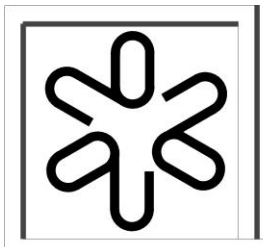

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ELECTRICAL CONDUCTIVITY OF VERY THIN METALLIC FILMS

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ELECTRICAL CONDUCTIVITY OF VERY THIN METALLIC FILMS

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Abstract.

This is a didactical paper written to graduate and postgraduate students of Physics and to researchers interested in electrical conductivity of nanometric metallic films.

1) Introduction.

In a preceding paper[1] we have show how to calculate the electrical and thermal conductivities of metallic bulks using the Boltzmann transport equation. With a similar formalism we will calculate the resistivity of very thin (nanometric) metallic films. Following the procedure adopted in our didactical articles, only a few references, books and papers, will be cited in this article.

We assume that the films are in a plane (x,y) with lengths L_x and L_y along the axes x and y, respectively, and thickness d along the z-axis. The thickness d is very small varying in the range $1\ nm \leq d \leq 20\ nm$. For these nanometric dimensions quantum size effects (QSE) play the main role[2-4] in the electronic conductivity. In this way a quantum mechanical approach is necessary to describe the conductivity.[2-4] The coordinates (x,y,z) origin is chosen in the middle point of the film, that is, $-L_x/2 \leq x \leq L_x/2$, $-L_y/2 \leq y \leq L_y/2$ and $-d/2 \leq z \leq d/2$. L_x and L_y are very large, that is, $L_x >> d$ and $L_y >> d$. As will be shown in what follows the electric resistivity is due to a bulk effect and to the roughness of the film surfaces. The height fluctuations of the film surfaces, located at the planes with $z = -d/2$ and $d/2$, will be indicated by $h(\boldsymbol{\rho})$ where $\boldsymbol{\rho} = x\,\boldsymbol{i} + y\,\boldsymbol{j}$, where $\boldsymbol{(i,j,k)}$ are the unit vectors along the axes (x.y,z), respectively.

Taking $L_x, L_y \rightarrow \infty$ and supposing that an applied electric field **E** is applied along the x-axis, that is, $\mathbf{E} = E\,\boldsymbol{i}$ the conducting electrons are represented by the wavefunctions

$$\varphi(x) = \exp(ik_x x)/\sqrt{L_x} \quad \text{and} \quad \varphi(y) = \exp(ik_y y)/\sqrt{L_y} \qquad (1.1),$$

respectively. These electrons have kinetic energies $\mathbf{p}^2/2m = (p_x^2 + p_y^2)/2m = \hbar^2\mathbf{k}^2/2m$, where $\mathbf{k}^2 = k_x^2 + k_y^2$. Due to the very small film thickness d the electronic states are quantized along the z-axis and are given by

$$\varphi_\nu(z) = (2/d)^{1/2}\cos(\nu\pi z/d) \qquad (1.2)$$

and their energies E_ν are given by

$$E_\nu = (\hbar^2/2m)(\nu\pi/d)^2 = \alpha\nu^2 \qquad (1.3),$$

where $\nu = 1,2,..,N$ and $\alpha = \hbar^2\pi^2/(2md^2)$. To obtain (1.1) and (1.2) it was assumed that the electrons are confined in a very large potential well V_o in the region $-d/2 \le z \le d/2$. The maximum energy E_ν is $E_N = (\hbar^2/2m)(N\pi/d)^2 = \varepsilon_F$ which is the Fermi energy given by $\varepsilon_F = 3^{2/3}\,\pi^{4/3}\,(\hbar^2/2m)(N/V)^{2/3}$. These quantum states ν are known as *Fermi subbands*.[2-4]

Thus, in our approach the free electrons in the film that are represented by the wavefunction

$$\Psi_{\mathbf{k}\nu}(x,y,z) = \varphi(x)\,\varphi(y)\,\varphi_\nu(z) = (1/\sqrt{L_x\,L_y})\exp(-\mathbf{k}\cdot\boldsymbol{\rho})\,\varphi_\nu(z) \qquad (1.4)$$

have energies $E_{\mathbf{k}\nu} = \hbar^2\mathbf{k}^2/2m + E_\nu$. Taking into account that $(\hbar^2/2m)(N\pi/d)^2 = E_N = \varepsilon_F$ we verify that the maximum ν value is

$$\nu_{max} = N = (3n/\pi)^{1/3}\,d \qquad (1.5).$$

Since the maximum value of the electronic energy is equal to the Fermi energy $\varepsilon_F = (h^2/2m)(3n/8\pi)^{2/3}$, the energies of the free electrons inside the film obey the following condition $\hbar^2\mathbf{k}^2/2m + E_\nu = \varepsilon_F$. In this way the maximum possible value for ν is given by the relation $(\hbar^2/2m)(N\pi/d)^2 = \hbar^2N^2/(2md^2) \approx \varepsilon_F$ and, consequently, $N \approx d\,(3n/\pi)^{1/3}$. The momentum $\mathbf{k}$ is sometimes written as $k_\nu = [(2m/\hbar^2)\,(\varepsilon_F - E_\nu)]^{1/2}$. The electronic mean free path will be indicated by ℓ.

At this point it would be interesting to present orders of magnitude of some relevant parameters for metallic thin films (Pt, Au, Cu,…):

$1\text{ nm} \le d \le 20\text{ nm}$,
$\Delta \sim 1\text{ nm}$, $n \sim 3\text{-}7\ 10^{28}/\text{cm}^3$,
$k_F = (3n\pi^2)^{1/3} \sim 10\text{ nm}^{-1}$,
$\lambda_F = 2\pi/k_F \sim 0.5\text{ nm}$
$\ell \sim 20\text{ nm}$.

For the Fermi subbands $\nu = 1,2,..,N$ we verify, using (1.5), that for $n \sim 5\ 10^{28}/\text{cm}^3$ and $d \sim 1.5$ nm we have $70 \ge N \ge 5$.

Quantum Size Effects" (QSE) become significant for thin metallic films conductivity when[2-4]

$$\begin{aligned} &\ell > d \\ &N \le 50 \\ &\lambda_F \ge \Delta \end{aligned} \qquad (1.6).$$

In the conditions (1.6) are satisfied to calculate the film conductivity it is necessary to modify the formalism adopted in Sections 2 and 3 of our preceding paper[1] introducing quantum effects that depend on the small thickness d and on the roughness of the film surfaces. The treatment for bulk metals shown in Sections 2 and 3 can be applied only for d > 20 nm.

The total resistivity $\rho(d)$ of a very thin film with thickness d is given by

$$\rho(d) = \rho_S(d) + \rho(\infty) = 1/\sigma_S(d) + \rho(\infty) \qquad (1.7),$$

where $\rho_S(d)$ and $\sigma_S(d)$ are, respectively, the surface resistivity and conductivity of the thin film and $\rho(\infty)$ the bulk conductor resistivity (or the resistivity of the film for $d \to \infty$). From the resistivity measurements we can determine the surface conductivity using (1.7):

$$\sigma_S(d) = 1/ [\rho(d) - \rho(\infty)] \qquad (1.8).$$

2) Quantum Calculation for the Surface Electrical Conductivity.

Taking into account the roughness of the film surfaces $h(\boldsymbol{\rho})$, where $\boldsymbol{\rho} = x\,\boldsymbol{i} + y\,\boldsymbol{j}$, the confinement potential of the electrons considered in Section 1 is now given by $V \approx V_o + U(\boldsymbol{\rho})$, where $U(\boldsymbol{\rho})$ is a perturbation due to $h(\boldsymbol{\rho})$. It can be estimated[2-4] using (1.3) taking $\nu = 1$:

$$U(\boldsymbol{\rho}) = \delta E \approx (\partial E/\partial d)\,\delta d = (\partial E/\partial d)\,h(\boldsymbol{\rho}) = -(\hbar^2\pi^2/md^3)\,h(\boldsymbol{\rho}) \qquad (2.1).$$

2.a) Surface Conductivity Without the Fermi Subbands.

Let us calculate, in a first approximation, the conductivity σ due to elastic electronic scattering generated by the surface roughness without taking into account the Fermi subbands. So, following the Boltzmann formalism developed in Section 2 of ref. 1 and that $\omega(\mathbf{p}' \to \mathbf{p}) = \omega(\mathbf{p} \to \mathbf{p}')$ we get,

$$\sum_{\mathbf{p}} \omega(\mathbf{p}' \to \mathbf{p})\, f(\mathbf{p}')\,[1 - f(\mathbf{p})] - \sum_{\mathbf{p}'} \omega(\mathbf{p} \to \mathbf{p}')\, f(\mathbf{p})\,[1 - f(\mathbf{p}')]$$

$$= \sum_{\mathbf{p}'} \omega(\mathbf{p} \to \mathbf{p}')\,[f(\mathbf{p}') - f(\mathbf{p})] \qquad (2.2).$$

Putting,

$$f(\mathbf{p}) = f_o(\varepsilon) + p_x\,\chi(\varepsilon) \quad \text{and} \quad f(\mathbf{p}') = f_o(\varepsilon) + p_x'\,\chi(\varepsilon) \qquad ,$$

we obtain

$$\sum_{\mathbf{p}'} \omega(\mathbf{p} \to \mathbf{p}')\,[p_x - p_x']\,\chi(\varepsilon) = W\,p_x\,\chi(\varepsilon) \qquad (2.3),$$

where $W = \sum_{\mathbf{p}'} \omega(\mathbf{p} \rightarrow \mathbf{p}')\,(1 - \cos\theta)$. So, we have,

$$-eE(\partial f/\partial p_x) + (p_x/m)(\partial f/\partial T)(\partial T/\partial x) = -W\, p_x\, \chi(\varepsilon) \qquad (2.4).$$

When there is no temperature gradient, that is, when $(\partial T/\partial x) = 0$ (2.4) can be easily solved giving

$$\chi(\varepsilon) = (eE/mW)(\partial f_o/\partial \varepsilon) \qquad (2.5).$$

Using (2.5) and taking into account that $\chi(\varepsilon) = eE(\ell/p)(\partial f_o/\partial \varepsilon)$ we get

$$W = p/m\ell = v/\ell \qquad (2.6).$$

As $(\partial T/\partial x) = 0$ we get (see ref.1),

$$J_x = e^2 E\, D^{(1)} \qquad (2.7).$$

Since $J_x = \sigma_x E$, $n = 2p_F^3/(3\pi^2\hbar^3)$ and putting (see ref.1) $D^{(1)} \approx [16\pi m/3(2\pi\hbar)^3]\,(\mu\ell)_{\varepsilon=\varepsilon F}$, $\mu_o = \varepsilon_F$, from (2.7) we obtain

$$\sigma_x = (e^2 n/m)(\ell/v)_{\varepsilon=\varepsilon F} = (e^2 n/m)\tau \qquad (2.8),$$

where $\tau = (\ell/v)_{\varepsilon=\varepsilon F}$ is the mean free time between collisions. As, according to (2.6), $(v/\ell)_{\varepsilon=\varepsilon F} = W(\varepsilon_F)$ we verify that the surface conductivity $\sigma_S = \sigma_x$, given by (2.8), can be written as

$$\sigma_S = (e^2 n/m) W(\varepsilon_F)^{-1} \qquad (2.9).$$

For very thin films it can be shown [4,5] that the electrical resistivity is created essentially to the surface roughness of the films. So, assuming that the bulk resistivity is negligible, the elastic electronic scattering $\mathbf{k} \rightarrow \mathbf{k}'$ due the surface roughness is described by[6]

$$\omega(\mathbf{k}' \rightarrow \mathbf{k}) = \omega(\mathbf{k} \rightarrow \mathbf{k}') = (2\pi/\hbar)\,|\langle \mathbf{k}\,|U(\boldsymbol{\rho})|\,\mathbf{k}'\rangle|^2\,\rho(k) \qquad (2.10),$$

where the surface roughness potential $U(\boldsymbol{\rho})$ is defined by (2.1), $\mathbf{k}$ for the 2-dim scattering is given by[6] $\mathbf{k} = k_x \boldsymbol{i} + k_y \boldsymbol{j}$, $k_x = (2\pi n_x/L_x)$, $k_y = (2\pi n_y/L_y)$, $\rho(k)dE_k = (L/2\pi)^2\, dk_x\, dk_y$ and $E_k = (\hbar^2 k^2/2m)$, taking $L_x = L_y = L$.

In these conditions $\rho(k)$ becomes

$$\rho(k) = (L/2\pi)^2\,(m/\hbar^2)\,d\theta \qquad (2.11).$$

Taking into account that $U(\boldsymbol{\rho}) = A\, h(\boldsymbol{\rho})$, where $A = -(\hbar^2\pi^2/md^3)$ we get

$$| < \mathbf{k} |U(\boldsymbol{\rho})| \mathbf{k}' >|^2 = A^2 | < k |h(\boldsymbol{\rho})|\mathbf{k}' > |^2 = A^2 |h_{\mathbf{k}\mathbf{k}'}|^2$$

where

$$|h_{\mathbf{k}\mathbf{k}'}|^2 = (1/L)^2 | \int d^2\boldsymbol{\rho}\, h(\boldsymbol{\rho}) \exp(i\mathbf{q}\,\boldsymbol{\rho}) |^2 \qquad (2.12),$$

with $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ and $q = |\mathbf{k} - \mathbf{k}'| = 2k \sin(\theta/2)$, taking into account that the resistivity effects are due essentially by elastic collisions, that is, $k' \approx k$. So, from (2.3),(2.10)-(2.12) we obtain

$$W(\varepsilon) = (\pi^3 \hbar/2md^6)\, \Phi(q) \qquad (2.13),$$

where $\Phi(q)$ is defined by

$$\Phi(q) = \int_o^{2\pi} |h_{\mathbf{k}\mathbf{k}'}|^2 (1-\cos\theta)\, d\theta \qquad (2.14).$$

Assuming that the energy ε of conducting electron is the Fermi energy, that is, $\varepsilon = \varepsilon_F$ and $q = q_F$ the surface conductivity $\sigma_S = \sigma_x = \sigma_E$ (along the E field), given by (2.9) becomes given by

$$\sigma_S = (e^2 n/m) W(\varepsilon_F)^{-1} = (2ne^2 d^6/\pi^3\, \hbar)\, \Phi(q_F)^{-1} \qquad (2.15).$$

For the particular case of the Gaussian model (see Appendix A) when the function $G(\rho)$ is given by $G(\rho/\xi) = \Delta^2 \exp(-\rho/\xi^2)$, where ξ is the "*surface correlation distance*" and Δ is the "*average surface roughness",* the function $\Phi(q_F)$ defined by (5.14) becomes (see Appendix A)

$$\Phi(q_F, \xi) = \int d^2\boldsymbol{\rho} \exp(i\mathbf{q}\cdot\boldsymbol{\rho})\, G(\rho/\xi) = \Delta^2 \int d^2\boldsymbol{\rho} \exp(i\mathbf{q}\cdot\boldsymbol{\rho}) \exp(-\rho/\xi^2) =$$

$$= (\xi\Delta)^2\, \pi \exp(-q^2\xi^2/4) \qquad (2.16).$$

Consequently, $W(\varepsilon_F)$ defined by (2.13) is written as

$$W(\varepsilon_F, \xi) = (\pi^4 \hbar/2md^6)\, (\xi\Delta)^2\, F_G(k_F\xi) \qquad (2.17),$$

where

$$F_G(k_F\xi) = \int_o^{2\pi} \exp[-k_F^2\xi^2 \sin 2(\theta/2)]\, (1-\cos\theta)\, d\theta$$

$$= 2 \exp(-k_F^2\xi^2/2)\, [I_o(k_F^2\xi^2/2) - I_1(k_F^2\xi^2/2)],$$

$I_o(z)$ and $I_1(z)$] are the modified Bessel functions of order 0 and 1.[7]

Thus, the surface conductivity $\sigma_S = \sigma_x = \sigma_E$, (2.9) becomes

$$\sigma_S(d) = (2ne^2 d^6/\pi^4\, \hbar\, \xi^2\Delta^2)\, F_G(k_F\xi)^{-1} \qquad (2.20).$$

For $k_F\xi << 1$, as $F_G(k_F\xi) \approx 2\pi$, (2.20) is given, simply, by[5]

$$\sigma_S(d) \approx (ne^2 d^6/\pi^5\, \hbar\, \xi^2\Delta^2) \qquad (2.21).$$

2.b) Surface Conductivity Considering the Fermi Subbands.

Now the calculation of the conductivity σ_x is improved taking into account the Fermi subbands ν. So, due to the surface roughness U(**ρ**) the electronic transitions are between the subbands $|\mathbf{k}\nu> \rightarrow |\mathbf{k}'\mu>$. Since the main contributions to the resistivity are due the elastic collisions it will assumed that $E_{\mathbf{k}\nu} = E_{\mathbf{k}'\mu}$, where $E_{\mathbf{k}\nu} = \hbar\mathbf{k}^2/2m + E_\nu$. The momentum k_ν is defined by $k_\nu^2 = (2m/\hbar^2)(\varepsilon_F - E_\nu)$. Rigorously, the momentum of the electron in the subband ν ought to be indicated by $\mathbf{k}_\nu$, but, sometimes, to simplify the notation it will be indicated simply by **k.**

The electric current density J_E along **E** due to the ν subbands contributions is given by[2]

$$J_E = -2e \sum_\nu \int d^2\mathbf{k}\, (L/2\pi\hbar)^2\, (\mathbf{E}\cdot\mathbf{k})\, f_\nu(\mathbf{k})\, (1/L^2 d) \qquad (2.22),$$

where $f_\nu(\mathbf{k})$ is the Fermi distribution for the subband ν and remembering that the film volume is $L^2 d$. It can be shown[2] that for elastic collisions between the subbands we have:

$$-(e\hbar/m)\, \mathbf{k}\cdot\mathbf{E}\, (\partial f_\nu/\partial\varepsilon) = (2\pi/\hbar) \sum_{\mu\mathbf{k}'} |<\mathbf{k}\nu|\, U(\boldsymbol{\rho})|\, \mathbf{k}'\mu>|^2\, \delta(E_{\mathbf{k}\nu} - E_{\mathbf{k}'\mu})$$

$$\times\, [f_\nu(\mathbf{k}_\nu) - f_\mu(\mathbf{k}_\mu')] \qquad (2.23).$$

where $k_{\mu\nu} = |\mathbf{k}_\mu - \mathbf{k}_\nu| = (\mathbf{k}_\mu^2 + \mathbf{k}_\nu^2 - 2\, \mathbf{k}_\mu\, \mathbf{k}_\nu \cos\theta)^{1/2}$.

Due to the coupling between the functions $f_\nu(\mathbf{k})$ in the system of differential equations (2.23) the exact determination of these functions is very complicated, long and tedious.[8,9] An approximate and simple way to solve (2.23) decoupling these equations is assuming that $f_\mu(\mathbf{k}') \approx f_\nu(\mathbf{k}')$. In this way, we can write, similarly to in ref.1,

$$f_\nu(\mathbf{k}_\nu) - f_\mu(\mathbf{k}_\mu') \approx f_\nu(\mathbf{k}_\nu) - f_\nu(\mathbf{k}_\nu') \approx \chi_\nu(\varepsilon)\, [k_{\nu x} - k'_{\nu x}] \qquad (2.24).$$

Since $k'_{\nu x} \approx k_{\nu x} \cos\theta$ (2.24) becomes

$$f_\nu(\mathbf{k}_\nu) - f_\mu(\mathbf{k}_\mu') \approx \chi_\nu(\varepsilon)\, k_{\nu x}\, (1-\cos\theta) \qquad (2.25).$$

Consequently, the Boltzmann equations without coupling between the subbands become given by,(putting to simplify the notation, $k_\nu = k$)

$$-e\,\hbar\, E\, (\partial f_\nu(\mathbf{k})/\partial k_x) \approx \sum_{\mu\mathbf{k}'} \omega(\mathbf{k}\nu \rightarrow \mathbf{k}'\mu)\, [f_\nu(\mathbf{k}) - f_\nu(\mathbf{k}')] =$$

$$= \sum_{\mu\mathbf{k}'} \omega(\mathbf{k}\nu \rightarrow \mathbf{k}'\mu)\, \chi_\nu(\varepsilon)\, k_{\nu x}\, (1-\cos\theta) \qquad (2.26),$$

where

$$\omega(\mathbf{k}\nu \rightarrow \mathbf{k}'\mu) = (2\pi/\hbar)\ |< \mathbf{k}\nu\ |U(\boldsymbol{\rho})|\ \mathbf{k}'\mu>|^2\ \Omega(E_{\mathbf{k}'\mu}),$$

where $\Omega(E_{\mathbf{k}'\mu})$ is the density of final states $|\mathbf{k}'\mu >$ given by (see (2.11)) $\Omega(E_{\mathbf{k}'\mu}) = (L/2\pi)\ (m/\hbar^2)\ d\theta$, $k_x = k'$ and $k'_x = k'\cos\theta = k_x \cos\theta$. It is important to note that in (2.26) the reference x-axis ("internal reference system" used to calculate the matrix element) is taken along the incident momentum **k**. So, the scattering angle θ is the angle between **k** and **k´**. It has nothing to do with the angle between **k** and **E,** that will be defined by α given by $\mathbf{E}\cdot\mathbf{k} = E\ k \cos\alpha$. In this case the **E** direction will be taken as reference direction to calculate the integral (2.22) $\int d^2\mathbf{k}\ (\mathbf{E}\cdot\mathbf{k})$…

From (5.26), following the same procedure adopted to get (2.3) we obtain

$$\chi_\nu(\varepsilon) = (eE/mW_\nu)\ (\partial f_{o\nu}/\partial\varepsilon) \qquad (2.27),$$

where W_ν is given by

$$W_\nu = (2\pi/\hbar)\ \Sigma_{\mu\mathbf{k}'}\ |<\mathbf{k}\nu\ |\ U(\boldsymbol{\rho})|\ \mathbf{k}'\mu >|^2\ \Omega(k_{\mu\nu})\ (1-\cos\theta)$$

$$= \Sigma_{\mu\mathbf{k}'}\ \omega(\mathbf{k}\nu \rightarrow \mathbf{k}'\mu)\ (1-\cos\theta) \qquad (2.28),$$

where $k_{\mu\nu} = q_{\mu\nu} = |\ \mathbf{k}_\mu - \mathbf{k}_\nu| = (\mathbf{k}_\mu^{\,2} + \mathbf{k}_\nu^{\,2} - 2\ \mathbf{k}_\mu\ \mathbf{k}_\nu \cos\theta)^{1/2}$.

Following a similar procedure used in Section (2.a) we can show that

$$\Sigma_{\mathbf{k}'}\omega(\mathbf{k}\nu \rightarrow \mathbf{k}'\mu)\ (1-\cos\theta) = (\pi^3\hbar/2md^6)\ \mu^2\nu^2 \int_o^{2\pi} |h_{\mathbf{k}\mathbf{k}'}|^2\ (1-\cos\theta)\ d\theta \qquad (2.29),$$

where $|h_{\mathbf{k}\mathbf{k}'}|^2 = \int d^2\boldsymbol{\rho}\ \exp(i\mathbf{q}_{\mu\nu}\cdot\boldsymbol{\rho})\ h(\boldsymbol{\rho})$. Defining $\Phi(q_{\mu\nu})$ by

$$\Phi(q_{\mu\nu}) = \int_o^{2\pi} |h_{\mathbf{k}\mathbf{k}'}|^2\ (1-\cos\theta)\ d\theta \qquad (2.30)$$

we see that W_ν given by (2.28) is written as

$$W_\nu = 1/\tau_x = (\pi^3\hbar/2md^6)\ \nu^2\ \Sigma_\mu\ \mu^2\ \Phi(q_{\mu\nu}) \qquad (2.31).$$

Taking into account (2.27)-(2.30) the conductivity J_E along the **E** field, defined by (2.22) becomes written as:

$$J_E \approx -(2e^2/m^2(2\pi\hbar)^2 d)\ \Sigma_\nu \int d^2\mathbf{p}\ (\mathbf{E}\cdot\mathbf{p}_\nu)^2/W_\nu)\ (\partial f_{o\nu}/\partial\varepsilon)$$

$$= -(e^2\hbar^2/2m^2\pi^2 d)\ \Sigma_\nu \int d^2\mathbf{k}\ (\mathbf{E}\cdot\mathbf{k}_\nu)^2/W_\nu)\ (\partial f_{o\nu}/\partial\varepsilon) \qquad (2.32).$$

Substituting (2.31) in (2.32) and remembering that $\sigma_S = \sigma_E = J_E/E$ we obtain the general expression for the surface conductivity σ_S:

$$\sigma_S(d) = (e^2\hbar d^5/m\pi^5) \sum_\nu \{\int d^2\mathbf{k}\, \mathbf{k}_{\nu x}^2 (\partial f_{o\nu}/\partial\varepsilon)/[\nu^2 \sum_\mu \mu^2 \Phi(q_{\mu\nu})]\} \qquad (2.33),$$

taking **E** as a reference direction, the x-axis, for instance, we have $\mathbf{E}\cdot\mathbf{k}_\nu = Ek_{\nu x} = Ek_\nu \cos\alpha$ and $d^2\mathbf{k} = k\, dk\, d\alpha$.

3) Limiting Cases of Physical Interest.

The calculation of the surface conductivity (2.33) can be simplified in special cases of physical interest for metals like, for instance, Pt, Au, Al and Cu. Since for these metals the main scattering contributions are due to electrons with $k \approx k' \approx k_F$ we can put (see (2.28))

$$k_{\mu\nu} = q_{\mu\nu} = |\mathbf{k}_\mu - \mathbf{k}_\nu| = q_F \approx 2k_F \sin(\theta/2) \qquad (3.1).$$

As $\varepsilon = \hbar^2\mathbf{k}^2/2m$, $k_x^2 = k^2\cos^2\alpha$ and taking into account that at $\varepsilon = \varepsilon_F$ we have $(\partial f_{o\nu}/\partial\varepsilon)_{\varepsilon F} = -\delta[\varepsilon - (\varepsilon_F - E_\nu)]$ the current J_x defined by (2.32) becomes

$$J_E = (e^2E\hbar^2/2m^2\pi^2 d)\,(\sum_\nu \int k^3\, dk \int_o^{2\pi} d\alpha \cos^2\alpha\,)/W_\nu)\delta[\varepsilon - (\varepsilon_F - E_\nu)],$$

that is,

$$J_E = (e^2E/2\pi md) \sum_\nu (k_\nu^2/W_\nu) \qquad (3.2),$$

where $k_\nu^2 = (2m/\hbar)(\varepsilon_F - E_\nu)$ and W_ν is defined by (2.28).Taking into account that the function W_ν is given by (see Appendix B)

$$W_\nu(q_F) = (\pi^3\hbar\nu^2/2d^6)\, \Phi(q_F)\, (\sum_0^N \mu^2) \qquad (3.3),$$

where

$$\Phi(q_F) = \int_0^{2\pi} d\theta\, (1 - \cos\theta)\, |h_{kk'}|^2$$

and

$$h_{kk'} = (1/L) \int d^2\boldsymbol{\rho}\, h(\boldsymbol{\rho}) \exp(i\mathbf{q}_F\, \boldsymbol{\rho}),$$

where $h(\boldsymbol{\rho}) = h(x,y)$ are the height fluctuations of the film surfaces at the points (x,y), according to Section 1.

Taking into account that $\sum_0^N \mu^2 = N(N+1)(2N+1)/6$ and that $\sigma = J/E$ the electric conductivity σ_S due to surface effects, using (3.2), is given by

$$\sigma_S(d) = (e^2/\hbar)[d^5/\pi^4\, \Phi(q_F)]\, [6/\, N(N+1)(2N+1)]\, \sum_{\nu=1}^N (k_\nu^2/\nu^2) \qquad (3.4),$$

which is a result similar to that found by Fishman and Calecki[9]

Eq.(3.4) was used to analyze the surface resistivity of very thin films measured[10] at the Laboratory of Thin Films (LFF) of the Department of Applied Physics (FAP) of the Institute of Physics (IFUSP) of the University of São Paulo.

The function $\Phi(q_F)$ depends on the model assumed to explain the surface roughness as is seen in our preceding papers.[10] In Appendix A it is shown how this function can be calculated taking into account the "*roughness correlation function*". Assuming the "Gaussian model" to calculate $\Phi(q_F)$ we get (see 2.16 and 2.17) $\Phi(q_F,\xi). = (\xi\Delta)^2\, F_G(k_F\xi)$ where $F_G(k_F\xi)= 2\exp(-k_F^2\xi^2/2)\,[I_o(k_F^2\xi^2/2) - I_1(k_F^2\xi^2/2)]$. For $k_F\xi << 1$ we verify that $\Phi(q_F,\xi). = (\xi\Delta)^2\pi$. In these conditions we verify that our prediction (3.4) for $\sigma_S(d)$ is exactly the same one obtained by Fishman and Calecki.[9]

Appendix A. Roughness Autocorrelation Function.

Let us calculate the function $\Phi(q)$ defined by (2.14) using the "*surface correlation function*" method:

$$\Phi(q) = \int_o^{2\pi} |h_{\mathbf{kk'}}|^2(1-\cos\theta)\, d\theta \qquad (A.1),$$

where

$$|h_{\mathbf{kk'}}|^2 = (1/L)^2\, |\int d^2\boldsymbol{\rho}\; h(\boldsymbol{\rho}) \exp(i\mathbf{q}\,\boldsymbol{\rho})\,|^2, \qquad (A.2),$$

and $\mathbf{q} = \mathbf{k} - \mathbf{k'}$.

In order to be didactical let us first calculate $|\langle \mathbf{k}\,|h(\boldsymbol{\rho})|\,\mathbf{k'}\rangle|^2$ for the 1-dim case

$$|\langle \mathbf{k}\,|h(x)|\,\mathbf{k'}\rangle|^2 = (1/L^2)\,(\int dx \exp(-ikx)h(x)\exp(ik'x))$$

$$x\,(\int dy \exp(-iky)h(y)\exp(ik'y)).$$

Putting $y = x + \lambda$ we get

$$|\langle \mathbf{k}\,|h(x)|\,\mathbf{k'}\rangle|^2 = (1/L)^2 \int dx \int d\lambda \exp(-ik\lambda)\, h(x)h(h+\lambda)\exp(ik'\lambda)$$

$$= (1^2/L)\,\{\int d\lambda \langle h(x)\, h(x+\lambda)\rangle \exp[i(k'-k)\lambda]\},$$

where

$$\langle h(x)\, h(x+\lambda)\rangle \equiv (1/L)\int dx\, h(x)\, h(x+\lambda)$$

is called "*height correlation function*".[4]

Similarly, for the 2-dim case, taking $\boldsymbol{\rho} = x\,\boldsymbol{i} + y\,\boldsymbol{j}$,

$$h_{\mathbf{kk'}} = \langle \mathbf{k'}|h(\boldsymbol{\rho})|\,\mathbf{k}\rangle = (1/L)\int d^2\boldsymbol{\rho}\; h(\boldsymbol{\rho})\exp(i\mathbf{q}\,\boldsymbol{\rho}),$$

we have

$$|h_{\mathbf{kk'}}|^2 = (1/L)^2 \int d^2\mathbf{X} \exp(-i\mathbf{q}\,\mathbf{X})\, h(\mathbf{X}) \int d^2\mathbf{Y} \exp(i\mathbf{q}\,\mathbf{Y})\, h(\mathbf{Y}). \quad (A.3).$$

Putting $\mathbf{Y} = \mathbf{X} + \boldsymbol{\rho}$ we get

$$|h_{\mathbf{k}\mathbf{k}'}|^2 = (1/L)^2 \int d^2\boldsymbol{\rho} \int d^2\mathbf{X} \exp(i\mathbf{q}\,\boldsymbol{\rho})\, h(\mathbf{X})\, h(\mathbf{X}+\boldsymbol{\rho}) =$$

$$= \int d^2\boldsymbol{\rho} \exp(i\mathbf{q}\,\boldsymbol{\rho}) < h(\mathbf{X})\, h(\mathbf{X}+\boldsymbol{\rho}) > \qquad (A.4),$$

where $< h(\mathbf{X})\, h(\mathbf{X}+\boldsymbol{\rho}) >$ defined by

$$G(\rho) = < h(\mathbf{X})\, h(\mathbf{X}+\boldsymbol{\rho}) > = (1/L)^2 \int d^2\mathbf{X}\, h(\mathbf{X})\, h(\mathbf{X}+\boldsymbol{\rho}) \qquad (A.5),$$

is the "*height autocorrelation function*".[4]

In this context $|h_{\mathbf{k}\mathbf{k}'}|^2$ given by (A.4) becomes written as

$$|h_{\mathbf{k}\mathbf{k}'}|^2 = (1/L)^2 \int d^2\boldsymbol{\rho} \int d^2\mathbf{X} \exp(i\mathbf{q}\,\boldsymbol{\rho})\, h(\mathbf{X})\, h(\mathbf{X}+\boldsymbol{\rho}) = \int d^2\boldsymbol{\rho} \exp(i\mathbf{q}\,\boldsymbol{\rho})\, G(\rho) \quad (A.6)$$

Several models have been proposed[4] to estimate $G(\rho)$. We can mention, for instance, two models, *Gaussian* and *Exponential*:

(1) Gaussian $\rightarrow$ $G(\rho/\xi) = \Delta^2 \exp(-\rho/\xi^2)$ (A.6)
(2) Exponential $\rightarrow$ $G(\rho/\xi) = \Delta^2 \exp(-\rho/\xi)$ (A.7),

where ξ is the "*surface correlation distance*" and Δ is the "*average surface roughness"*.

Appendix B. Calculation of the Function W_ν.

Let us calculate the function W_ν defined by (2.28):

$$W_\nu = \sum_{\mu\mathbf{k}'} \omega(\mathbf{k}\nu \rightarrow \mathbf{k}'\mu)\,(1-\cos\theta), \qquad (B.1),$$

where

$$\omega(\mathbf{k}\nu \rightarrow \mathbf{k}'\mu) = (2\pi/\hbar) \sum_{\mu\mathbf{k}'} | < \mathbf{k}\nu\, |U(\boldsymbol{\rho})|\, \mathbf{k}'\mu > |^2\, \Omega(k_{\mu\nu}),$$

$\mathbf{k}_\nu$ and $\mathbf{k}'_\mu$ are written simply as $\mathbf{k}$ and $\mathbf{k}'$, respectively,

$$U(\boldsymbol{\rho}) = -(\hbar^2\pi^2/md^3)\, s^2 h(\boldsymbol{\rho}) = -As^2 h(\boldsymbol{\rho}),\ (\ s = \mu \text{ or } \nu),$$

and $\quad |\mathbf{k} > = (1/L)\exp(i\mathbf{k}\,\boldsymbol{\rho}),\ k_x = k',\ k'_x = k'\cos\theta = k_x\cos\theta.$

To calculate $\omega(\mathbf{k}\nu \rightarrow \mathbf{k}'\mu)$ let us take the x-axis along the $\mathbf{k}$ direction of the incident electron as a reference direction. So, $\mathbf{i}\cdot\mathbf{k} = k_x = k\cos\theta$ and $d^2\mathbf{k} = k\,dk\,d\theta$. So, the density of final states $\Omega(E_{\mathbf{k}'\mu})$ is given by (see (2.11)),

$$\Omega(E_{\mathbf{k}'\mu}) = (L/2\pi)\,(m/\hbar^2)\,d\theta$$

and

$$k_{\mu\nu} = q_{\mu\nu} = |\mathbf{k}_\mu - \mathbf{k}_\nu| = (\mathbf{k}_\mu^2 + \mathbf{k}_\nu^2 - 2\,\mathbf{k}_\mu\,\mathbf{k}_\nu \cos\theta)^{1/2}\,.$$

Assuming that, according to section 3, that $k \approx k' \approx k_F$ we can put

$$k_{\mu\nu} = q_{\mu\nu} = |\mathbf{k}_\mu - \mathbf{k}_\nu| = q \approx 2k_F \sin(\theta/2).$$

In this way (B.1) becomes

$$W_\nu = (\pi^3 \hbar v^2/2d^6)\, \Phi(q)\, (\textstyle\sum_0^N \mu^2) \qquad \text{(B.2)},$$

where

$$\Phi(q) = \textstyle\int_o^{2\pi} |h_{\mathbf{k}\mathbf{k}'}|^2 (1-\cos\theta)\, d\theta,$$

$$h_{\mathbf{k}\mathbf{k}'} = (1/L)\textstyle\int d^2\boldsymbol{\rho}\, \exp(i\mathbf{q}\,\boldsymbol{\rho})\, h(\boldsymbol{\rho}) \qquad \text{and} \qquad \mathbf{q} = \mathbf{k'} - \mathbf{k}.$$

REFERENCES

1)M.Cattani. "Boltzmann Equation and the Electrical and Thermal Conductivities of Metallic Bulks". http://publica-sbi.if.usp.br/PDFs/pd1671.pdf (09maio12).

2) T. Ando, A.B. Fowler and F. Stern. Rev. Mod. Phys. 54, 437 (1982); G.Fisher and H.Hoffmann. Z.Physik 39,287(1980). Z.Tesanovic and M.V.Jaric Phys.Rev.Lett.57,2760(1986); H.Sasaki, T.Noda, K.Hirakawa, M.Tanaka and T.Matsusue. Appl. Phys. Lett. 51,1974 (1987);

3) J.M.Ziman. "Electrons and Phonons". Oxford Univ.Press (1960).

4) R.E.Prange and Tsu-Wei Nee. Phys.Rev.168,779 (1968).

5) H. Sasaki, T. Noda, K. Hirakawa, M. Tanaka and T.Matsusue. Appl. Phys. Lett. 51, 1934 (1987).

6) L.I.Schiff. "Quantum Mechanics", McGraw-Hill (1965).

7) J.M.F.Bassalo and M.Cattani. "Elementos de Física Matemática" vol.1. Editora Livraria da Física, São Paulo (2010).

8) E.D.Siggia and P.C. Kwok, Phys.Rev.B2 1024 (1970).

9) G.Fishman and D.Calecki Phys.Rev.Lett.62,1032 (1989); Phys.Rev. B43, 11581(1991).

10) M.Cattani, M.C.Salvadori, F.S.Teixeira and R.S.Wiederkehr. Surf. Rev. Lett.14, 345 (2007).