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Theory of electrical transport and scattering at a metal–metal interface

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Abstract. The Schrödinger equation for an electron near a randomly rough metal–metal (or metal–vacuum) interface is approximately solved. The wavefunction and probability currents are averaged over all realisations of the interface characterised by its root-mean-square departure from flatness and the extent of its lateral correlation, and the results are used to set up simple boundary conditions for the Boltzmann transport equation. These are in the form of angle-dependent transmission and reflection coefficients, generalising Fuchs' reflectivity parameter, but given as explicit functions of observable properties of the interface. These results are further applied to the calculation of the electrical conductivity of thin films and foils, and of double-layer metallic films.

1. Introduction

Most quantitative treatments of surface and size effects in the transport properties of solids have been based on semiclassical methods in which the Boltzmann equation is solved in conjunction with Fuchs' (1938) boundary conditions (Sondheimer 1952, Chambers 1969). These conditions assert that in each surface a fixed fraction p ($0 \leq p \leq 1$) of the incident electrons are reflected specularly, while the rest are scattered into the equilibrium distribution function.

Formerly, this *specularity* parameter p was taken to be a phenomenological quantity, which could be varied freely in order to fit the theory to the experiments. As the accuracy of the data improved, however, it has become increasingly apparent that the physical nature of the surface scattering should be considered more seriously. Parrot (1965), for instance, has found that size effects in Bi could be explained only by supposing that p is strongly dependent on the angle of incidence θ ; it can be taken that $p = 0$ for $\theta < \theta_c$ and $p = 1$ for $\theta_c < \theta < \pi/2$, where θ_c is a certain cut-off angle. Brändli and Cotti (1965) used a specularly of the same form in a study of eddy current resistance of thin films.

Ziman (1960) calculated the quantum-mechanical scattering of conduction electrons by the asperities of the surface of the sample. As the detailed distribution of these asperities is in general unknown, Ziman characterised them by statistical parameters, supposing that the departure of the actual surface from flatness and the surface auto-correlation function were both Gaussian. From the angular spectrum of the reflected wave, Ziman extracted a formula for the specularity p as a function of these parameters. Soffer (1967, 1970) generalised Ziman's calculation by considering angles of incidence

other than normal and by thoroughly enforcing the law of conservation of the number of particles. A calculation of similar scope was performed by Falkovsky (1970a, b, 1980), who solved the Boltzmann equation approximately in the presence of a surface composed of random flat sections of known average characteristics.

Greene (1966a, b) investigated the scattering properties of surfaces with roughness smaller in extent than the electron wavelength, and derived boundary conditions significantly different than those of Fuchs. Greene's conditions were expressed in terms of another parameter, different from the specularity p , called the *kinetic specularity*, and which is always smaller than the former. Indeed, in the calculation of Greene and O'Donnell (1966) of the scattering of electrons by random surface charges in semiconductors, the kinetic specularity shows a very strong angular dependence, while p is practically a constant.

These conclusions were somewhat marred because Greene made an incorrect usage of the Pauli principle. Nevertheless, Greene's ideas have recently been corrected and extended, and a number of so-called boundary conditions in integral form have been obtained (Okulov and Ustinov 1979).

For a number of years, Soffer's boundary conditions were considered to be the best available. They have been applied, for instance, to the calculation of the electrical conductivity of thin films and wires (Sambles *et al* 1982b), of thermoelectric effects in thin films (Sambles and Priest 1984), etc. It has been found that, in contrast to theories based on Fuchs' conditions, calculations using Soffer's specularity do not require unphysical assumptions to give satisfactory agreement with experiments (Sambles and Elsom 1980, 1985, Sambles and Preist 1982, Stesmans 1982, 1983, Sambles *et al* 1981, 1982a, Sambles and Mundy 1983).

Recently I have obtained another, closed-form expression for a specularity p depending on angle, generalising Soffer's formula, and applied it to the calculation of transport properties of thin films and wires (Moraga 1987, 1988). These results will be discussed further in the following.

All these considerations apply to the scattering of electrons by a solid-vacuum interface. However, it is clear that the effects on the conduction electrons due to the scattering at the interface between two solids is of comparable importance. For instance, there is a considerable amount of experimental research on the influence of thin metallic overlayers on the electrical conductivity of various metals (Lucas 1964, 1968, 1971, Chopra and Randlett 1967, Berman and Juretschke 1971). Further, recently it has become possible to manufacture artificial metallic superlattices in the form of multilayer films (Schuller 1980, Falco *et al* 1985). Earlier theoretical treatments of the transport properties of these materials had to proceed under the unlikely assumption that there was no scattering at the boundary between the metals. An improved theoretical model for the electrical conductivity of multilayer films was proposed by Carcia and Suna (1983), who introduced a phenomenological probability t of coherent passage across each interface. Recently, Dimmich (1985) noted that, due to the difference in electron wavelengths of the two metals, the probability t_{AB} of passage from metal A to metal B ought to be different from the probability t_{BA} of transit in the opposite direction, and obtained a solution of the Boltzmann transport equation appropriate for this case.

These theories underestimate, however, the resistivity of a multilayer system, because the boundary conditions at each interface are erroneously prescribed. Thus, as will be demonstrated in the detailed calculations given below, it becomes necessary to introduce further probabilities r_{AA} and r_{BB} of *coherent reflection* at the interface between metals A and B, in direct analogy with Fuchs' specularity p . Clearly in this case

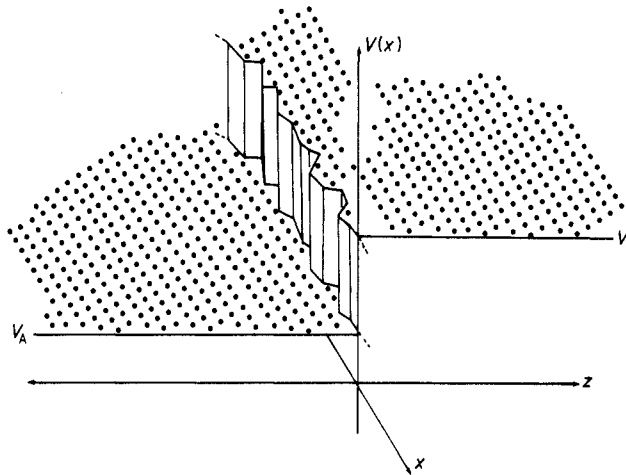


Figure 1. The interface between metals A and B is modelled by a potential step equal to V_A for $z < \zeta$ and V_B for $z > \zeta$, where ζ (the departure of the surface from flatness) is a random function of x, y .

$t_{AB} + r_{AA} < 1$, since it is always possible that the scattering of each electron by the interface will not only preclude its passage to the adjoining metal, but can also remove it from the out-of-balance distribution and thus from the entire transport process.

The purpose of this paper is to calculate, in closed form and in terms of observable properties of the interface, these probabilities of coherent reflection and passage. It will be seen that: (i) they are proportional to the corresponding quantum-mechanical reflection and transmission coefficients, and to the exponential of a function depending on the root-mean-square (RMS) amplitude of the surface asperities, and on its lateral correlation length; (ii) they are strongly dependent on the angle of incidence, so that in practice both the coherent passage and the specular reflection are generally suppressed except for the case of glancing electrons; and (iii) in the case of a metal-vacuum interface the probability r reduces to the specularity p calculated previously (which in the appropriate limit further reduce to the earlier result of Soffer), while in this case t clearly vanishes.

This paper also contains two applications of these new boundary conditions. First, I calculate the electrical resistivity of thin aluminium films and foils as a function of temperature, and compare the results with the measurements of Sambles *et al* (1981), which are perhaps the best available at present. Furthermore, the conductivity of a double-layer metal film is calculated and contrasted with experimental results of Lucas (1968).

2. The wavefunction of an electron in the vicinity of a randomly rough surface

In this section I shall calculate the wavefunction of a conduction electron traversing a system composed of two metals joined on an irregular surface. These metals, to be called A and B (see figures 1 and 2), fill the half-spaces $z < \zeta(x, y)$ and $z > \zeta(x, y)$ respectively,

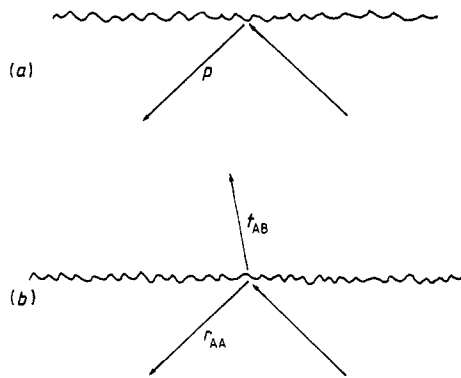


Figure 2. (a) In a metal–vacuum interface p is the fraction of electrons that are reflected specularly. (b) In a metal–metal interface, r_{AA} is the fraction of electrons coming from metal A that are reflected specularly back into A, and t_{BA} is the fraction passing from B to A along the classical trajectory.

where the *profile function* ζ specifies the departure of the actual from the average (or ideal) surface, which we take here to be the x, y plane.

As we intend to develop boundary conditions to be used in ordinary applications of the Boltzmann transport equation, the physical nature of the interface will be simplified as much as possible. Thus, we shall neglect the detailed contributions of the periodic ionic potentials of each metal and the effects of the impurities, and shall represent them by an average that has constant values V_A and V_B at each side of the surface with imaginary parts equal to $\hbar/2\tau_A$ and $\hbar/2\tau_B$, where τ_A and τ_B are the respective relaxation times. Further, the actual band structure of the bulk metals will be replaced by simple parabolic-type bands.

Some of these simplifications are not essential and can be relaxed if necessary. The quantum-mechanical problem of calculating the transmission and reflection coefficients of such a system will be solved here, however, without further assumptions by means of the so-called smoothing method (Keller 1962, Watson and Keller 1984, Brown 1984). In order to have explicit formulae for the resulting transmission and reflection coefficients, a number of approximations of a mathematical nature will be introduced at the end of the calculations. These, of course, are not of a fundamental character. On the other hand, I believe that no solution of this problem has a physical meaning except a statistical treatment based on averaged properties of the rough surface. The process of averaging will introduce difficulties of another kind, which will be discussed at that point.

In these circumstances, the wavefunction $\psi(x)$ is everywhere determined by its values at the interface, i.e.

$$\psi(x)\delta_{x,A} = \psi_A(x) + \lambda \int d^2X_b [\psi(x_b)D_1G_A(x_b, x) - G_A(x_b, x)D\psi(x_b)] \quad (1)$$

and

$$\psi(x)\delta_{x,B} = \lambda \int d^2X_b [-\psi(x_b)D_1G_B(x_b, x) + G_B(x_b, x)D\psi(x_b)] \quad (2)$$

where $X = xe_x + ye_y$ denotes the component of $x = X + ze_z$ parallel to the plane of the

average surface; $\lambda = \hbar^2/2m$; the symbol $\delta_{x,A}$ is equal to 1 if the point x lies in metal A and is 0 otherwise (and similarly for $\delta_{x,B}$); ψ_A is a source function of arbitrary strength

$$\psi_A(x) = \int \frac{d^2K}{(2\pi)^2} A_K \exp[i(\mathbf{K} \cdot \mathbf{X} - \gamma_K z)] \tag{3}$$

G_a ($a = A, B$) denotes the electron Green function in each (unbounded) metal, which in the simple model employed here is given by

$$G_a(x, x') = - \int \frac{d^2K}{(2\pi)^2} (2\lambda\gamma_K^a)^{-1} \exp\{i[\mathbf{K} \cdot (\mathbf{X} - \mathbf{X}') - \gamma_K^a |z - z'|]\} \tag{4}$$

$D\psi(x_b)$ is, except for a scale factor, the normal derivative of ψ evaluated at the surface $x_b = \mathbf{X} + \zeta(\mathbf{X})\mathbf{e}_x$, viz.

$$D\psi(x_b) = \left(- \frac{\partial \zeta(\mathbf{X})}{\partial x} \frac{\partial}{\partial x} - \frac{\partial \zeta(\mathbf{X})}{\partial y} \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \right) \psi(x) \Big|_{x=x_b} \tag{5}$$

and $D_1G_a(x, x')$ denotes the same derivative applied to the first argument of the Green function.

In these formulae $\mathbf{K} = k_x\mathbf{e}_x + k_y\mathbf{e}_y$ is a two-dimensional vector parallel to the $z = 0$ plane; and γ_K^a denotes the function

$$\gamma_K^a = \begin{cases} [K^2 + (-E_F + V_a)/\lambda]^{1/2} & \text{if } \lambda K^2 > E_F - V_a \\ -i[(E_F - V_a)/\lambda - K^2]^{1/2} & \text{otherwise} \end{cases} \tag{6}$$

where $a = A, B$ and E_F denotes the Fermi energy common to the two metals in contact.

The two unknowns in (1) and (2) are $\psi(x_b)$ and $D\psi(x_b)$. These will be approximately determined by means of an asymptotic condition. Let us first make $z \gg \delta$ in (1) and $z \ll \delta$ in (2), where δ is the RMS amplitude of the surface asperities. We have that

$$0 = 2\gamma_K^A A_K + \int d^2Y \int \frac{d^2R}{(2\pi)^2} \exp[i(\mathbf{R} - \mathbf{K}) \cdot \mathbf{Y} + \gamma_K^A \zeta_Y] \\ \times \{ - [i(\mathbf{K} + \mathbf{R})\nabla\zeta_Y + \gamma_K^A] \psi_R(\zeta_Y) + \psi'_R(\zeta_Y) \} \tag{7}$$

and

$$0 = \int d^2Y \int \frac{d^2R}{(2\pi)^2} \exp[i(\mathbf{R} - \mathbf{K}) \cdot \mathbf{Y} - \gamma_K^B \zeta_Y] \\ \times \{ [i(\mathbf{K} + \mathbf{R})\nabla\zeta_Y - \gamma_K^B] \psi_R(\zeta_Y) - \psi'_R(\zeta_Y) \} \tag{8}$$

where we have denoted the profile function simply by ζ_Y , and have put

$$\psi(x) = \int \frac{d^2K}{(2\pi)^2} e^{i\mathbf{K} \cdot \mathbf{x}} \psi_K(z). \tag{9}$$

We note that equations (7) and (8) are consequence of

$$0 = 2\gamma_K^A A_K (2\pi)^2 \delta(\mathbf{K} - \mathbf{R}) + \int d^2Y \exp[i(\mathbf{R} - \mathbf{K}) \cdot \mathbf{Y} + \gamma_K^A \zeta_Y] \\ \times \{ - [i(\mathbf{K} + \mathbf{R})\nabla\zeta_Y + \gamma_K^A] \psi_R(\zeta_Y) + \psi'_R(\zeta_Y) \} \tag{10}$$

and

$$0 = \int d^2 Y \exp[i(\mathbf{R} - \mathbf{K}) \cdot \mathbf{Y} - \gamma_K^B \zeta_Y] \{ [i(\mathbf{K} + \mathbf{R}) \nabla \zeta_Y - \gamma_K^B] \psi_R(\zeta_Y) - \psi'_R(\zeta_Y) \}. \tag{11}$$

These equations will be Fourier-transformed. We start by defining

$$g_{K;P}^{(\pm)a} = \int d^2 Y e^{-i\mathbf{P} \cdot \mathbf{Y}} \exp(\pm \gamma_K^a \zeta_Y) \tag{12}$$

$$\tilde{\psi}_{K;P} = \int d^2 Y e^{-i\mathbf{P} \cdot \mathbf{Y}} \psi_R(\zeta_Y) \tag{13}$$

and

$$\tilde{\psi}'_{K;P} = \int d^2 Y e^{-i\mathbf{P} \cdot \mathbf{Y}} \psi'_R(\zeta_Y) \tag{14}$$

and obtain, as a consequence of the Fourier theorem, the inverse formulae

$$\exp(\pm \gamma_K^a \zeta_Y) = \int \frac{d^2 P}{(2\pi)^2} e^{i\mathbf{P} \cdot \mathbf{Y}} g_{K;P}^{(\pm)a} \tag{15}$$

$$\psi_R(\zeta_Y) = \int \frac{d^2 P}{(2\pi)^2} e^{i\mathbf{P} \cdot \mathbf{Y}} \tilde{\psi}_{R;P} \tag{16}$$

$$\psi'_R(\zeta_Y) = \int \frac{d^2 P}{(2\pi)^2} e^{i\mathbf{P} \cdot \mathbf{Y}} \tilde{\psi}'_{R;P} \tag{17}$$

and also that

$$\exp(\pm \gamma_K^a \zeta_Y) \nabla \zeta_Y = \int \frac{d^2 P}{(2\pi)^2} e^{i\mathbf{P} \cdot \mathbf{Y}} (\pm i\mathbf{P} / \gamma_K^a) g_{K;P}^{(\pm)a}. \tag{18}$$

Thus, we have instead of (10) and (11),

$$0 = 2\gamma_R^A A_R (2\pi)^2 \delta(\mathbf{K}) + \int \frac{d^2 P}{(2\pi)^2} g_{K+R;K-P}^{(+A)} (\alpha_{R;K,P}^A \tilde{\psi}_{R;P} + \tilde{\psi}'_{R;P}) \tag{19}$$

and

$$0 = \int \frac{d^2 P}{(2\pi)^2} g_{K+R;K-P}^{(-B)} (\alpha_{R;K,P}^B \tilde{\psi}_{R;P} - \tilde{\psi}'_{R;P}) \tag{20}$$

where we denote ($a = A, B$)

$$\alpha_{R;K;P}^a = (\mathbf{K} + 2\mathbf{P}) \cdot (\mathbf{K} - \mathbf{P}) / \gamma_{K+R}^a - \gamma_{K+R}^a. \tag{21}$$

These much simpler equations will be solved presently. In order to do this, the properties of the profile function ζ_X must first be prescribed. It is clear that in practice this function is not known in great detail. Usually only a number of statistical properties of the surface are amenable to measurements, such as some average value of the departure of the actual surface from flatness, or the extent of the lateral correlation. Correspondingly, one should calculate quantities that do not depend on a particular realisation of the surface roughness profile, but are averages taken over ensembles of such functions, characterised by some statistical parameters.

On the other hand, it is clear that not every averaged quantity is physically meaningful. Thus, although it is correct to base a given calculation on averaged particle densities or particle currents—or more generally, averaged Green functions—the concept of an averaged wavefunction probably has no proper meaning. In this paper we calculate transmission and reflection coefficients, that is, quotients of random (reflected and transmitted) currents over a deterministic one. Then, even if we utilise such averaged wavefunctions in intermediate mathematical steps, our final results will have, I believe, reasonable counterparts in reality.

Customarily, the function ζ_X is assumed to be a random variable with a Gaussian probability distribution having zero mean and a standard deviation

$$\langle \zeta_X \zeta_Y \rangle = \delta^2 W(|X - Y|) \tag{22}$$

where $\langle \dots \rangle$ denotes the average taken over the probability distribution. Here δ is the RMS value of the roughness amplitude, and $W(X)$ is taken to be

$$W(X) = \exp(-X^2/a^2) \tag{23}$$

where a is the lateral correlation length.

Other probability functions (and other forms of the correlation function W) have been considered, but experimental determinations of the statistical properties of real surfaces tend to favour those hypothesised here (Rasigni *et al* 1984).

In these circumstances, it is easy to show that, for the function defined in (12)

$$\langle g_{K;P}^{(\pm)a} \rangle = \bar{g}_K^a (2\pi)^2 \delta(\mathbf{P}) \tag{24}$$

with

$$\bar{g}_K^a = \exp[\frac{1}{2}(\gamma_K^a \delta)^2]. \tag{25}$$

Let us further denote Δh the fluctuation of a random quantity h

$$\Delta h = h - \langle h \rangle. \tag{26}$$

Then, we can write equations (19) and (20) as a pair of Fredholm inhomogeneous integral equations

$$\begin{aligned} \gamma_{K+R}^A \tilde{\psi}_{R;K} - \tilde{\psi}'_{R;K} &= (2\gamma_{R;K}^A A_R / \bar{g}_R^A) (2\pi)^2 \delta(\mathbf{K}) \\ &+ \int \frac{d^2P}{(2\pi)^2} f_{K+R;K-P}^{(+A)} (\alpha_{R;K,P}^A \tilde{\psi}_{R;P} + \tilde{\psi}'_{R;P}) \end{aligned} \tag{27}$$

and

$$\gamma_{K+R}^B \tilde{\psi}_{R;K} + \tilde{\psi}'_{R;K} = \int \frac{d^2P}{(2\pi)^2} f_{K+R;K-P}^{(-B)} (\alpha_{R;K,P}^B \tilde{\psi}_{R;P} - \tilde{\psi}'_{R;P}) \tag{28}$$

where we have put

$$f_{K,Q}^{(\pm)a} = \Delta g_{K,Q}^{(\pm)a} / \bar{g}_K^a. \tag{29}$$

The pair (27) and (28) can now be written in its final form

$$\Psi_{R;K} = \Psi_{R;K}^{(0)} + \int \frac{d^2P}{(2\pi)^2} c_{R;K,P} \Psi_{R;P} \tag{30}$$

where the matrices Ψ , $\Psi^{(0)}$ and c are given by

$$\Psi_{R;K} = \begin{bmatrix} \tilde{\psi}_{R;K} \\ \tilde{\psi}'_{R;K} \end{bmatrix} \tag{31}$$

$$\Psi_{R;K}^{(0)} = \frac{2\gamma_R^A A_R}{\bar{g}_R^A (\gamma_R^A + \gamma_R^B)} (2\pi)^2 \delta(\mathbf{K}) \begin{bmatrix} 1 \\ -\gamma_R^B \end{bmatrix} \tag{32}$$

and

$$c_{R;K,P} = \begin{bmatrix} c^{(1,1)} & c^{(1,2)} \\ c^{(2,1)} & c^{(2,2)} \end{bmatrix} \tag{33}$$

with

$$c^{(1,1)} = (\alpha_{R;K,P}^A f_{K+R;K-P}^{(+A)} + \alpha_{R;K,P}^B f_{K+R;K-P}^{(-B)}) / \Gamma_{K+R}^{AB} \tag{34}$$

$$c^{(1,2)} = (f_{K+R;K-P}^{(+A)} - f_{K+R;K-P}^{(-B)}) / \Gamma_{K+R}^{AB} \tag{35}$$

$$c^{(2,1)} = (-\alpha_{R;K,P}^A \gamma_{K+R}^B f_{K+R;K-P}^{(+A)} + \alpha_{R;K,P}^B \gamma_{K+R}^A f_{K+R;K-P}^{(-B)}) / \Gamma_{K+R}^{AB} \tag{36}$$

$$c^{(2,2)} = (-\gamma_{K+R}^B f_{K+R;K-P}^{(+A)} - \gamma_{K+R}^A f_{K+R;K-P}^{(-B)}) / \Gamma_{K+R}^{AB} \tag{37}$$

and

$$\Gamma_Q^{AB} = \gamma_Q^A + \gamma_Q^B. \tag{38}$$

We now apply the smoothing method in order to solve equation (30) approximately. The method was developed originally by Keller (1962), and has recently been applied by Watson and Keller (1984) to the case of surface scattering of scalar waves, and by Brown (1984) and Maradudin (1986) to the electromagnetic problem. Let us first write equation (30) schematically as

$$\Psi = \Psi^{(0)} + \int c\Psi. \tag{39}$$

Then, it is easy to see that

$$\Psi = \chi + \int K\langle\Psi\rangle \tag{40}$$

where the new inhomogeneous part and kernel are given, respectively, by

$$\chi = \Psi^{(0)} + \int c\Delta\chi \tag{41}$$

and

$$K = c + \int c\Delta K. \tag{42}$$

We note, also, that (40) implies that

$$\langle\Psi\rangle = \langle\chi\rangle + \int \langle K\rangle\langle\Psi\rangle \tag{43}$$

and

$$\Delta\Psi = \Delta\chi + \int \Delta K\langle\Psi\rangle. \tag{44}$$

In practice, (40) will be solved by successive application of these two equations. As the operation of taking averages restores the translational symmetry in the plane of the ideal surface, (43) is an algebraic rather than an integral equation. Thus (re-establishing the indices suppressed in passing from (30) to (39)),

$$\langle K_{R;K,P} \rangle = \bar{K}_{R;K} (2\pi)^2 \delta(\mathbf{K} - \mathbf{P}) \quad (45)$$

and

$$\langle \Psi_{R;K} \rangle = (1 - \bar{K}_{R;K})^{-1} \Psi_{R;K}^{(0)} \quad (46)$$

because in this case $\Psi^{(0)}$ is not a random variable, so that $\chi = \Psi^{(0)}$ by (41). From this value of the average $\langle \Psi \rangle$, equation (44) gives directly the value of the fluctuation $\Delta \Psi$, and thus the complete Ψ .

In the present case, it can be shown without difficulty that

$$\langle f_{K;R}^{(+a)} f_{Q;S}^{(+b)} \rangle = \langle f_{K;R}^{(-a)} f_{Q;S}^{(-b)} \rangle = (2\pi)^2 \delta(\mathbf{R} + \mathbf{S}) F_{K,Q}^{(+a,b)}(\mathbf{R}) \quad (47)$$

and

$$\langle f_{K;R}^{(+a)} f_{Q;S}^{(-b)} \rangle = (2\pi)^2 \delta(\mathbf{R} + \mathbf{S}) F_{K,Q}^{(-a,b)}(\mathbf{R}) \quad (48)$$

where

$$F_{K,Q}^{(\pm)a,b}(\mathbf{R}) = \int d^2 X e^{-i\mathbf{R} \cdot \mathbf{X}} \{ \exp[\pm \delta^2 \gamma_K^a \gamma_Q^b W(\mathbf{X})] - 1 \} \quad (49)$$

by the assumptions preceding (24). Thus, one has that

$$\bar{K}_{R;K} = \begin{bmatrix} \bar{K}^{(1,1)} & \bar{K}^{(1,2)} \\ \bar{K}^{(2,1)} & \bar{K}^{(2,2)} \end{bmatrix} \quad (50)$$

where we write

$$\bar{K}^{(1,1)} = \int \frac{d^2 P}{(2\pi)^2} [\alpha_{R;P,K}^A (U_{KPR}^{A,B} + V_{KPR}^{B,A}) + \alpha_{R;P,K}^B (V_{KPR}^{A,B} + U_{KPR}^{B,A})] / C_{KPR}^{AB} \quad (51)$$

$$\bar{K}^{(1,2)} = \int \frac{d^2 P}{(2\pi)^2} (U_{KPR}^{A,B} + V_{KPR}^{B,A} - V_{KPR}^{A,B} - U_{KPR}^{B,A}) / C_{KPR}^{AB} \quad (52)$$

$$\begin{aligned} \bar{K}^{(2,1)} = \int \frac{d^2 P}{(2\pi)^2} [& \alpha_{R;P,K}^A (-\gamma_{P+R}^B U_{KPR}^{A,B} + \gamma_{P+R}^A V_{KPR}^{B,A}) \\ & + \alpha_{R;P,K}^B (-\gamma_{P+R}^B V_{KPR}^{A,B} + \gamma_{P+R}^A U_{KPR}^{B,A})] / C_{KPR}^{AB} \end{aligned} \quad (53)$$

$$\bar{K}^{(2,2)} = \int \frac{d^2 P}{(2\pi)^2} [\gamma_{P+R}^B (-U_{KPR}^{A,B} + V_{KPR}^{B,A}) + \gamma_{P+R}^A (-V_{KPR}^{A,B} + U_{KPR}^{B,A})] / C_{KPR}^{AB} \quad (54)$$

and

$$U_{KPR}^{A,B} = (\alpha_{R;P,K}^A - \gamma_{P+R}^B) F^{(+A,A)}(\mathbf{K} - \mathbf{P}) \quad (55)$$

$$V_{KPR}^{A,B} = (\alpha_{R;P,K}^A + \gamma_{P+R}^A) F^{(-A,B)}(\mathbf{K} - \mathbf{P}) \quad (56)$$

$$C_{KPR}^{AB} = (\gamma_{K+R}^A + \gamma_{K+R}^B)(\gamma_{P+R}^A + \gamma_{P+R}^B). \tag{57}$$

Further,

$$(1 - \bar{K}_{R,K})^{-1} = d^{-1} \begin{bmatrix} 1 - \bar{K}^{(2,2)} & \bar{K}^{(1,2)} \\ \bar{K}^{(2,1)} & 1 - \bar{K}^{(1,1)} \end{bmatrix} \tag{58}$$

where (also neglecting terms containing products of functions F)

$$d^{-1} = 1 + \int \frac{d^2P}{(2\pi)^2} [(\alpha^A - \gamma^B)(\alpha^A - \gamma^B)F^{(+)\text{A,A}} + (\alpha^B + \gamma^B)(\alpha^A + \gamma^A)F^{(-)\text{A,B}} + (\alpha^A + \gamma^A)(\alpha^B + \gamma^B)F^{(-)\text{B,A}} + (\alpha^B - \gamma^A)(\alpha^B - \gamma^A)F^{(+)\text{B,B}}] / (\Gamma^{\text{AB}})^2. \tag{59}$$

The values of $\tilde{\psi}_{K;P}$ and $\tilde{\psi}'_{K;P}$ —the unknowns in (27) and (28)—are obtained by inserting formulae (51)–(54) and (59) into (58), and then into (43). The resulting terms have, however, quite different magnitudes. From (21), for instance, we have that

$$\alpha_{R;0,P'}^A + \gamma_{P'+R}^A = \alpha_{R;0,0}^A + \gamma_R^A = 0$$

while

$$\alpha_{R;0,P'}^B + \gamma_{P'+R}^B = \gamma_R^A - \gamma_R^B$$

after multiplication by the respective function F and integration over P . Thus we have, retaining only the terms that are important in this sense,

$$\langle \tilde{\psi}_{R;K} \rangle = \frac{2\gamma_R^A A_R}{\bar{g}_R^A (\gamma_R^A + \gamma_R^B)} (2\pi)^2 \delta(\mathbf{K}) \left(1 + \int \frac{d^2P}{(2\pi)^2} F_{P+R,R}^{(+)\text{A,A}}(\mathbf{R}) \right) + O(F^2) \tag{60}$$

and

$$\langle \tilde{\psi}'_{R;K} \rangle = -\frac{2\gamma_R^A \gamma_R^B A_R}{\bar{g}_R^A (\gamma_R^A + \gamma_R^B)} (2\pi)^2 \delta(\mathbf{K}) \left(1 + \int \frac{d^2P}{(2\pi)^2} F_{P+R,R}^{(+)\text{A,A}}(\mathbf{R}) \right) + O(F^2) \tag{61}$$

exactly up to terms of order F . We see that, with the same accuracy, we can write

$$\langle \tilde{\psi}_{R;K} \rangle = \frac{2\gamma_R^A A_R}{\bar{g}_R^A (\gamma_R^A + \gamma_R^B)} (2\pi)^2 \delta(\mathbf{K}) \exp(L_R) \tag{62}$$

and

$$\langle \tilde{\psi}'_{R;K} \rangle = -\frac{2\gamma_R^A \gamma_R^B A_R}{\bar{g}_R^A (\gamma_R^A + \gamma_R^B)} (2\pi)^2 \delta(\mathbf{K}) \exp(L_R) \tag{63}$$

with

$$L_R = \int \frac{d^2P}{(2\pi)^2} F_{P+R,R}^{(+)\text{A,A}}. \tag{64}$$

By (16) and (17) we have determined the average value of the wavefunction and its derivative at the interface

$$\langle \psi_K(\zeta_X) \rangle = \frac{2\gamma_R^A A_R}{\bar{g}_R^A (\gamma_R^A + \gamma_R^B)} \exp(L_R) \tag{65}$$

and

$$\langle \psi'_K(\zeta_X) \rangle = -\frac{2\gamma_R^A \gamma_R^B A_R}{\bar{g}_R^A (\gamma_R^A + \gamma_R^B)} \exp(L_R) \tag{66}$$

with a source in metal A.

3. The average wavefunction

We are now in a position to calculate the average wavefunction in the entire system, and then the diverse particle currents, which will give the reflection and transmission coefficients. Of course, the averaged currents cannot be computed merely as simple products of average wavefunctions. Rather, the smoothing method will be applied in a way epitomised by the passage from equation (70) to (76). Thus, in order to calculate the mean of a given product of random functions one sets up, and approximately solves, a suitable integral equation whose kernel and inhomogeneous part have been previously calculated from simpler averages.

Let us consider first metal A. Setting $z \ll -\delta$ in (1), we have

$$\begin{aligned} \psi_K(z) = & A_K \exp(-\gamma_K^A z) + \exp(\gamma_K^A z) \frac{1}{2\gamma_K^A} \\ & \times \int d^2 Y \int \frac{d^2 P}{(2\pi)^2} \exp[i(\mathbf{R} - \mathbf{K}) \cdot \mathbf{Y} - \gamma_K^A \zeta_Y] \\ & \times \{-[i(\mathbf{K} + \mathbf{R}) \nabla \zeta_Y - \gamma_K^A] \psi_R(\zeta_Y) + \psi'_R(\zeta_Y)\}. \end{aligned} \quad (67)$$

According to (12)–(14), this equation can be written

$$\begin{aligned} \psi(z) = & A_K \exp(-\gamma_K^A z) + \exp(\gamma_K^A z) \frac{1}{2\gamma_K^A} \int \frac{d^2 P d^2 R}{(2\pi)^4} \\ & \times g_{K;K-R-P}^{(-)A} (-\alpha_{R;K-R,P}^A \tilde{\psi}_{R;P} + \tilde{\psi}'_{R;P}). \end{aligned} \quad (68)$$

We see that the average wavefunction $\langle \psi(z) \rangle$ depends on the averages $\langle g_{K;Q}^{(-)A} \tilde{\psi}_{R;P} \rangle$ and $\langle g_{K;Q}^{(-)A} \tilde{\psi}'_{R;P} \rangle$, or, by (31), on $\langle g_{K;Q}^{(-)A} \Psi_{R;P} \rangle$, where we have put $\mathbf{Q} = \mathbf{K} - \mathbf{R} - \mathbf{P}$.

This average can be calculated as follows. First, we note from (30) that $g_{K;Q}^{(-)A} \Psi_{R;P}$ satisfies the integral equation

$$g_{K;Q}^{(-)A} \Psi_{R;P} = g_{K;Q}^{(-)A} \Psi_{R;P}^{(0)} + \int \frac{d^2 P'}{(2\pi)^2} c_{R;P,P'} g_{K;Q}^{(-)A} \Psi_{R;P'} \quad (69)$$

or, by (43)

$$\langle g_{K;Q}^{(-)A} \Psi_{R;P} \rangle = J_{K,Q,R,P} + \int \frac{d^2 P'}{(2\pi)^2} \langle K_{R;P,P'} \rangle \langle g_{K;Q}^{(-)A} \Psi_{R;P'} \rangle \quad (70)$$

where $\langle K_{R;P,P'} \rangle$ is given by (39) and (50)–(54). On the other hand,

$$J_{K,Q,R,P} = \langle g_{K;Q}^{(-)A} \Psi_{R;P}^{(0)} \rangle + \int \frac{d^2 P'}{(2\pi)^2} \langle c_{R;P,P'} \Delta g_{K;Q}^{(-)A} \Psi_{R;P'}^{(0)} \rangle + \dots \quad (71)$$

exactly up to terms of order F . The first term of (71) is

$$\frac{2\gamma_R^A A_R \bar{g}_K^A}{\gamma_R^A + \gamma_R^A \bar{g}_R^A} (2\pi)^4 \delta(\mathbf{P}) \delta(\mathbf{K} - \mathbf{R}) \begin{bmatrix} 1 \\ -\gamma_K^A \end{bmatrix} \quad (72)$$

while the second term is given by

$$\frac{2\gamma_K^A A_K}{(\gamma_K^A + \gamma_K^B)(\gamma_{P+K}^A + \gamma_{P+K}^B)} (2\pi)^2 \delta(\mathbf{K} - \mathbf{R}) \begin{bmatrix} S_{K;P}^{A,A} + S_{K;P}^{B,A} \\ -\gamma_{P+K}^B S_{K;P}^{A,A} + \gamma_{P+K}^A S_{K;P}^{B,A} \end{bmatrix} \quad (73)$$

where

$$S_{\hat{K};\hat{P}}^{\hat{A},\hat{A}} = (\alpha_{\hat{K};\hat{P},0}^{\hat{A}} - \gamma_{\hat{K}}^{\hat{A}})F_{\hat{P}+\hat{K};\hat{K}}^{(-)\hat{A},\hat{A}}(\mathbf{P}) \tag{74}$$

and

$$S_{\hat{K};\hat{P}}^{\hat{B},\hat{A}} = (\alpha_{\hat{K};\hat{P},0}^{\hat{B}} + \gamma_{\hat{K}}^{\hat{B}})F_{\hat{P}+\hat{K};\hat{K}}^{(+)\hat{B},\hat{A}}(\mathbf{P}) \tag{75}$$

and we have used (47) and (48). From (70) we see that

$$\langle g_{\hat{K};\hat{Q}}^{(-)\hat{A}}\Psi_{R;\hat{P}} \rangle = (1 - \bar{K}_{R;\hat{P}})^{-1}J_{\hat{K},\hat{Q},R,\hat{P}}. \tag{76}$$

The first factor has been calculated in (58), while the second is given by (71). Thus, we obtain the required averages. In order to determine the wavefunction we need the linear combination of averages

$$\int \frac{d^2P d^2R}{(2\pi)^4} (-\alpha_{\hat{R};\hat{K}-R,\hat{P}}^{\hat{A}} \langle g_{\hat{K};\hat{K}-R-\hat{P}}^{(-)\hat{A}} \tilde{\psi}_{R;\hat{P}} \rangle + \langle g_{\hat{K};\hat{K}-R-\hat{P}}^{(-)\hat{A}} \tilde{\psi}'_{R;\hat{P}} \rangle). \tag{77}$$

This is given, neglecting terms of order F^2 , by five terms, which can be obtained in a straightforward way from previous formulae. Of these, we can neglect two by the same reasoning leading to (60) and (61). We have then

$$(76) \approx 2\gamma_{\hat{K}}^{\hat{A}}A_{\hat{K}} \frac{\gamma_{\hat{K}}^{\hat{A}} - \gamma_{\hat{K}}^{\hat{B}}}{\gamma_{\hat{K}}^{\hat{A}} + \gamma_{\hat{K}}^{\hat{B}}} (1 + M_{\hat{K}}^{\hat{A},\hat{A}}) + O(F^2) \tag{78}$$

$$\approx 2\gamma_{\hat{K}}^{\hat{A}}A_{\hat{K}} \frac{\gamma_{\hat{K}}^{\hat{A}} - \gamma_{\hat{K}}^{\hat{B}}}{\gamma_{\hat{K}}^{\hat{A}} + \gamma_{\hat{K}}^{\hat{B}}} \exp(M_{\hat{K}}^{\hat{A},\hat{A}}) + O(F^2) \tag{79}$$

where

$$M_{\hat{K}}^{\hat{A},\hat{A}} = \int \frac{d^2P}{(2\pi)^2} [F_{\hat{P}+\hat{K};\hat{K}}^{(+)\hat{A},\hat{A}}(\mathbf{P}) - F_{\hat{P}+\hat{K};\hat{P}}^{(-)\hat{A},\hat{A}}(\mathbf{P})]. \tag{80}$$

Thus, by (68), the average wavefunction for an electron in metal A (but travelling not too near the interface) is given by the simple formula

$$\langle \psi_{\hat{K}}(z) \rangle = A_{\hat{K}} \left(\exp(-\gamma_{\hat{K}}^{\hat{A}}z) + \exp(\gamma_{\hat{K}}^{\hat{A}}z) \frac{\gamma_{\hat{K}}^{\hat{A}} - \gamma_{\hat{K}}^{\hat{B}}}{\gamma_{\hat{K}}^{\hat{A}} + \gamma_{\hat{K}}^{\hat{B}}} \exp(-M_{\hat{K}}^{\hat{A},\hat{A}}) \right). \tag{81}$$

Proceeding in an exactly parallel way, we have that the average wavefunction for an electron lying in metal B (but, again, not too near the interface) is given by

$$\langle \psi_{\hat{K}}(z) \rangle = -A_{\hat{K}} \exp(-\gamma_{\hat{K}}^{\hat{B}}z) \frac{2\gamma_{\hat{K}}^{\hat{A}}}{\gamma_{\hat{K}}^{\hat{A}} + \gamma_{\hat{K}}^{\hat{B}}} \frac{\bar{g}_{\hat{K}}^{\hat{B}}}{\bar{g}_{\hat{K}}^{\hat{A}}} \exp(N_{\hat{K}}^{\hat{A},\hat{B}}) \tag{82}$$

where $\bar{g}_{\hat{K}}^{\hat{a}}$ is given in (25), and

$$N_{\hat{K}}^{\hat{A},\hat{B}} = \int \frac{d^2P}{(2\pi)^2} [F_{\hat{P}+\hat{K};\hat{K}}^{(+)\hat{A},\hat{A}}(\mathbf{P}) - F_{\hat{P}+\hat{K};\hat{P}}^{(+)\hat{A},\hat{B}}(\mathbf{P})]. \tag{83}$$

The first term in (81) represents a source of arbitrary strength located in metal A. Consequently, the second term in (81) is the reflected wave, while (82) represents the transmitted wave. Thus we see that, if one neglects correlations that are necessarily short-ranged, the reflection and transmission coefficients of the metal-metal interface are given, respectively, by

$$r_{A,A}(\mathbf{K}) = R_{\hat{K}} \exp(-2 \text{Re } M_{\hat{K}}^{\hat{A},\hat{A}}) \tag{84}$$

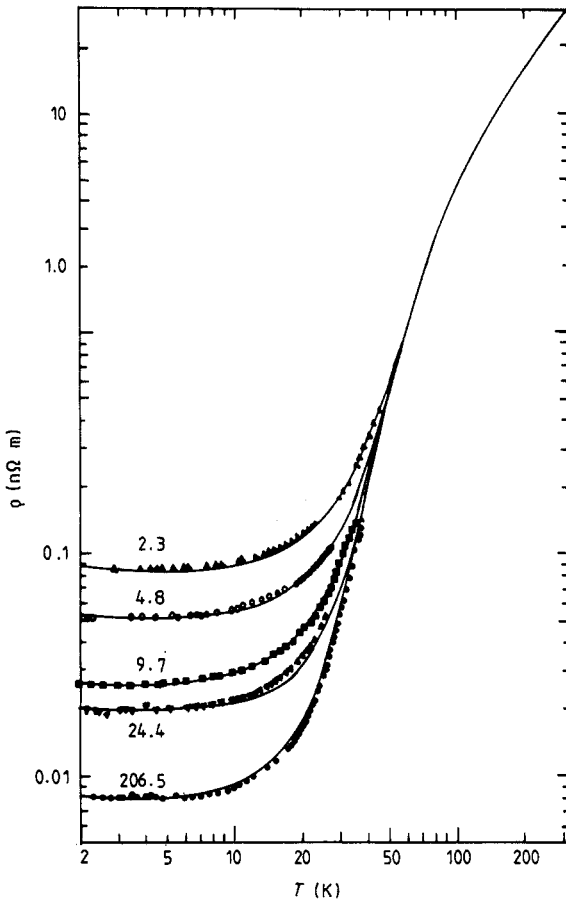


Figure 3. Fit of equations (86) and (87) (full curves) to data obtained from Sambles *et al* (1981, figure 3). Thickness (μm) is shown on each curve.

and

$$t_{A,B}(\mathbf{K}) = D_K |\bar{g}_K^B / \bar{g}_K^A|^2 \exp(2 \text{Re } N_K^{A,B}) \tag{85}$$

where R_K and D_K are the quantum-mechanical reflection and transmission coefficients of the *ideal surface* (Landau and Lifshitz 1958) if one further neglects the detailed structure of the diffusely reflected and transmitted components (Moraga 1987).

4. Applications

4.1. Electrical conductivity of thin films and foils

In this section I shall specialise the expressions for the reflection and transmission probabilities to the case of the metal-vacuum interface. In this case $V_A < E_F < V_B$ and, by (6), γ^A is nearly pure imaginary while γ^B is real. Thus, $R_K = 1$ while $D_K = 0$ and

$$p(u) \equiv r_{A,A}(\mathbf{K}) = \exp(2 \text{Re } M_K^{A,A}) \tag{86}$$

by (84), where u is the cosine of the angle of incidence and $M_K^{A,A}$ is given by (80). Formula (86) has been obtained previously by means of a number of resummations of a series

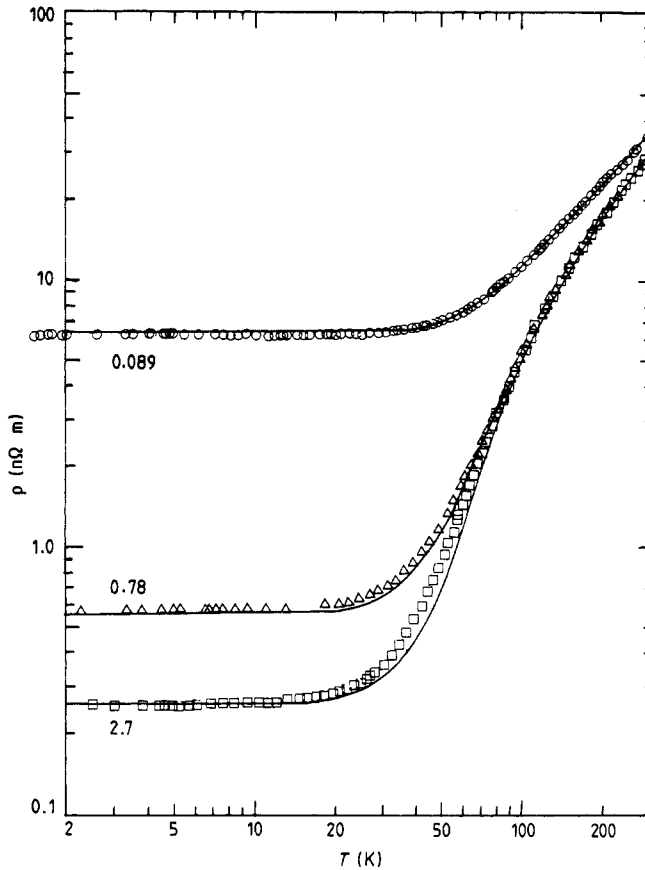


Figure 4. Fit of equations (86) and (87) (full curves) to data obtained from Sambles *et al* (1981, figure 5). Thickness (μm) is shown on each curve.

expansion in powers of δ (Moraga 1987); we can see now that its validity depends neither on the correctness of that approach nor on the adequacy of the infinite barrier model.

The experimental accuracy of the present theory can be tested at this point. As is well known, the electrical conductivity σ of a metallic film of thickness κ (in units of the mean free path of the conduction electrons) is given by (Fuchs 1938)

$$\frac{\sigma}{\sigma_{\infty}} = 1 - \frac{3}{8\kappa} \int_0^1 u(1-u^2) \frac{(1-p)[1 - \exp(-\kappa/u)]}{1 - p \exp(-\kappa/u)} du \quad (87)$$

where σ_{∞} is the conductivity of the bulk metal and p is given by (86). This conductivity has been subject to a number of precise measurements, of which perhaps the best—in terms of the high purity of the samples used and the range of thicknesses explored—are those made on thin aluminium films and foils by Sambles *et al* (1981). I have fitted equations (86) and (87) to these data (figures 3 and 4), supposing, perhaps too arbitrarily, that both the RMS departure from flatness δ and the lateral correlation length of all surfaces was equal to 5 au.

It is seen that the fit is good, although not perfect. The fit can certainly be improved by taking into account, for instance, the effects of small-angle scattering (Olsen 1958,

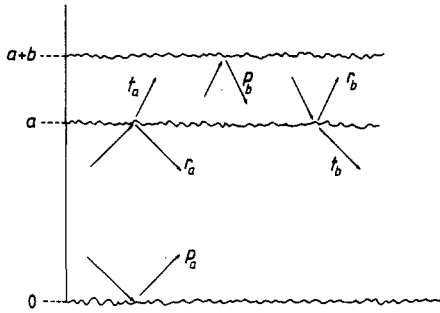


Figure 5. Thin film $0 < z < a$ with an overlayer $a < z < a + b$. Scattering occurs at all the rough surfaces, with the transmission and reflection coefficients shown.

Azbel' and Gurzhi 1962) which are absent in (87). On the other hand, in the resistivity of the bulk used in these calculations I have included a term $10.0T^2 f \Omega \text{ m}$ coming from the effects of the electron-electron scattering. The adequacy of such a term seems now, however, to be debatable and, if I have to drop it, the fit will surely be somewhat spoiled.

4.2. Electrical conductivity of double-layer films

In order to explore further the influence of the surfaces on the conductivity of solids, a number of measurements have been made on double-layer thin films. Experimentally it has been found that the resistance of a thin-film sample can be increased by the deposition of a layer of a different (or even of the same) metal. This increment has been attributed to a change of the Fuchs' parameter of the surface from $p \approx 1$ to $p \approx 0$ as a result of the added overlayer (Lucas 1964, 1968, 1971, Chopra and Randlett 1967, Berman and Juretschke 1971).

Unfortunately, the theoretical analysis of this phenomenon had to proceed under the hypothesis that no additional scattering occurred at the interfaces between the layers. It is, of course, very unlikely that this assertion holds even approximately true. By using the results of the previous section we can, however, obtain a new theoretical description that is free from this limitation.

We shall solve here the Boltzmann equation for the double-layer metallic film shown in figure 5 for the case of an electric field applied in the x direction. According to the results of the last section, the appropriate boundary conditions applying at the rough surfaces $z = 0$, $z = a$ and $z = a + b$, respectively, are

$$f_{\text{A}}^{(+)}(0, v_z) = p_a f_{\text{A}}^{(-)}(0, v_z) + g_{\text{A}} \quad (88)$$

$$f_{\text{A}}^{(+)}(0, -v_z) = r_a f_{\text{A}}^{(+)}(a, v_z) + t_b f_{\text{B}}^{(-)}(a, -v_z) + g'_{\text{A}} \quad (89)$$

$$f_{\text{B}}^{(+)}(a, v_z) = t_a f_{\text{A}}^{(+)}(a, v_z) + r_b f_{\text{B}}^{(-)}(a, -v_z) + g_{\text{B}} \quad (90)$$

and

$$f_{\text{B}}^{(-)}(a + b, -v_z) = p_b f_{\text{B}}^{(+)}(a + b, v_z) + g'_{\text{B}} \quad (91)$$

where v_z is the z component of the electron velocity, and the indices $+$ and $-$ of the distribution function $f_a^{(\pm)}(z, v_z)$ denote the branches of this function corresponding to the cases $v_z > 0$ and $v_z < 0$, respectively, for electrons travelling in metal $a = \text{A, B}$.

These conditions suffice for determining a unique solution of the transport linearised in the usual way (together with the *diffuse components* g_a and g'_a). The longitudinal conductivity of the system is

$$\sigma = \frac{1}{a+b} [a\sigma_A(1 - \frac{3}{4}I_1) + b\sigma_B(1 - \frac{3}{4}I_2)] \quad (92)$$

where σ_A and σ_B are the bulk conductivities of the respective metals,

$$I_1 = \frac{1}{\kappa_a} \int_0^1 \frac{u(1-u^2)}{\Delta} (U_{a,b} + V_{a,b})(1 - \varepsilon_a) du \quad (93)$$

and

$$I_2 = \frac{1}{\kappa_b} \int_0^1 \frac{u(1-u^2)}{\Delta} (U_{b,a} + V_{b,a})(1 - \varepsilon_b) du \quad (94)$$

with

$$\Delta = 1 - p_a r_a \varepsilon_a^2 - p_b [r_b + p_a (t_a t_b - r_a r_b) \varepsilon_a^2] \varepsilon_b^2 \quad (95)$$

$$U_{a,b} = (1 - p_a)(1 - r_b p_b \varepsilon_b^2) + p_a \{ (1 - r_a - t_b) + t_b(1 - p_b) \varepsilon_b + p_b [t_b(1 - r_b - t_a) - r_b(1 - r_a - t_b)] \varepsilon_b^2 \} \varepsilon_a \quad (96)$$

and

$$V_{a,b} = 1 - r_a - t_b + t_b(1 - p_b) \varepsilon_a + p_a \{ 1 - r_a - t_b + t_b(1 - p_b) \varepsilon_b + p_b [t_b(1 - r_b - t_a) - r_b(1 - r_a - t_b)] \varepsilon_b^2 \} \varepsilon_a. \quad (97)$$

Here $U_{b,e}$ and $V_{b,e}$ are obtained from these formulae by interchanging everywhere a by b , κ_a and κ_b are the film thicknesses over their respective mean free paths, and $\varepsilon_j \equiv \exp(-\kappa_j/u)$ ($j = a, b$).

In figure 6 we compare values calculated from equations (92)–(97) with experimental measurements of the electrical resistance of a number of metallic overlayers deposited over gold substrata made by Lucas (1968). It is seen that there is a good fit when the thickness of the added material is not too small. The curves, however, are qualitatively different, since the experimental values show a maximum as a function of thickness, while the theoretical curves are monotonic.

Again, a better fit (together with a resistance maximum) could have been obtained by adjusting the reflectivity of the added layer according to an empirical function of its thickness (Lucas 1968). But it is likely that this procedure would have been erroneous, because ordinary transport theory in fact fails for samples that are too thin. The reason for this may not only lie in the failure of the transport equation to take into account quantum effects appearing when one of the dimensions of the specimen is comparable with the electron wavelength; it may also be a consequence of the fact that, when the specimen size is diminished beyond a certain point, the boundary conditions cannot be prescribed any more in each surface entirely independently of each other.

Thus, in order to obtain significant improvements of the theory in this respect, one can proceed only in two directions. Either one develops more generalised boundary conditions, taking into account the reflectivity effects of the entire overlayer (and not, as done here, as an incoherent superposition of two surfaces); or one entirely abandons the programme of transport theory and employ methods that are quantum-mechanical throughout (Rammer and Smith 1986).

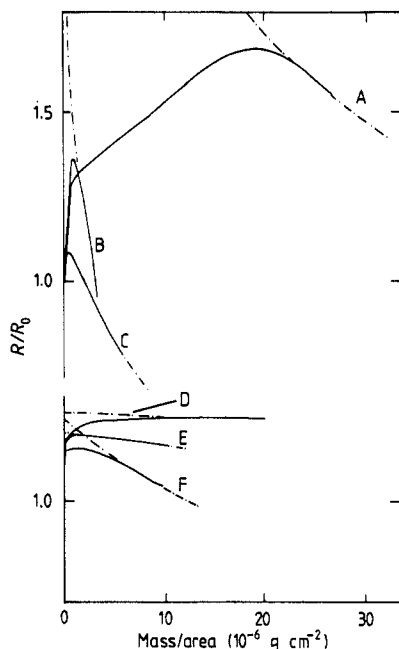


Figure 6. Electrical resistance of metallic overlayers in units of the substrate resistance as a function of the added mass/area: full curves, experimental data from Lucas (1968); chain curves, calculated values; (A) Pb over Au, (B) Al over Au, (C) Ag over Au, (D) Bi over Au, (E) Cr over Au, (F) Fe over Au.

These developments are, however, well outside the scope of this paper.

5. Conclusions

Okulov and Ustinov (1978) have pointed out that a rigorous formulation of the boundary conditions for the Boltzmann equation should begin by solving the problem of an electron being transmitted or reflected by an *ideal* surface. This limited objective has, of course, never been fully fulfilled. In order to do this, one should calculate first the wavefunction describing the stationary state of a conduction electron in the field of the potential barrier created at the interface, taking into account the effects of the ionic lattice whose periodicity is broken by the boundary. Even then, it is not automatically assured that a perfect surface would conserve the tangential component of the momentum, because a vicinal surface, for instance, would form steps and act as a cross-grating (Müser 1954). Further, even in cases in which the two-dimensional Bloch theorem is valid and a simple dispersion relation exists between the energy and the tangential component of the momentum, the analysis becomes complicated by the necessity to distinguish between normal and umklapp transmission and reflection processes at the interface.

In this paper I have obtained boundary conditions for the Boltzmann transport equation at a rough metallic interface by a drastic simplification of the problem. First, the complicated fields at the potential barrier are replaced by a simple potential step of a suitable energy. Further, the contributions of the periodic ionic potential are simply ignored, the tangential component of the momentum is supposed to be unrestrictedly conserved, and a simple parabolic-type dispersion relation is assumed. Thus, an electron traversing an interface can only be refracted (due to its change of wavelength) or be

incoherently scattered into the equilibrium distribution, or, alternatively, it can be specularly reflected back into the original metal. For a given event, either of these processes can occur according to well defined probabilities. These probabilities are obtained here by means of a well defined procedure that amounts to solving the Schrödinger equation for the simplified model just described, and then calculating the quantum-mechanical reflection and transmission coefficients. Proceeding in this way, we find that, in spite of their approximate character, these probabilities are coherently related and do not, for instance, add to more than 1 for these exclusive processes. They are, furthermore, calculable in terms of observable properties of the interface, i.e. the height of the potential step, the value of the Fermi energy and the two statistical parameters that characterise here the surface roughness profile.

I believe that these new results are a valid generalisation of the ordinary (Fuchs 1938) boundary conditions for the Boltzmann transport equation. First, in the case of a metal-vacuum interface, these conditions reduce to the use of an angle-dependent reflection coefficient, which in the proper limits coincides with the well known Soffer and Shen-Maradudin forms and are thus well validated (Moraga 1987). Further, one can solve the Boltzmann equation plus these new boundary conditions and calculate transport properties for systems that have an experimental counterpart. In this paper I have done this for the case of the electrical resistivity of thin films and foils, and also of a substratum with a thin metallic overlayer. These results have been compared with the experiments, and satisfactory agreements have been obtained.

One may in the future hope to see these new boundary conditions tested in other real systems, thereby increasing our grasp of their domain of validity and thus our understanding of the interesting phenomena arising in the transport properties of small samples.

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