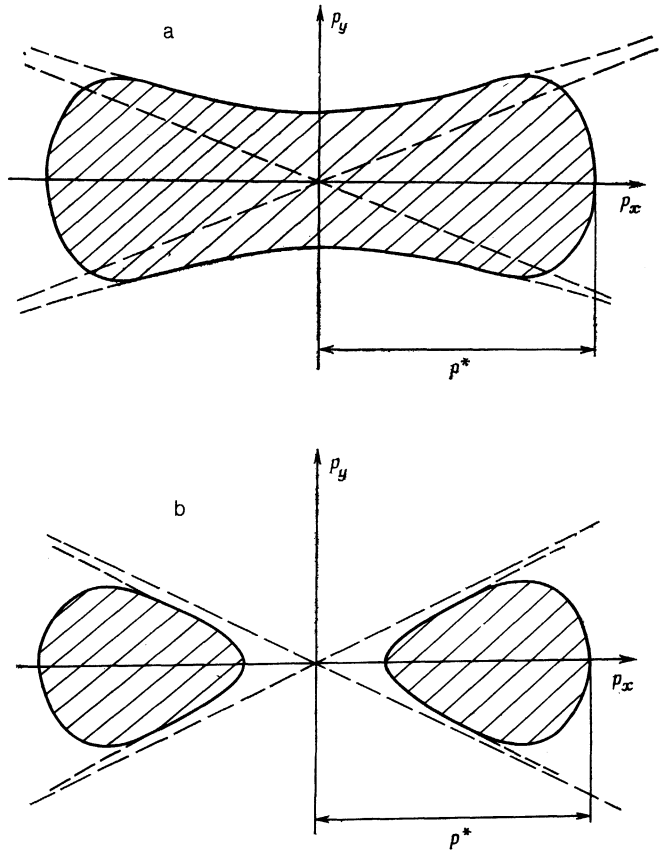

FIG. 1. Neck-breaking model of an electron topological transition. a—$\Delta > 0$; b—$\Delta < 0$.

3D model.[1,12] As a result we find

$$\tau(\omega)=\tau_0\left(2\ln\frac{4\varepsilon_0}{|\omega+\Delta|}\right)^{-1}, \quad (10)$$

where τ_0 is again given by expression (5), but now m is replaced by $(m_x m_y)^{1/2}$, $\omega = \varepsilon - \mu$, and $\varepsilon_0 = p^{*2}/2m_x$. Actually, ε_0 also depends on the energy, but this dependence is far weaker than that in the denominator. In the calculations below we will accordingly assume that $\varepsilon_0(\varepsilon) = \varepsilon_0(\mu)$ is independent of the energy.

Expression (10) differs substantially from expression (15), which describes the electron relaxation in the isotropic case. A logarithmic dependence $\tau(\omega)$ arises in the case of the spectrum (9), and as $\omega + \Delta \to 0$ we find $\tau \to 0$. We should also stress the distinction between (10) and the expression for the relaxation time in the 3D model.[9] In the 3D case we know that the relaxation time, like the density of states, can be written as a sum of two terms, a smooth function of the energy and an increment which vanishes on one side of the transition. The 2D functional dependence cannot be represented in this manner, and as a result there are important differences between the Δ dependence of the thermoelectric power in the 2D case and that in the 3D case.

We turn now to a calculation of the thermoelectric power in the case of an electron topological transition. Substituting (10) into general expression (7), and integrating over the constant-energy curves ε = const, we find

$$\frac{\beta_{xx}^{sing}}{\beta_0} = -\frac{3}{2\pi^2}\frac{\varepsilon_0}{T}\left(\frac{m_y}{m_x}\right)^{1/2}\int_{-\infty}^{\infty}\frac{x\,dx}{\mathrm{ch}^2 x}\ln^{-1}\frac{2\varepsilon_0/T}{|x+\Delta/2T|}+O(1), \tag{11}$$

where β_0 is given by expression (8). We see that the background value (i.e., that far from the transition) of the thermoelectric power is equal to β_0 in order of magnitude. The last term in (11) is small over the entire range of Δ ($|\Delta| \ll \varepsilon_0$) [cf. (13) and (14) below].

We first note that the result $\beta^{sing}(\Delta) = \beta^{sing}(-\Delta)$ follows from (11). The reason is that in this case there is a symmetry under a simultaneous change in the sign of Δ and a replacement of the electron gas by a hole gas in this system, in contrast with the $3D$ case with $\alpha = 0$. Let us examine the asymptotic behavior of $\beta^{sing}(\Delta)$ in two limiting cases. (In accordance with the discussion above, we assume $\Delta > 0$.) We rewrite the expression for $\beta^{sing}(\Delta,T)$ in the following form:

$$\frac{\beta_{xx}^{sing}}{\beta_0} = -\frac{3}{2\pi^2}\frac{\varepsilon_0}{T}\left(\frac{m_y}{m_x}\right)^{1/2}\int_0^{\infty}\frac{x\,dx}{\mathrm{ch}^2 x}\left(\ln^{-1}\frac{2\varepsilon_0/T}{x+\Delta/2T}-\ln^{-1}\frac{2\varepsilon_0/T}{x-\Delta/2T}\right). \tag{12}$$

1) $\Delta \gg T$ (the region far from the transition). In this case, because of the rapid convergence of the integral in (12), the difference between the inverse logarithms can be expanded in a series in $2Tx/\Delta$ (although this expansion becomes illegitimate for $x \geqslant \Delta/2T$, the region $x \ll \Delta/2T$ becomes important in the integral because of the divisor of $\cosh^2 x$ in the integrand). We then write

$$\frac{\beta_{xx}^{sing}}{\beta_0} = -\frac{\varepsilon_0}{2\Delta}\left(\frac{m_y}{m_x}\right)^{1/2}\ln^{-2}\frac{4\varepsilon_0}{\Delta}. \tag{13}$$

2) $\Delta \ll T$ (the immediate vicinity of the transition). In this region the integral in (12) can be broken up into the sum of two integrals: one from 0 to γ and one from γ to ∞ ($\Delta/2T \ll \gamma \ll 1$). In the former we replace $\cosh^2 x$ by one; as a result, this integral becomes

$$\propto \frac{\Delta}{T}\gamma\ln^{-2}\frac{4\varepsilon_0}{\Delta}.$$

In the second integral we can expand the difference between inverse logarithms in a series in $\Delta x/T$. As a result we find

$$\propto \frac{\Delta}{T}\ln^{-2}\frac{2\varepsilon_0}{\Delta}.$$

To first order in Δ/T we thus have

$$\frac{\beta_{xx}^{sing}}{\beta_0} = -\frac{3}{2\pi^2}\frac{\varepsilon_0\Delta}{T^2}\left(\frac{m_y}{m_x}\right)^{1/2}\ln^{-2}\frac{2\varepsilon_0}{T}. \tag{14}$$

Figure 2 shows the results of a numerical calculation of $\beta^{sing}(\Delta)/\beta_0$ from (11).

4. DISCUSSION OF RESULTS

The expressions found here for the electron-impurity relaxation time and for the thermoelectric power in $2D$ systems are quite different from those in the $3D$ case. In the first place, although the thermoelectric power in (10) can again be written as the sum of a background value of the thermoelectric power and a singular part which is greater than the background component by a factor of a large parameter, in this case the singular part β^{sing} is an odd function of the parameter Δ. As a result, $\beta^{sing}(\Delta)$ is a double-humped curve (Fig. 2). The electron-impurity relaxation time in (10), on the other hand, cannot in general be written as the sum of a regular component and a singular component, and it is nonzero on both sides of the transition. The reason for this behavior is the symmetry of the system under a change in the sign of the carriers and a simultaneous change in the sign of Δ in the case $\alpha = 0$, which we mentioned above. We might add that in a $2D$ system, in contrast with a $3D$ system,[4,9] the part of the relaxation time which is associated with the electron topological transition is a strong function of the parameter ε_0 which characterizes the peripheral regions of the Fermi surface.

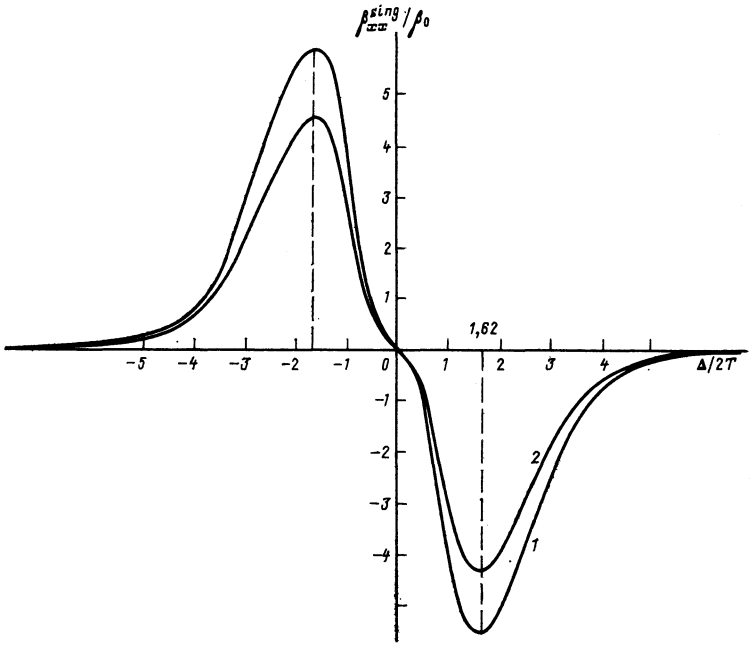

FIG. 2. Results of a numerical calculation of $\beta_{xx}^{sing}/\beta_0$, in units of $(3/2\pi^2)(\varepsilon_0/T)(m_x/m_y)^{1/2}$, as a function of $\Delta/2T$ [see (11)]. 1—$\varepsilon_0 = 100$T; 2—$\varepsilon_0 = 500$T.

In the analysis of the thermoelectric power near an electron topological transition in a quasi-2D electron structure above, we made several assumptions, which require special discussion.

First, in describing the transverse quantization of the motion of the electron we used the model of an infinitely deep potential well. That model substantially simplifies the energy spectrum of the conduction electrons, (1). Actually, the potential well in an MIS structure or a heterostructure is approximately triangular, and an Airy function or even more-complex model functions would have to be used as the electron wave functions in the transverse direction.[7] Second, an important circumstance in an analysis of thin MIS structures is the presence of fluctuations in the surface potential in the insulating layer.[13] Nevertheless, we would expect that these factors would play a role only in a numerical comparison of theoretical and experimental results. Our simplified model is therefore adequate as long as we are not attempting to reproduce the experimental results accurately.

Third, in analyzing the scattering of electrons by impurities we used a 3D screened Coulomb potential.[10] That approach actually means that we are arbitrarily breaking the electron system up into two subsystems: the electrons which are screening the charged centers and the electrons which are participating directly in the transport. This is a legitimate approximation since our main purpose here is to discuss features of the thermoelectric power which are linked with the electron topological transition, and the main requirement on our choice of scattering potential is that it be of short range $[q_0 \gg (\varepsilon_0 m)^{1/2}]$. The actual shape of the potential is again important only in a numerical comparison of theory and experiment.[14] Furthermore, in actual experimental studies of the kinetic characteristics of MIS structures, the history of the sample is important. In the standard procedure, the experimentalist first applies a voltage to the gate of the MIS structure and only then cools the sample. In this case the screening of the Coulomb centers is caused primarily by 3D electrons, which localize near these centers and which participate no further in transport processes.[1)]

Despite the number of limitations involved here, the results found on the thermoelectric power near the electron topological transition in the 2D system which we have considered agree well with the experimental data of Ref. 6, which we have already cited (Fig. 3). In analyzing the results we should note that the results in Ref. 6 were given as functional dependences $EW^{-1}(V_g)$, where E is the electric field, W is the heat flux, and V_g is the gate voltage. Since $\mathbf{W} \propto -\nabla T$, we plot the thermoelectric power with the opposite sign in the figure. For the left-hand side of the figure, the vector W is directed along the superlattice. For the right-hand side, it runs perpendicular to this superlattice. Clearly, the two structural features which have been singled out, A and B, are observed at the same values of $N_S(V_g)$ in the two cases. Feature A corresponds to tangency, and feature B corresponds to the formation of an electron cavity. Unfortunately, it is difficult to analyze the experimental situation since these two types of topological transitions lie close together. Nevertheless, it is clear from Fig. 3 that—in agreement with (11)—feature A consists of a maximum and a minimum. The fact that the thermoelectric power of an MIS structure and a superlattice has an anisotropy was explained previously.[3,15] Here we wish to point out that the feature

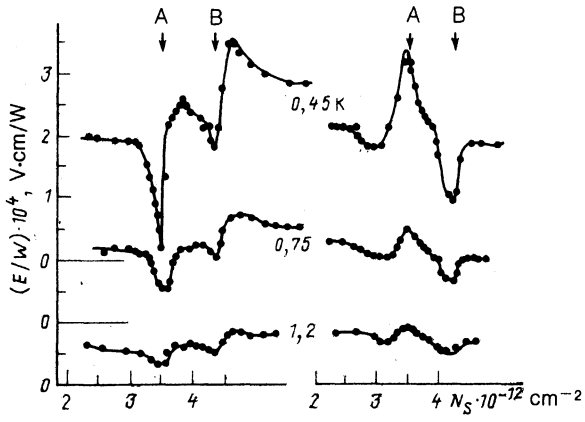

FIG. 3. Experimental results[6] on the thermoelectric power as a function of the density N_S. A—Transition corresponding to the appearance of a neck; B—transition corresponding to the appearance of a cavity. Curves at left—The heat flux is directed along the superlattice; at right—it is directed perpendicular to the superlattice.

spreads out with increasing temperature according to (14). The asymmetry of the feature in the thermoelectric power between topological transitions A and B is apparently caused not only by phonon drag, as was assumed in Ref. 6, but also by the joint effects of transitions on the kinetics of the conduction electrons.

According to Ref. 6, the thermal spreading of the characteristics of a metal near an electron topological transition does not require a special analysis. It can be found by substituting the temperature T for Δ in the final expressions. For example, to calculate the singular part of the diffusion component of the thermoelectric power (without phonon drag), it is sufficient to use the Mott formula and to replace Δ by T at $T \ll \Delta$. The analysis above shows that the situation becomes more complicated in a calculation of kinetic properties because the energy dependence of the relaxation time near an electron topological transition is not a trivial point. In the limit $\Delta \to 0$, the relaxation time is a logarithmic function of the energy, so the Mott formula, which is based on an expansion of τ in powers of ω, should not be used.

As can be seen from a comparison of our results with experimental data of Ref. 6, a calculation of the singular part of the diffusion component of the thermoelectric power leads to a $\beta^{\text{sing}}(\Delta)$ dependence which is reminiscent of the singular thermoelectric power component associated with the phonon drag as found in Ref. 6. For the latter, the following expression was derived in Ref. 6:

$$\beta_{ph} \propto -\beta_0 \frac{T^2 \Lambda^2 \varepsilon_c l_{ph}}{s^5 \rho (|\Delta|/m)^{1/2}} \ln \frac{\varepsilon_c}{|\Delta|}, \qquad (15)$$

where Λ is the strain component, l_{ph} is the phonon mean free path, s is the sound velocity, and ρ is the density of the metal. The large number of constants involved here makes it difficult to make a direct comparison with expressions (13) and (14), but if we set $\Delta \approx T$ in (13)–(15) we find that two cases are possible: (a) The mechanism due to the $\tau(\varepsilon)$ dependence outweighs the phonon-drag mechanism. In particular, this may be the case at low temperatures (this conclusion agrees with the theory of Ref. 16, which asserts that the phonon-drag effect does not influence an electron topological transition at low temperatures). (b) The opposite is true. The

effect can thus apparently be attributed to the joint effects of a diffusion of conduction electrons and a phonon drag. Each of these effects may outweigh the other under certain conditions.

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