IMPURITY SCATTERING OF ELECTRONS IN THIN FILMS

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The Born approximation is inapplicable for the scattering of electrons in thin (quantizing) films if the electrons' energy is sufficiently close to any of the thin-film levels, even if the impurity potential is small. In this article it is shown that an arbitrarily weak attraction of the impurity atom leads to the appearance of a bound state of the electron with an energy in the forbidden band. The dependence of the conductivity on the film's thickness turns out to be substantially more complicated than the result obtained in the ordinary Born approximation.

IT is well known that the oscillations of the kinetic coefficients in thin films are related to the discontinuous dependence of the density of states at the Fermi level on the film's thickness (see, for example,[1]). In this connection it is usually assumed that one can calculate the matrix element describing the scattering of an electron in the first Born approximation, and then the probability of an elementary scattering event turns out to be a smooth and monotonic function of the film's thickness.

In the present article it will be shown that a more complicated situation occurs in the case of elastic scattering by impurities. If the electron's energy is sufficiently close to some kind of level ϵ_n of transverse quantization, the Born approximation turns out to be inapplicable even for an arbitrarily small impurity potential. Taking this circumstance into account leads to the result that the probability for an elementary scattering event becomes an oscillating function of the film's thickness. As a result the dependence of the kinetic coefficients on the thickness is complicated although it retains the oscillating character.

Let us start with an examination of the corrections associated with the second term in the Born series: $V^{(1)} + V^{(2)} + \ldots$ (see Fig. 1). The graph representing the quantity $V^{(2)}$ (without any external lines) corresponds to the following expression:

$$V^{(2)} \sim \sum_s \int \frac{U_{ns}(\mathbf{p}-\mathbf{q})\,U_{sm}(\mathbf{q}-\mathbf{p}')}{E - E_s(\mathbf{q}) + i\delta}\,\frac{d\mathbf{q}}{(2\pi)^2}, \tag{1}$$

where

$$U_{ns}(\mathbf{p}-\mathbf{q}) = \int \psi_n^*(z)\,U(\mathbf{r})\,\psi_s(z)\,e^{-i(\mathbf{p}-\mathbf{q})\rho}\,dr;$$

$U(\mathbf{r})$ is the potential of the impurity atom, ρ is a two-dimensional vector in the plane of the film, which is perpendicular to the z axis; the $\psi_n(z)$ denote the eigenfunctions of the electron's transverse motion, and $E_s(\mathbf{q}) = \epsilon_s + (q^2/2)$ where ϵ_s are the film levels of energy ($\hbar = m^* = 1$).

The integral in (1) diverges logarithmically in the region of small momenta if $E = \epsilon_s$. Thus, the contribution of the second approximation is of the order of $U^2 \ln|E - \epsilon_s|/q_{\max}^2$, where $q_{\max}$ is the characteristic size of $U(\mathbf{q})$, and the smallness of the perturbation $U(\mathbf{r})$ may be compensated by the large magnitude of the logarithm. In order to obtain the correct result it is necessary to sum the entire Born series, which is equivalent to solving an integral equation for the Green's function:

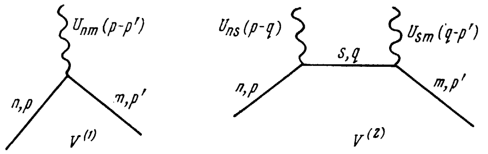

FIG. 1

$$(E - E_n(\mathbf{p}) + i\delta)\,G_{nm}(\mathbf{p}\mathbf{p}') = -\delta_{nm}\delta(\mathbf{p}-\mathbf{p}') + \sum_{sq} U_{ns}(\mathbf{p}-\mathbf{q})\,G_{sm}(\mathbf{q},\mathbf{p}'). \tag{2}$$

Below a model is considered in which $U_{ns}(p)$ does not depend on p (a short-range potential): $U_{ns} = U_0\psi_n^*(z)\psi_s(z_0)$ where z_0 denotes the z coordinate of the impurity atom, which is located at the point $\mathbf{R}_0(\rho_0, z_0)$. Integrals which diverge at large momenta are cut-off at $q_{\max}$. Under these assumptions the solution of Eq. (2) has the form (S denotes the area of the film)

$$G_{nm}(\mathbf{p}\mathbf{p}'\mathbf{R}_0) = -\frac{4\pi^2}{S}\frac{\delta_{nm}\delta(\mathbf{p}-\mathbf{p}')}{E-E_n(\mathbf{p})+i\delta} + \frac{g(E)\,\psi_n^*(z_0)\,\psi_m(z_0)\,e^{-i(\mathbf{p}-\mathbf{p}')\rho_0}}{S(E-E_n(\mathbf{p})+i\delta)(E-E_m(\mathbf{p}')+i\delta)}, \tag{3}$$

$$g(E,\mathbf{R}_0) = -U_0\left[1 - U_0\sum_s \frac{|\psi_s(z_0)|^2}{4\pi^2}\int \frac{dq}{E - E_s(\mathbf{q}) + i\delta}\right]^{-1}. \tag{4}$$

In the $\mathbf{r}$-representation one has $G(\mathbf{r}, \mathbf{r}_0) = G^0(\mathbf{r}, \mathbf{r}_0) + G^0(\mathbf{r}, \mathbf{R}_0)\,g(E, \mathbf{R}_0)\,G^0(\mathbf{R}_0, \mathbf{r}_0)$. It is clear that the electron scattering amplitude is determined by the quantity g(E) which, for E close to a certain film level ϵ_n, is given by

$$g(E) = -U_0\left[1 + \frac{U_0}{2\pi}|\psi_n(z_0)|^2 \ln\frac{q_{\max}^2}{2|E-\varepsilon_n|} + \frac{iU_0}{2}\sum_{s=1}^{N(E)}|\psi_s(z_0)|^2\right]^{-1}. \tag{5}$$

Here N(E) denotes the number of levels of transverse quantization having energies less than E. In order of magnitude $|\psi_n(z_0)|^2 \sim 1/a$ where a denotes the thickness of the film. If the potential of the impurity center is a small perturbation ($U_0/a \ll 1$) and $U_0 > 0$, then $|g(E)|$ does not exceed U_0. However, in the case of attraction ($U_0 < 0$) the quantity $|g(E)|$ has maxima near $E = \epsilon_n$, and there reaches a value of the order of a, but in the intervals between the maxima $|g(E)| \sim U_0 \ll a$. On the segment of the real energy axis $0 \leq E \leq \epsilon_1$ the function g(E) is real since $N(E) \equiv 0$, and it has a pole at the point

$$E_p = \varepsilon_1 - \frac{q_{max}^2}{2} \exp\left(-\frac{2\pi}{|U_0|\,|\psi_1(z_0)|^2}\right).$$

Thus, a bound state of the electron arises with an energy below the first film level, i.e., in the forbidden band. This fact should be related to the following well-known result of quantum mechanics: for a two-dimensional problem in an arbitrarily shallow potential well there always exists a level of negative energy which is exponentially shallow in comparison with the depth of the well. The thin (quantizing) film makes the electron's motion effectively two-dimensional, and therefore an arbitrary attractive potential leads to the occurrence of localized states.

As is clear from the expression for E_p, the energy of such a state depends on z_0, i.e., on the position of the impurity atom. Since the impurities are randomly distributed over the thickness of the film, an impurity band arises which merges with the bottom of the conduction band. One can calculate the density of states in the impurity band, having assigned a specific model for the film, i.e., having chosen a specific form for $\psi_n(z)$. For the model of a rectangular well having infinitely high walls, $\psi_n(z) = \sqrt{2/a}\sin(n\pi z/a)$. Assuming the impurities to be uniformly distributed in the film, we obtain the following result for the density of states in the impurity band for a single impurity atom:

$$\nu(E) = \frac{2}{a}\frac{dz_0}{dE_p} = \ln^{1/2}\frac{2(\varepsilon_1 - E_c)}{q_{max}^2}\left[\left(\ln^{1/2}\frac{\varepsilon_1 - E}{\varepsilon_1 - E_c}\right)(\varepsilon_1 - E)\ln\frac{2(\varepsilon_1 - E)}{q_{max}^2}\right]^{-1}, \tag{6}$$

where E_c is the bottom of the impurity band: $E_c = \epsilon_1 - (1/2)q_{max}^2 \exp(-\pi a/|U_0|)$.

The function $\nu(E)$ has singularities at the edges of the impurity band: for $E \to E_c$ we have $\nu(E) \sim (E - E_c)^{-1/2}$, and as $E \to \epsilon_1$ one will have $\nu(E) \sim (\epsilon_1 - E)^{-1}\ln^{-3/2}[2(\epsilon_1 - E)/q_{max}^2]$. Strictly speaking the result for $E \to \epsilon_1$ is not valid within a certain neighborhood of ϵ_1 due to the overlap between the wave functions of electrons localized on different impurity atoms. This neighborhood is small for a small impurity concentration and will not be considered in detail in the present article.

The pole of g(E) investigated above turns out to be the only one associated with fulfillment of the condition $U_0 \ll a$. In fact, for real and positive values of E outside the interval $0 \leq E \leq \epsilon_1$ the equation $[g(E)]^{-1} = 0$ does not have any solutions since $N(E) \neq 0$ and g(E) becomes complex (see Eq. (5)). However, if the existence of poles in the complex E plane is postulated, then assuming $E = E_0 + i\Gamma$, from Eq. (4) we obtain two equations for the determination of E_0 and Γ:

$$1 - \frac{|U_0|}{a\pi}\sum_s |\psi_s(z_0)|^2 \ln\frac{q_{max}^2}{2((\varepsilon_s - E_0)^2 + \Gamma^2)^{1/2}} = 0,$$

$$\sum_s |\psi_s(z_0)|^2 \operatorname{arc\,tg}\frac{\Gamma}{\varepsilon_s - E_0} = 0. \tag{7}$$

Investigation of the system (7) leads to the following conclusions. In the case $|U_0| \ll a$ no solutions exist on the physical energy sheet apart from the solution already found: $\Gamma = 0$, $E = E_p$. The remaining resonances in the scattering amplitude correspond to poles lying on other sheets of the Riemann surface, namely: the resonance associated with E close to ϵ_n corresponds to a pole on the n-th sheet. Thus, only the first pole belongs to the physical energy sheet and corresponds to a real bound state. Quasi-stationary levels of the electron do not appear (one should keep in mind that the quantity $E - \epsilon_n$ plays the role of the particle's kinetic energy; at a resonance $E - \epsilon_n \sim q_{max}^2 \exp(-\pi a/|U_0|)$ and the width ΔE of the resonance at half-maximum turns out to be numerically larger: $\Delta E \sim e^{2\pi} q_{max}^2 \exp(-\pi a/|U_0|)$, i.e., the resonances are not narrow and they do not correspond to metastable states).[1)]

One can eliminate the explicit dependence on the cut-off parameter q_{max} and express all of the results in terms of the amplitude f for the scattering of a zero-energy electron by a potential U(**r**) in an infinite crystal. In the case of scattering by short-range impurities in a magnetic field, this problem was solved by Skobov.[2] The starting point is the Lippmann-Schwinger[3] integral equation or the expression for the electron's Green's function in the **r**-representation without taking the impurity field into account. The latter is given by (see[4]):

$$G_E(\rho, \rho', zz') = \int e^{i\mathbf{p}(\rho-\rho')}\frac{\sin Rz' \sin R(a-z)\,d\mathbf{p}}{4\pi^2 \sin Ra} \quad \text{for } z > z',$$
$$z \rightleftarrows z' \text{ for } z < z', \tag{8}$$

where $R = R(p) = \sqrt{2E - p^2 + i\delta}$. The following treatment is completely analogous to article[2]. The matrix element of the transition $n\mathbf{p} \to m\mathbf{q}$ has the form

$$M(n\mathbf{p}, m\mathbf{q}) = \frac{4\pi f}{aS} e^{i(\mathbf{q}-\mathbf{p})\rho_0}\tilde{g}(E)\sin\frac{n\pi z_0}{a}\sin\frac{m\pi z_0}{a},$$

$$\tilde{g}(E) = \left[1 + 2f\int_0^{\sqrt{2E}} \sin Rz_0 \sin R(a - z_0)\operatorname{cosec}(Ra) R^{-1}p\,dp + i\frac{2\pi f}{a}\sum_{n=1}^{N(E)} \sin^2\frac{n\pi z_0}{a}\right]^{-1}. \tag{9}$$

For $E = (n\pi)^2/2a^2$ the integral in expression (9) diverges logarithmically, and a formula of type (5) is obtained. Thus, the matrix element of the scattering oscillates upon variation of E or a.

The relaxation time and the kinetic characteristics of the electrons are determined by the quantity $|M(n\mathbf{p}, m\mathbf{q})|^2$, averaged over the positions of the impurity atoms. In the problem under consideration the scattering is isotropic, that is, $|M|^2$ does not depend on the angle between **p** and **q**. Therefore the transport relaxation time is determined by the usual scattering cross section:

$$\frac{1}{\tau_n(\mathbf{p})} = 2\pi\sum_{mq}\overline{|M(np, mq)|^2}\,\delta(\varepsilon_n + p^2/2 - \varepsilon_m - q^2/2)$$
$$= \frac{16\pi c|f|^2}{a}\sum_m\int_0^\pi |\tilde{g}(E;\varphi)|^2\,\Theta(E - \varepsilon_m)\sin^2 m\varphi \sin^2 n\varphi\,d\varphi. \tag{10}$$

Here $\varphi = \pi z_0/a$, $E = \epsilon_n + (p^2/2)$, $\Theta(x) = 1$ for $x > 0$, $\Theta(x) = 0$ for $x < 0$, and c denotes the impurity concentration.

[1)] The author thanks V. L. Pokrovskiĭ for a discussion of this part of the work.

In connection with averaging over the distribution of the impurity atoms, one should keep in mind the single property which distinguishes a film from a bulk sample. As a consequence of the dependence of the scattering amplitude on the z-coordinate of the impurity atom, the quantity

$$\frac{1}{a}\int_0^a \psi_m^*(z)\, g(E;z)\, \psi_n(z)\, dz$$

does not vanish for m ≠ n. Because of this $\overline{M^2}$ contains, in addition to the usual terms that are diagonal with respect to the number of the impurity atom and correspond to incoherent scattering by different atoms, the contributions of nondiagonal terms coming from coherent scattering by atoms that are located "one above the other," that is, the x and y coordinates of these atoms are the same but their z coordinates are different. The relative magnitude of this correction is of the order of caa_0^2, where a_0 is the linear size of the region in which the impurity atom is localized. It is natural to assume that a_0 is of the order of the lattice parameter. Then $caa_0^2 \lesssim 1$ for $a \lesssim 1000$ Å up to values of $c \sim 10^{20}\ \text{cm}^{-3}$. In this work it is assumed that the impurity concentration does not attain such a high value, so that $caa_0^2 \ll 1$, and one can neglect the contribution due to coherent scattering.

In the limit of a strongly degenerate electron gas, the electrical conductivity of the film is expressed by the following formula:

$$\sigma = \frac{e^2}{16\pi^2|f|^2c}\sum_{n=1}^{N(\mu)}(\mu-\varepsilon_n)\Big[\sum_{m=1}^{N(\mu)}\int_0^\pi |\tilde{g}(E;\varphi)|^{-2}\sin^2 m\varphi\,\sin^2 n\varphi\, d\varphi\Big]^{-1}, \tag{11}$$

where μ denotes the Fermi level and e is the electron charge. In the first Born approximation $\tilde{g}(E;\varphi) \equiv 1$, and the well-known saw-tooth dependence of the conductivity on the thickness is obtained: $\sigma_0 = e^2na/4\pi^2|f|^2c[N(\mu) + (1/2)]$, where n denotes the electron concentration. This dependence is depicted by the dashed line shown in Fig. 2. In the neighborhood of the critical points a_1, a_2, ..., which are determined by the equation $\mu(a_j) = \epsilon_{j+1}$, the inapplicability of the Born approximation becomes important, and one must use formula (9) for $\tilde{g}(E, \varphi)$.

In the general case the evaluation of the integral in (11) leads to extremely cumbersome expressions; therefore, below only the neighborhood of the point a_1 will be investigated. Qualitatively the same thing happens near the other critical values of the film thickness. In the region $a < a_1$ one finds

$$\sigma = \frac{s^2(\mu-\varepsilon_1)}{16\pi^2|f|^2c}\Big[\int_0^\pi \frac{\sin^4\varphi\, d\varphi}{(1-2\Lambda|f|a^{-1}\sin^2 2\varphi)^2 + 4\pi^2|f|^2a^{-2}\sin^4\varphi}\Big]^{-1}; \tag{12a}$$

for $a > a_1$ one finds

$$\sigma = \frac{e^2}{16\pi^2|f|^2c}\Big\{(\mu-\varepsilon_1)\Big[\int_0^\pi L(\varphi)\sin^2\varphi\, d\varphi\Big]^{-1} + (\mu-\varepsilon_2)\Big[\int_0 L(\varphi)\sin^2 2\varphi\, d\varphi\Big]^{-1}\Big\}, \tag{12b}$$

where

$$L(\varphi) = \frac{5-\sin 5\varphi/\sin\varphi}{(1-2|f|\Lambda a^{-1}\sin^2 2\varphi)^2 + 4\pi^2|f|^2a^{-2}\sin^4\varphi(1+4\cos^2\varphi)}$$

$$\Lambda = \ln(4\pi/a^2|\mu-\varepsilon_2|).$$

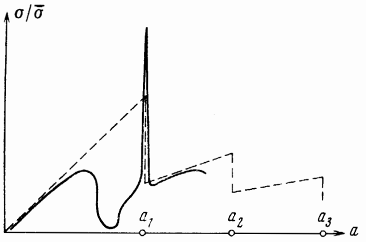

FIG. 2

If $\lambda \equiv 2\Lambda|f|/a < 1$, $a < a_1$, then the conductivity at first increases linearly, and then falls with increase of a, and at the minimum it becomes substantially smaller than its characteristic value $\bar{\sigma} = e^2na/4\pi^2|f|^2c$. Namely, in the region $1 \gg 1 - \lambda \gg |f|/a$ one finds

$$\sigma \approx \frac{e^2na}{2\pi^2|f|^2c}(1-\lambda)^{3/2} \ll \bar{\sigma}. \tag{13}$$

It should be emphasized that σ calculated in the Born approximation is of the order of $\bar{\sigma}$ everywhere. However, if $\lambda > 1$ then the conductivity increases with increasing thickness (as before $a < a_1$). Upon fulfillment of the inequality $\lambda - 1 \gg |f|/a$

$$\sigma \approx \frac{e^2na}{4\pi^2|f|^2c}\Big(\frac{\pi|f|}{2a}\Big)\big[(2\lambda-1+2\sqrt{\lambda^2-\lambda})^{1/2} - (2\lambda-1-2\sqrt{\lambda^2-\lambda})^{1/2}\big]. \tag{14}$$

If $\lambda - 1 \sim |f|/a$ the conductivity is of the same order of magnitude as in formula (13), i.e., $\sigma \sim \bar{\sigma}(|f|/a)^{3/2}$. But for $\lambda \to \infty$, which corresponds to $a \to a_1$, $\mu \to \epsilon_2$, σ formally tends to infinity:

$$\sigma \sim \bar{\sigma}(|f|/a)^{3/2}\sqrt{\ln(4\pi/a_2|\mu-\varepsilon_2|}.$$

This is related to the fact that the scattering amplitude vanishes for $\mu = \epsilon_n$ (see Eq. (9)).

Actually, for a finite impurity concentration, a finite damping appears in the Green's function, and the conductivity remains finite. Taking the temperature broadening of the Fermi distribution into account or taking other scattering mechanisms into consideration leads to the same result. However, it hardly makes sense to consider these refinements since σ becomes substantially larger than $\bar{\sigma}$ in an extremely narrow region near a_1. The size of this region is proportional to $\exp(-a^3/|f|^3)$ where $a \gg |f|$. A graph of $\sigma(a)$ is shown in Fig. 2 (the solid line). For scattering by screened Coulomb centers and for a temperature close to zero ($T \ll \epsilon_2 - \epsilon_1$), the width of the region near a_1 where the difference between σ and σ_0 is appreciable amounts to approximately 20% of the period of oscillations.

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