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# *SCATTERING OF CONDUCTION ELECTRONS IN VERY THIN FILMS*

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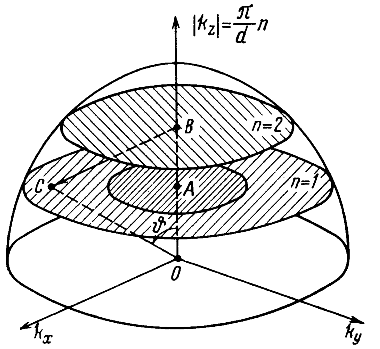
The scattering of conduction electrons is calculated in the effective mass approximation for very thin semimetal films in which the de Broglie wavelength is comparable with the film thickness. The probability of the electron scattering by phonons, electrons, and geometric defects of the film surface is determined. It is assumed that the electron mean free path is large in comparison with the film thickness, and that the reflection of electrons from the boundaries is mainly specular. The allowed electrons states are then arranged in layers in momentum space (see the figure), each layer having its value of the quantized transverse energy. It is therefore necessary to distinguish between longitudinal and transverse electron scattering. The longitudinal scattering is connected only with the rotation of the longitudinal quasimomentum of the electron. The transverse scattering is accompanied by a transition of the electron from one layer to another. Owing to the conservation of the longitudinal momentum, elastic transverse transitions can be caused only by phonons of finite energy. At very low temperatures, when the latter are missing, transverse electron-phonon scattering is therefore due entirely to spontaneous phonon emission. If this emission is forbidden, as in a normal metal, the scattering probability decreases exponentially with temperature. In a film with identical conditions on both surfaces, the transverse electron-electron scattering connected with transitions between layers of different parity is forbidden in virtue of symmetry. Therefore there is no electron-electron transverse scattering in the second layer. The probability of longitudinal electron-electron scattering is proportional to the third power of the longitudinal quasimomentum. Owing to the quantization of transverse motion, the transverse diffusivity of the electron reflection from the film surface is strongly inhibited in comparison with the diffusivity of a single surface.

## 1. INTRODUCTION

IN this paper we deal with the scattering of conduction electrons in very thin films; "very thin" means that the film thickness d is comparable with the de Broglie wavelength $\lambda$ of the electron, $\lambda \sim d$. If T denotes the kinetic energy in eV and m* the effective mass of the electron, then $\lambda = 12.3\,\text{Å}/(Tm^*/m)^{1/2}$. In normal metals $m^*/m \sim 1$ and the Fermi energy is $E_F \sim 5$ eV, so we obtain $\lambda \sim 5\,\text{Å}$. In metals with small effective masses, $m^*/m \sim 0.1$, and small Fermi energies, $E_F \sim 0.1$ eV, we obtain $\lambda \sim 100$ Å. In semimetals of the Bi type, where $m^*/m \sim 0.01$ and $E_F \sim 0.01$ eV, we obtain $\lambda \sim 10^3$ Å. In practice it is possible to prepare sufficiently homogeneous films of thicknesses down to 100 Å. Therefore, the very thin films considered here can be prepared from metals with sufficiently low electron concentration, from semimetals, and finally, from semiconductors.

It is assumed that the volume mean free path $\Lambda$ of the electron is much larger than the film thickness, $\Lambda \gg d$, so that $\Lambda \gg \lambda$, because $d \sim \lambda$. This means that the scattering over one wavelength is small, which is always so if one may use the quasimomentum concept. It is also assumed that the film is sufficiently "good," i.e., the height $\Delta h$ of the roughnesses and other geometrical defects of the film is small in comparison with its thickness; thus $\Delta h \ll \lambda$. Hence, the reflection of conduction electrons from the film surface is mainly specular, i.e., the diffusivity is small, $\rho \ll 1$.

When these conditions are fulfilled, the electrons in the film form a sort of Knudsen gas, with specific features resulting from the quantization of the transverse motion of electrons. The quantization is due to the fact that electrons interfere in the thin film just like light interferes in thin transparent sheets. Interference may lead to resonant electron tunneling through the system of dielectric barriers.[1, 2] Thin-film electron interferometers using these effects have been proposed.[3] These devices will probably be utilized in due time. The study of interference resonances may yield new



In a very thin film the electron states form a system of discrete layers (n = 1, 2, ...) in momentum space, this being caused by the quantization of the transverse energy. The elastic transition of an electron from the point B of the second layer to point C of the first one corresponds to a scattering by an angle $\vartheta = \pi/3$.

information on electron behavior in thin films, particularly on the properties of comparatively hot electrons. Unfortunately, there is no experimental work in this direction as yet, except the short communication[4] on the observation of interference resonances in a thin aluminum film.

The sharpness of the interference resonances depends upon the electron scattering in the film.[5] The study of electron scattering in very thin films is therefore of interest for the construction of thin-film electron interferometers. This was the reason for undertaking the present calculations. It has turned out, however, that electron scattering in very thin films has a number of interesting features which seem to be of physical interest per se, and is worth investigating regardless of the prospects of its practical application.

The question of electron scattering in very thin films was first raised in connection with the discovered anomalies of the electric conductivity of thin nickel films.[6] An idea was expressed that the quantization of the transverse motion should reduce the scattering, but no calculations were made in either [6] or in later work. The only published calculation deals with scattering by phonons in very thin semiconductor films,[7] assuming that all electrons lie in the lowest transverse level, i.e., that they actually form a two-dimensional gas.

In the present work we calculate the electron scattering by phonons, electrons, and geometrical defects of the surface. It is shown first that the substantial difference between the electron scattering in a very thin film and in a thick sample arises from anisotropy caused by the quantization of the transverse motion. So, in a film with absolutely impenetrable walls the transverse motion of the electron is described by a standing wave with nodes on the surface: $\lambda_n = 2d/n$ (n = 1, 2, 3, ...), with quantized transverse quasimomentum

$$|p_\perp| = \pi\hbar n / d$$

and transverse energy

$$E_\perp = p_\perp^2 / 2m^* = 0.0038\ \mathrm{eV} \cdot (m / m^*)\,(100\ \text{Å} / d)^2 n^2.$$

The longitudinal energy $E_\| = p_\|/2m^*$ is not quantized. Because of quantization, the momentum distribution of the electrons in a thin film is substantially modified. The distribution is shown in the figure, where $|k_z| = |p_\perp|/\hbar$ is the transverse component of the electron wave vector, and $k_x$ and $k_y$ are the longitudinal components. The electron states are located in layers, each layer having its corresponding definite transverse quasimomentum and energy. The number of filled layers increases with electron concentration $n_0$. Thus, for example, the filling of the second layer begins at point B under condition that the longitudinal electron energy in the first layer reaches a value

$$E_\| = 3\pi^2\hbar^2 / 2m^* d^2,$$

equal to the difference between the transverse energies of the second and first layers. Assuming that any electron state in the layer has in the phase-space a corresponding unit cell of volume $(2\pi\hbar)^2$, we find that electrons fill up the lower layer, while the second and next layers are unpopulated, if $n_0 \leq 3\pi/2d^3$. For d = 100 Å this yields $n_0 \leq 5 \times 10^{18}\ \mathrm{cm}^{-3}$, corresponding to the electron concentration in the Bi type metals.

For the electrons in the first layer there is only a longitudinal elastic scattering connected with the rotation of the longitudinal quasimomentum; the transverse quasimomentum cannot change, and the electrons actually behave like a two-dimensional gas. On the contrary, an electron situated at point B in the second layer does not participate in the longitudinal motion but can pass to point C of the first layer as a result of elastic scattering. Its transverse momentum changes then from $2\pi\hbar/d$ to $\pi\hbar/d$; owing to momentum conservation, a longitudinal momentum $p_\| = \sqrt{3}\pi\hbar/d$ appears simultaneously, corresponding to scattering by an angle $\vartheta = \pi/3$. Elastic transverse scattering by a smaller angle is impossible because the energy and momentum conservation laws would not be simultaneously satisfied. In the general case, an electron from the second and higher levels can undergo both longitudinal and transverse scattering. Longitudinal scattering by any small angle is possible, whereas transverse scattering is always connected with a large-angle rotation of the quasimomentum; therefore it can be caused by mechanisms which are capable of ensuring sufficiently large scattering angles.

## 2. SCATTERING BY PHONONS

Transverse scattering. Let us find the average time $\tau_{21f}$ an electron can spend in the second layer before experiencing a transition to the first layer due to interaction with longitudinal acoustical phonons. We shall use the deformation potential method, as in [7].

The wave functions of an electron in a plane-parallel layer with absolutely impenetrable walls are chosen in the form

$$\psi_{\mathbf{k},n}(\mathbf{r})=\left(\frac{2}{Sd}\right)^{1/2}e^{i\mathbf{kr}}\left\{\begin{matrix}\cos(n\pi z/d)\\ \sin(n\pi z/d)\end{matrix}\right\},\quad -\frac{d}{2}\leqslant z\leqslant\frac{d}{2},\tag{1}$$

where $\mathbf{r}$ is the radius vector of the electron, $\hbar\mathbf{k}$ is its longitudinal momentum, and S is the area of the film; sin corresponds to even, and cos to odd values of n, n being the number of the layer.

Calculation in the first approximation of perturbation theory yields for the probability of a transition with phonon emission

$$\frac{1}{\tau_{21f}}=2^6\pi^2\frac{C^2}{\rho_0 v_l}\int d\mathbf{q}\cdot q\left([\exp(\hbar v_l q/kT)-1]^{-1}+1\right)$$
$$\times\frac{(q_z d)^2\cos^2(q_z d/2)}{[\pi^2-(q_z d)^2]^2[(3\pi)^2-(q_z d)^2]^2}$$
$$\times\delta\left\{\frac{\hbar^2}{2m^*}[\mathbf{k}_2^2-(\mathbf{k}_2-\mathbf{q}_{\parallel})^2]+\frac{3\pi^2\hbar^2}{2m^*d^2}-\hbar v_l q\right\}.\tag{2}$$

Here C is the electron-phonon interaction constant, $\rho_0$ is the mass density of the film, $v_l$ is the longitudinal sound velocity, k is the Boltzmann constant, and $\hbar\mathbf{q}$ is the momentum of the phonon.

We assume that the phonon spectrum in the film is the same as in a large sample. We replaced the number of phonons by the average value at the given temperature T; the $\delta$-function in the integral takes care of energy conservation.

The probability of a transition with absorption of a phonon differs from (2) by not having the unity, which accounts for spontaneous emission, in the brackets in the integral, and by the changed sign of q-containing terms in the argument of the $\delta$-function. In what follows we shall neglect the phonon energy $\hbar v_l q$ in comparison with the change in the transverse electron energy $3\pi^2\hbar^2/2m^*d^2$.

We consider the case $k_2 = 0$, which corresponds to a state represented by the point B in the figure. Calculation of the integrals yields for the total probability of the transition

$$\frac{1}{\tau_{21f}}\approx\frac{\pi C^2 m^*}{\rho_0 v_l\hbar^2 d^2}\left\{(1+\sqrt{3})+\frac{2}{e^{T_0/T}-1}+\frac{2\sqrt{3}}{e^{\sqrt{3}\,T_0/T}-1}\right\},\tag{3}$$

where

$$T_0=2\pi\hbar v_l/kd.\tag{4}$$

The term $(1+\sqrt{3})$ represents the contribution from spontaneous phonon emission, and the exponential terms are connected with induced emission and absorption.

At sufficiently low temperatures, $T \ll T_0$, (for $d = 100$ Å and $v_l = 3\times10^5$ cm/sec we obtain $T_0 = 14.4$°K) all phonons able to cause scattering are frozen, and scattering is due totally to spontaneous phonon emission. However, if a degenerate electron gas partially fills the two lower layers, then, because of the Pauli principle, radiative transitions are forbidden as in a usual metal. Therefore with decreasing temperature the probability of transverse scattering on phonons tends exponentially to zero. This effect is caused by the fact that the transition from the second layer to the first one is associated by a change in longitudinal electron quasimomentum of the order of $\sqrt{3}\pi\hbar/d$; phonons with smaller momentum cannot give rise to scattering because the longitudinal momentum is conserved.

At sufficiently high temperatures, $T \gg T_0$, one may neglect the spontaneous emission in comparison with the induced one; then

$$1/\tau_{21f}\approx 2C^2 m^* kT/\rho_0 v_l^2\hbar^3 d.\tag{5}$$

We have considered the case $k_2 = 0$, but in the case $0 < k_2 < \pi/d$ the results will not differ noticeably.

Longitudinal scattering. Longitudinal scattering of electrons of the first layer has been discussed by Demikhovskiĭ and Tavger.[7] For second-layer electrons the result does not differ qualitatively.

## 3. SCATTERING OF ELECTRONS BY ELECTRONS

Transverse scattering. Let us find the probability of an electron transition from the second (or third, etc.) layer into the first one due to interaction with the electrons which fill up the first layer. We write the matrix element of the screened inter-electron interaction in the form

$$\langle\mathbf{k}'_1,(1);\ \mathbf{k}'_2,(1)\ |\hat{H}_{ee}|\ \mathbf{k}_1,(1);\ \mathbf{k}_2,(2)\rangle$$
$$=e^2\int\psi^*_{\mathbf{k}_1',1}(\mathbf{r}_1)\psi^*_{\mathbf{k}_2',1}(\mathbf{r}_2)\frac{\exp(-|\mathbf{r}_1-\mathbf{r}_2|/r_D)}{|\mathbf{r}_1-\mathbf{r}_2|}$$
$$\times\psi_{\mathbf{k}_1,1}(\mathbf{r}_1)\psi_{\mathbf{k}_2,2}(\mathbf{r}_2)\,d\mathbf{r}_1\,d\mathbf{r}_2,\tag{6}$$

$\mathbf{k}_i$ and $\mathbf{k}'_i$ are the longitudinal momenta of the i-th electron before and after scattering, respectively, and $r_D$ is the Debye screening radius; we assume that $r_D \ll d$.

It turns out that in a film with identical conditions on both surfaces the matrix element (6) vanishes for transitions between layers of different parity, in particular for transitions between neighboring layers. This is caused by the fact that by virtue of the symmetry of the problem the electron wave-functions in odd layers are symmetrical (antisymmetrical in even layers) relative to reflections from the central plane of the film. The integrand in (6) is therefore an odd function $z_2$ and the integration between symmetrical limits yields zero. This can easily be proved by substituting, say, the functions (1). We note, however, that the zero result is a consequence of the problem's symmetry and does not depend on the explicit form of the wave functions. Thus the transverse interelectron scattering is forbidden for electrons of the second layer.

Let us now find the probability of a transition from the third layer to the first one. The matrix element for such a transition, calculated with the aid of the functions (1), is

$$\frac{2\pi e^2}{(Sd)} \frac{\delta_{\mathbf{k}_2-\mathbf{k}_2',\,\mathbf{k}_1-\mathbf{k}_1'}}{|\mathbf{k}_1'-\mathbf{k}_1|^2+1/r_D^2}, \tag{7}$$

and the use of any other functions of z leads to a change in the numerical coefficient only, which is of no importance to us.

The probability of the corresponding transition is, in the first approximation,

$$\frac{1}{\tau_{31\,e}} = \frac{2\pi}{\hbar} \sum_{\mathbf{k}_2',\,\mathbf{k}_1,\,\mathbf{k}_1'} |\langle \mathbf{k}_1', (1); \mathbf{k}_2', (1)\,|H_{ee}|\,\mathbf{k}_1, (1); \mathbf{k}_2, (3)\rangle|^2$$
$$\times\,\delta\left\{\frac{\hbar^2}{2m^*}\left(k_1^2+k_2^2+\frac{8\pi^2}{d^2}-k_1'^2-k_2'^2\right)\right\}$$
$$\times f_1(\mathbf{k}_1)[1-f_1(\mathbf{k}_1')][1-f_1(\mathbf{k}_2')]. \tag{8}$$

Here $f_1(\mathbf{k})$ is the longitudinal momentum distribution of the electrons in the first layer. In place of it we take the Fermi function at T = 0. We assume that the second and next layers are unpopulated, so that the longitudinal Fermi momentum is $\hbar k_{1F} \le \sqrt{3}\pi\hbar/d$. Calculating (8) in the case $r_D \ll d$, we obtain

$$\frac{1}{\tau_{31\,e}} = \frac{2\pi m^* e^4}{\hbar^3 d^2} r_D^4 k_{1F}^2. \tag{9}$$

The scattering probability (9) is proportional to $k_{1F}^2$, i.e., to the number of electrons in the first layer. This should be expected because it was assumed that the transverse energy of the scattered electron is much larger than the Fermi energy. The appearance of factors $1/d^2$ and $r_D^2$ is due to the matrix element (7).

Taking, for an estimate, d = 100 Å, $k_{1F} = 1/d$, $m^* = 0.1\,m$, and $r_D = 10$ Å, we obtain $\tau_{31e} = 3.9 \times 10^{-13}$ sec. The corresponding transit time of the electron across the film is $\tau_0 = 0.92 \times 10^{-14}$ sec, so that during the time $\tau_{31e}$ the electron accomplishes 42 transits. However one should have in mind that expression (9) was obtained in the Born approximation and certainly has therefore too large a coefficient.

Longitudinal scattering. Let us find the probability of longitudinal scattering of an electron from the second layer, due to collisions with electrons which fill up the first layer. Proceeding as in the calculation of the transverse scattering, we obtain

$$\frac{1}{\tau_{22e}} = \frac{2^7}{9\pi} \frac{m^* e^4}{\hbar^3 d^2} r_D^4 k_{1F}^2 \left(\frac{k_2}{k_{1F}}\right)^3, \quad k_2 \ll k_{1F} \ll \frac{1}{r_D}. \tag{10}$$

the factor $k_2^3$ results from the conservation laws, by virtue of which the longitudinal momentum transfer for $k_2 \ll k_{1F}$ can take place only in a narrow range of angles $\sim(k_2/k_{1F})$, the increment of the longitudinal momentum being $(k_1' - k_1) \lesssim k_2^2/k_{1F}$. The probability (10) of longitudinal scattering decreases therefore quickly with $k_2$. Thus, if for $k_2 \sim k_{1F} \sim 1/d$ we have $\tau_{22e} \sim 10^{-13}$ sec, as in the foregoing example, then already for $k_2 = 0.1 k_{1F}$ we obtain $\tau_{22e} \sim 10^{-10}$ sec. Therefore, longitudinal scattering of electrons with sufficiently small longitudinal quasimomentum, $k_2 \ll k_{1F}$, is insignificant. If these electrons, moreover, lie in the second layer, then their transverse scattering is forbidden, too.

## 4. SCATTERING FROM SURFACE DEFECTS OF THE FILM

For electrons in a thin film one has to consider separately the coefficients of longitudinal diffusivity $\rho_{\parallel}$ and of transverse diffusivity $\rho_{\perp}$. We shall estimate the transverse diffusivity for second-layer electrons using the diffraction method developed in [8]. It is shown there that for normal incidence of a plane wave on a rough surface, the angular intensity distribution of the reflected wave is

$$|F(s)|^2 = \exp(-\pi\varphi^2)\,\delta(s)$$
$$+\,\{1-\exp(-\pi\overline{\varphi^2})\}\frac{\Delta x}{\lambda(\pi\overline{\varphi^2})^{1/2}}\exp\left(-\frac{\Delta x^2 s^2}{\lambda^2\overline{\varphi^2}}\right), \tag{11}$$

where $\overline{\varphi^2} = 16\pi^2(\Delta h)^2/\lambda^2$; $s = \sin\vartheta$, $\vartheta$ is the scattering angle, and $\Delta x$ is the longitudinal dimension of the roughness. The first term in (11) describes a specularly reflected wave. The second term describes a bundle of scattered beams and characterizes the diffuse reflection. The diffusivity of a single surface is

$$\rho = 1 - \exp(-\pi\overline{\varphi^2}). \tag{12}$$

It depends on the ratio of the height $\Delta h$ of the roughnesses to the wavelength $\lambda$. The angular intensity distribution of the reflected light depends on the form of the roughnesses. If these are mildly sloping, so that $4\pi\Delta h \ll \Delta x$, small angle scattering occurs, and vice versa.

The small-angle transverse scattering is inhibited in thin films; only scattering by large angles of the order of $\vartheta$ is allowed. For example, it was shown above that for the state represented on the figure by point B, we have $\vartheta_0 = \pi/3$. Taking into account the inhibition of the small angle scattering, we obtain the transverse diffusivity in a thin film by integrating the second term in (11) over angles larger than $\vartheta_0$ (we put $s_0 = \sin\vartheta_0$):

$$\rho_\perp = \{1 - \exp(-\pi\overline{\varphi^2})\}\frac{\Delta x}{\lambda(\pi\overline{\varphi^2})^{1/2}} \times 2\int_{s_0}^{1} \exp\left(-\frac{\Delta x^2}{\lambda^2\overline{\varphi^2}}s^2\right) ds. \tag{13}$$

The transverse scattering is largely inhibited in the case when the roughnesses are mildly sloping and the average scattering angle in (11) is small, so that the parameter

$$\Theta_0^2 = (s_0\Delta x / 4\pi\Delta h)^2 \gg 1.$$

Then we obtain instead of (12)

$$\rho_\perp \approx \{1 - \exp(-\pi\overline{\varphi^2})\} \exp(-\Theta_0^2) / \sqrt{\pi}\Theta_0. \tag{14}$$

It is seen that with increasing $\Theta_0$ the transverse diffusivity in a very thin film decreases exponentially in comparison with the diffusivity (12) of a single surface. Expression (14) can hardly be used to obtain safe quantitative estimates. It can be assumed, however, that it represents the qualitative aspect of the phenomenon. The complexity of the considered problem lies in the fact that an accurate description of the rough surface is not an easy problem, and there is therefore as yet no safe method of calculating the degree of diffusivity.

In the present paper it is everywhere assumed that the electron scattering from the surface is specular. However, the obtained results can be generalized to include the case of diffuse reflection, as was kindly pointed out to the author by M. Ya. Azbel'.

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