

RELAXATION TIMES OF ELECTRONS IN QUASI-TWO-DIMENSIONAL DISORDERED SYSTEMS

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Abstract: The Faber-Ziman diffraction model was reformulated so that to describe the behavior of the quasi-two-dimensional electron gas in a two-dimensional system of disordered potentials. Elastic scattering of charge carriers in the plane determined by the potentials was assumed. Some model calculations of the transport relaxation time were performed. The inverse transport relaxation times for subbands with a minimum and maximum in-plane Fermi vector components were calculated as a function of Cs layer width. The oscillations for the latter subband with a period equal to the atomic diameter were obtained for very thin layers.

1. INTRODUCTION

The transport properties of two-dimensional electron systems have recently attracted considerable attention because they open new perspectives for applications in nanoelectronics based on quantum transport processes of spin and charge. One of the most important problems in this matter is conductivity (or resistivity) which should apparently depend on the size of the system. Moreover, we can observe the quantization of conductivity due to geometrical confinement or external magnetic field applied perpendicularly to the plane of motion of electrons [1]. Such phenomena should exist in a very thin metallic stripe where the electron gas can be treated as quasi two-dimensional and its properties should differ from those of three-dimensional one.

The purpose of this paper is to consider a quasi two-dimensional electron gas moving through a system of randomly located potentials which has a thickness of several atomic monolayers. The wave function of an electron is formally three-dimensional but its z -dependence is completely different from the xy one because of constraints given by surfaces. This should give rise to a dependence of the scattering process and – furthermore – the kinetic coefficient on the thickness of the film, at least for the samples of a nanometer size.

2. THEORETICAL MODEL

We consider the motion of non-interacting electrons in presence of random potential in the two-dimensional system which extends unlimitedly in xy plane but has a finite thickness L_z in z -direction. The wave function of such electrons is a solution of the Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + U(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad (1)$$

where the potential $U(\mathbf{r})$ is given by the superposition of atomic potentials.

We assume that the potential $U(\mathbf{r})$ can be separated into two parts, namely in-plane $U_1(x, y)$ and perpendicular-to-plane $U_2(z)$.

$$U(\mathbf{r}) = U_1(x, y) + U_2(z), \quad (2)$$

where $U_1(x, y)$ is a random set of potentials, and $U_2(z)$ corresponds to geometrical confinement and can be represented by a quantum well.

This choice of potential allows us to relate it with the width of layer in z -direction. Thus the wave function can be factorized as follows

$$\Psi(\mathbf{r}) = \phi(x, y)\zeta(z). \quad (3)$$

Substituting Eq. (2) and Eq. (3) into Eq. (1) we can separate the latter into two [2]

$$-\frac{d^2}{dz^2}\zeta(z) + \frac{2m}{\hbar^2}U_2(z)\zeta(z) = k_z^2\zeta(z), \quad (4)$$

and

$$-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\phi(x, y) + \frac{2m}{\hbar^2}U_1(x, y)\phi(x, y) = k_\rho^2\phi(x, y), \quad (5)$$

where $\rho = (x, y)$ is a vector in xy plane, k_ρ and k_z are the wave vectors of electron in xy plane and z -direction, respectively, correlated as below

$$k_\rho^2 + k_z^2 = k^2, \quad (6)$$

and

$$k^2 = \frac{2m}{\hbar^2}E. \quad (7)$$

Let us assume that the potential well in the z -direction is of infinite depth. It is a realistic assumption if the sample lies on an insulating substrate and is placed in vacuum or an inert gas atmosphere. Then the solution of Eq. (4) is very simple

$$\zeta(z) = C_z \sin k_z z, \quad (8)$$

where

$$k_z = m\pi / L_z, \quad (9)$$

and $m = 1, 2, \dots$

In this picture only the component \mathbf{k}_ρ undergoes the scattering. If we assume elastic scattering, its absolute value is given by Eq. (6). Now we can solve the scattering problem in two dimensions.

A formal solution of Eq. (5) has the form

$$\phi(\boldsymbol{\rho}) = \phi_0(\boldsymbol{\rho}) + \frac{2m}{\hbar^2} \int d^2\rho' G(\boldsymbol{\rho}, \boldsymbol{\rho}') U_1(\boldsymbol{\rho}') \phi(\boldsymbol{\rho}'), \quad (10)$$

where the Green function $G(\rho, \rho')$ is given by the formula

$$G(\rho, \rho') = -\frac{1}{(2\pi)^2} \int d^2q \frac{\exp[i\mathbf{q}\rho(\rho - \rho')]}{q^2 - k_p^2}, \quad (11)$$

and $\phi_0(\rho)$ is a solution of Eq. (5) without a source

$$\phi_0(\rho) = \exp[-i\mathbf{k}_p \cdot \rho] \quad (12)$$

normalized such that one incident particle falls into a unit area in xy plane. We can solve the integral equation (10) in the first Born approximation [3] putting $\phi_0(\rho)$ instead of $\phi(\rho)$ under the integral sign then

$$\phi(\rho) \approx e^{-i\mathbf{k}_p \cdot \rho} + \frac{1}{\sqrt{8\pi k_p}} \frac{e^{-i\mathbf{k}_p \cdot \rho}}{\sqrt{\rho}} e^{-3i\pi/4} \int d^2\rho' U_1(\rho') e^{i\mathbf{q} \cdot [\mathbf{k}_p - k_p(\rho/\rho)]}, \quad (13)$$

The differential cross-section $d\sigma/d\varphi$ determines only the probability of scattering into the planar angle $[\varphi, \varphi + d\varphi]$

$$\frac{d\sigma}{d\varphi} = \frac{1}{8\pi k_p} \left(\frac{m}{2\pi \hbar^2} \right)^2 \left| \int d^2\rho' U_1(\rho') \exp[i\mathbf{q} \cdot \rho'] \right|^2, \quad (14)$$

where $\mathbf{q} = \mathbf{k} - k(\rho/\rho)$ is the scattering vector in xy plane.

For a disordered system the potential $U_1(\rho)$ is a superposition of atomic potentials $u_a(\rho)$ located at random positions \mathbf{R}_i

$$U_1(\rho) = \sum_{i=1}^N u_a(\rho - \mathbf{R}_i)$$

After some manipulations, analogous to those in Ziman's work [4] we obtain

$$\frac{d\sigma}{d\varphi} = \frac{1}{8\pi k_p} \left(\frac{m}{2\pi \hbar^2} \right)^2 N S(q) |u_a(q)|^2, \quad (15)$$

where N is the total number of atoms in the system, $S(q)$ is a two-dimensional structure factor, $u_a(q)$ is a Fourier transform of $u_a(\rho)$, and

$$q = 2k_p \sin \frac{\varphi}{2}.$$

The inverse transport relaxation time τ_{tr}^{-1} can be expressed by this cross section [5]

$$\tau_{tr}^{-1} = 2 \frac{v_F}{A} \int_0^\pi d\varphi \frac{d\sigma}{d\varphi} (1 - \cos \varphi), \quad (16)$$

where v_F is the two-dimensional Fermi velocity, A is the area of the sample, and the factor of 2 comes from the fact that electron may scatter “to the left” or “to the right” from its primary direction.

This is the general formula of our model. The very interesting fact is that relaxation times form discrete set of values, dependent on the quantum number m . It can be easily seen from the equations (6) and (9) because k is actually equal to k_F (three-dimensional Fermi vector) and is constant for a specific material. However, to obtain a quantitative results we have to make some further assumptions.

3. SCATTERING BY 2D SCREENED POTENTIAL

Assume the Coulomb screened potential in an usual form

$$u_a(\rho) = u_0 \frac{e^{-\lambda\rho}}{\rho},$$

where λ^{-1} is a screening length.

Its Fourier transform in two dimensions can be easily calculated

$$u_a(q) = \frac{2\pi u_0}{\sqrt{\lambda^2 + q^2}}.$$

The two-dimensional structure factor was calculated by Khan and Toan [6] up to $q = 6q_F$. For our purposes we need $S(q)$ only in the range from 0 to $2q_F$ and it can be approximated by a parabola $\alpha(q/q_F)^2$ in this range. Then τ_{tr}^{-1} is given by

$$\tau_{tr}^{-1} = \frac{m v_F}{2\pi k_p} \left(\frac{m_e}{2\pi \hbar^2} \right)^{2k_p} \int_0^{2k_p} \frac{dq}{k_p} \alpha \left(\frac{q}{k_p} \right)^2 \frac{4\pi^2 u_0^2 \left(\frac{q}{2k_p} \right)^2}{\lambda^2 + q^2} \frac{1}{\sqrt{1 - \left(\frac{q}{2k_p} \right)^2}}, \quad (17)$$

where n is the areal density of electrons, or if we come back to the angular variable φ

$$\tau_{tr}^{-1} = \frac{1}{(2\pi)^2} \frac{m_e}{\hbar^3} \alpha U_0^2 \int_0^\pi d\varphi \frac{\sin^4(\varphi/2)}{\left(\frac{\lambda}{2k_p} \right)^2 + \sin^2(\varphi/2)} \quad (18)$$

where we used the relation [7]

$$k_p = (2\pi n)^{1/2}$$

valid for 2D electron gas.

The dependence of τ_{tr}^{-1} on the quantum number m is hidden in k_p because of equations (6) and (9). After simple calculations we obtain

$$\left(\frac{\lambda}{2k_p}\right)^2 = \frac{1}{\pi} \frac{1}{k_F \alpha_0} \frac{1}{1 - \left(\frac{m\pi}{L_z k_F}\right)^2}, \quad (19)$$

where we made use of the relation [7]

$$\left(\frac{\lambda}{k_F}\right)^2 = \frac{4}{\pi} \frac{1}{k_F a_0},$$

a_0 being the Bohr radius.

Equation (19) provides us with a condition for the allowed values of m

$$\frac{m\pi}{L_z k_F} < 1. \quad (20)$$

The inequality (20) also defines a maximum value of m . It comes from equation (19) but is not related to the screening parameter λ . It only expresses the fact that the denominator on the right-hand side of the equation (19) should not be negative. Thus for a specific material (definite k_F) and a definite sample thickness L_z only a finite set of m is possible, hence the relaxation times are quantized.

4. NUMERICAL RESULTS

We have done numerical calculations for a very thin disordered film of cesium of variable thickness $L_z < 100 \times 10^{10}$ m. The Fermi vector for Cs was taken as $k_F 0.65 \times 10^{10}$ m⁻¹. It gives maximum value of m : $m_{\max} = 20$. The coefficient α in 2D structure factor we took equal to 0.28 after [6].

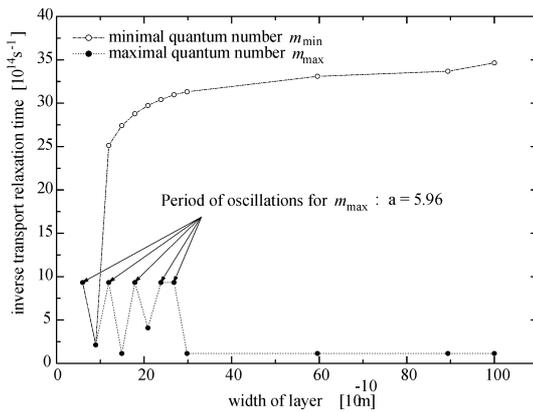


Fig. 1. The inverse transport relaxation time τ_{tr}^{-1} as a function of the width of layer L_z for minimum quantum number m_{\min} and maximum quantum numbers m_{\max}

We performed calculations only for minimum value of m (always equal to unity) and the maximum one (m_{\max}) for each value of L_z which corresponded to multiple of the atomic

diameter of Cs (5.96×10^{10} m). The results are given in Fig. 1. The relaxation times for minimal m are of the order of 10^{15} which is a reasonable value for disordered metals. The relaxation times for m_{\max} show interesting oscillations. They come from the inequality (20): m_{\max} can be the same for two neighboring but different L_z 's in case of very thin films and the respective integrals apparently differ from each other in this situation.

5. CONCLUSIONS

We obtained a general formula for the inverse transport relaxation time of electrons moving in a system of random potentials which has a finite width in one direction. A plausible realization of such system is a very thin film of disordered metal. Electrons which form the conduction band in such sample can be divided into a finite number of subbands. These subbands can be numbered by means of a quantum number m which describes electron states in a potential well of a width L_z . Each subband has its own transport relaxation time. Estimating the experimental conductivity of such sample needs taking into account all these subbands with appropriate weights. This is intended to be done in the next paper.

References

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