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The effect of a magnetic field on the transport and scattering properties of randomly rough surfaces

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Abstract. The quantum reflectivity of a randomly rough surface in the presence of a uniform magnetic field parallel to the mean surface is approximately calculated. The resulting specularity function—depending on the RMS roughness amplitude, the lateral correlation length, the angle of incidence of a conduction electron and the angle between its classical trajectory and the magnetic field—is used in conjunction with the Boltzmann equation in order to calculate the magnetoresistance of thin films as a function of field strength and thickness. For intermediate fields, we find considerable disagreements between these results and the usual theory in which the surface specularity is represented by a phenomenological parameter.

1. Introduction

It is well known that the electrical resistivity of good conductors at low temperatures turns out to depend on the size and shape of the sample. This is due to the fact that the mean-free path of the conduction electrons becomes long in comparison with the dimensions of the material, resulting in increased contributions to the resistivity from surface scattering of these electrons (Chopra 1969, Brandli and Olsen 1969).

Most experimental studies of this size effect measure the apparent DC conductivity of thin films or wires as a function of thickness. In order to interpret such results, however, it has been necessary to assume that the mean-free path is the same function of temperature for all different specimens. Alternatively, one can measure conductivity effects with the added presence of a magnetic field B. By varying B, it is possible to obtain information about the surface effect (along with other properties of the conduction electrons) by measurements performed on a single sample. For instance, it has been found that the longitudinal magnetoresistance of thin films increase with B in the low field region, in a way that depends sensitively on the amount of diffuse surface scattering (Way and Kao 1972).

It is obvious that the amount of information one can extract from these measurements depends critically on the reliability of the theories to which they are compared. These usually proceed from a solution of the Boltzmann transport equation in the approximation of a time of relaxation, to which three other premises are added: it is supposed that the Fermi surface is spherical, that the mean free path is isotropic, and that the surface scattering is represented by a parameter p equal to the probability that an electron is reflected specularly at the surface (Fuchs 1938). The first two assumptions can be somewhat patched up—the case of ellipsoidal Fermi surfaces, for instance, can be easily accommodated (Ham and Mattis 1960, Price 1960). However, the third hypothesis is, in the words of Sambles and Preist (1982), 'an unacceptable over-simplification'. In order to improve upon it, the physical mechanism of surface scattering had to be investigated more closely. Thus, as long as the source of surface diffusiveness lies in the presence of surface asperities, the specularity parameter can be replaced by a surface specularity function obtained by Soffer (1967) from a quantum mechanical calculation. This function depends on the angle of incidence of the electrons upon the surface and the root-mean square height of its roughness. With this change in the usual transport theory, excellent accord is found between theoretical and experimental results in the DC conductivity of thin foils and wires (Sambles and Elsom 1980, Sambles *et al* 1982).

The same approach was applied to the calculation of the magnetoresistance and Hall effect of thin films (Preist and Sambles 1986), and to the longitudinal magnetoresistance of thin wires (Golledge *et al* 1987). But here the use of Soffer's expression for the surface specularity becomes suspect. As is well known, the effect of magnetic fields, in opposition to the case of electric fields, results in surface states whose existence profoundly modifies the scattering properties of the boundary. Thus, one expects that the specularity function develops a dependence on the magnitude of the magnetic field (as well as on its orientation) and, consequently, that no comparison of the results of the usual theory to magnetoresistance measurements made at different values of B can have much meaning.

On the other hand, by means of an improved infinite order perturbative method, one of us has calculated another expression for the reflectivity function for the case $B = 0$ (Moraga 1987). This function not only gives better account of higher order effects of the amplitude of the surface roughness, but is also a function of the lateral correlation of these asperities—a factor ignored in Soffer's treatment. The procedure has been applied to the calculation of the DC conductivity of thin films and wires, of size effects on thermoelectric properties, and of the general scattering properties of rough interfaces (Moraga 1989, 1990). By a generalization of these methods, we calculate approximately in this paper a new reflectivity function p for the case of a magnetic field parallel to the surface. This is done by solving the Schrödinger equation for an electron near a randomly rough surface and by extracting the appropriate quantum reflectivity coefficient, which we identify with p, from the resulting wavefunction. This reflectivity coefficient differs in two significant respects with the specularity parameter used up until now. First, it is very anisotropic, depending not only on the angle of incidence as in the case $B = 0$ but also on the angle between the classical trajectory of the electron as it hits the surface and that of the magnetic field. Furthermore, its magnitude depends on B in such a way that, on the average for a given surface, p is found to be an increasing function of B.

In order to illustrate the applications of the present theory, we calculate in this paper the magnetoresistance of a thin metallic film in the longitudinal case, i.e. the case in which the electric and magnetic fields are parallel to each other and to the plane of the surfaces. For intermediate values of the magnetic field there are considerable discrepancies between the usual description in which the specularity parameter is independent of B, and the more rigorous treatment given here.

2. Surface perturbation theory

We suppose that the metal fills the half-space limited by a randomly rough surface, while the remaining space is empty. The average (or ideal) surface coincides with the x–y plane (figure 1). The wavefunction $\psi(\boldsymbol{x})$ for an electron in this metal is given by the Schrödinger equation in integral form

$$\psi(\boldsymbol{x})\delta_{\boldsymbol{x},V} = \psi_V(\boldsymbol{x}) + \int_S \{(\hbar^2/2m)[\nabla G(\boldsymbol{s},\boldsymbol{x})\psi(\boldsymbol{s}) - G(\boldsymbol{s},\boldsymbol{x})\nabla\psi(\boldsymbol{s})] + (\mathrm{i}\hbar e/mc)G(\boldsymbol{s},\boldsymbol{x})\boldsymbol{A}\psi(\boldsymbol{s})\}\,\mathrm{d}^2 s \tag{1}$$

where $G(\boldsymbol{x},\boldsymbol{x}')$ is the Green function for the infinite domain, $\boldsymbol{A}$ is the vector potential whose curl is the magnetic field $\boldsymbol{B}$, $\psi_V(\boldsymbol{x})$ is a source of arbitrary strength, S is the surface which bounds the domain V and $\delta_{\boldsymbol{x},V}$ is equal to one if the point $\boldsymbol{x}$ lies in the domain V and is zero otherwise (Morse and Feshbach 1953). This equation simplifies considerably in the infinite barrier model

$$\psi(\boldsymbol{x})\delta_{\boldsymbol{x},V} = \psi_V(\boldsymbol{x}) - \lambda\int G(\boldsymbol{s},\boldsymbol{x})\nabla\psi(\boldsymbol{s})\,\mathrm{d}^2 s \tag{2}$$

with $\lambda \equiv \hbar^2/2m$. It is well known that this approximation suffices for the calculation of reflectivity coefficients. We shall adhere to it in what follows.

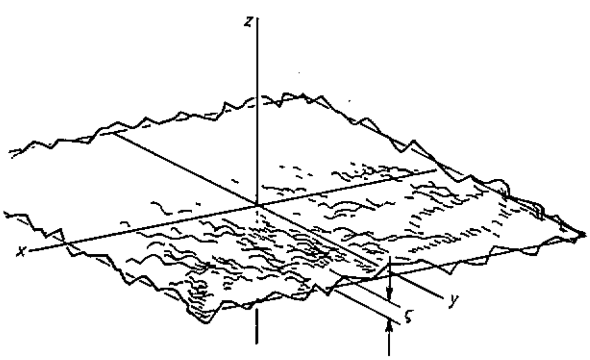

Figure 1. The metal occupies the half-space $z < \zeta$, the other half-space $z > \zeta$ being empty. The random surface profile function $\zeta(x,y)$ has mean zero and, thus, the average or ideal surface is the x–y plane.

We shall suppose that the magnetic field lies in the plane of the ideal surface. Putting $\boldsymbol{B} = B\boldsymbol{e}_x$, we have that $\boldsymbol{A} = -Bz\boldsymbol{e}_y$. Then, the problem can be simplified further by Fourier transforming both the wave and Green function in the x–y plane,

$$\psi(x,y,z) \equiv \psi(\boldsymbol{x}) = \int \frac{\mathrm{d}k_x\mathrm{d}k_y}{(2\pi)^2}\exp[\mathrm{i}(k_x x + k_y y)]\psi_{k_x,k_y}(z) \equiv \int \frac{\mathrm{d}^2 K}{(2\pi)^2}\mathrm{e}^{\mathrm{i}\boldsymbol{K}\boldsymbol{X}}\psi_{\boldsymbol{K}}(z) \tag{3}$$

$$G(\boldsymbol{x},\boldsymbol{x}') = \int \frac{\mathrm{d}^2 K}{(2\pi)^2}\mathrm{e}^{\mathrm{i}\boldsymbol{K}\boldsymbol{X}}G_{\boldsymbol{K}}(z,z'). \tag{4}$$

We note that the Fourier component of the Green function is given by

$$G_K(z,z') = -\frac{1}{\lambda W_K}\phi_K^{(+)}(z_>)\phi_K^{(-)}(z_<) \tag{5}$$

where $\phi^{(\pm)}$ is the solution of the one-dimensional Schrödinger equation

$$\left[\mathcal{E} - \frac{\hbar^2 k_x^2}{2m} - \frac{1}{2m}\left(\hbar k_y + \frac{eB}{c}z\right)^2\right]\phi_K^{(\pm)}(z) + \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}^2 z}\phi_K^{(\pm)}(z) = 0 \tag{6}$$

which is regular at $z \to \pm\infty$, respectively. Also, W is the Wronskian of these two functions and $z_>$ ($z_<$) is the larger (smaller) quantity of z and z'. As is well known (Landau and Lifshitz 1958), the solutions of this one- dimensional problem are parabolic cylinder functions (Abramowitz and Stegun 1965)

$$\phi_K^{(\pm)}(z) = U\left[\alpha, \pm(2m\omega/\hbar)^{1/2}(z+z_0)\right] \tag{7}$$

where we find for the angular frequency $\omega = |eB|/mc$, the centre of the orbit $z_0 = e\hbar k_y/eB$, the parameter

$$\alpha = \frac{1}{\hbar\omega}\left(\frac{\hbar^2 k_x^2}{2m} - \mathcal{E}\right) \tag{8}$$

and the Wronskian

$$W_K = \left(\frac{4m\pi\omega}{\hbar}\right)^{1/2}\frac{1}{\Gamma(\alpha+\frac{1}{2})}. \tag{9}$$

In this notation, the source function is given by

$$\psi_V(\boldsymbol{x}) = \int \frac{\mathrm{d}^2 K}{(2\pi)^2}\mathrm{e}^{\mathrm{i}KX}A_K\phi_K^{(+)}(z). \tag{10}$$

where A_K is an arbitrary amplitude.

3. The effects of the surface roughness

We turn now to the specification of the surface roughness. We shall suppose that the actual surface is described by a random profile function $z = \zeta(\boldsymbol{x})$ which we assume to be distributed as a Gaussian process with zero mean, and correlation

$$\langle\zeta(\boldsymbol{X})\zeta(\boldsymbol{X}')\rangle = \delta^2 W(\boldsymbol{X}-\boldsymbol{X}') \tag{11}$$

where δ is the root-mean square (RMS) amplitude of the surface roughness. We also assume that the pair correlation function W is

$$W(\boldsymbol{X}) = \exp(-|\boldsymbol{X}|^2/a^2) \tag{12}$$

where a is the correlation length.

We note that, if the expressions for ψ, ψ_V and G—given respectively by formulae (3), (10) and (4)—are substituted into (2), the value of the exact wavefunction is obtained, provided that the derivative of its Fourier component is known at the surface. This latter quantity can be obtained from an asymptotic condition analogous to an extinction theorem. Thus, for $z \gg \delta$, it is seen that equation (2) can be written as

$$0 = W_{\boldsymbol{K}} A_{\boldsymbol{K}} (2\pi)^2 \delta(\boldsymbol{K} - \boldsymbol{R}) + \int \mathrm{d}^2 Y \, \mathrm{e}^{\mathrm{i}\boldsymbol{Y}(\boldsymbol{R}-\boldsymbol{K})} \phi_{\boldsymbol{K}}^{(-)} \psi'_{\boldsymbol{R}}(\zeta(\boldsymbol{Y})) \quad (13)$$

where

$$\psi'_{\boldsymbol{K}}(z) \equiv \frac{\mathrm{d}}{\mathrm{d}z} \psi_{\boldsymbol{K}}(z) \quad (14)$$

is the unknown quantity to be determined. Now we define Fourier transforms of all these quantities:

$$g_{\boldsymbol{K};\boldsymbol{P}}^{(\pm)} \equiv \int \mathrm{d}^2 Y \, \mathrm{e}^{-\mathrm{i}\boldsymbol{P}\boldsymbol{Y}} \phi_{\boldsymbol{K}}^{(\pm)}(\zeta(\boldsymbol{Y})) \quad (15)$$

$$\tilde{\psi}_{\boldsymbol{K};\boldsymbol{P}} \equiv \int \mathrm{d}^2 Y \, \mathrm{e}^{-\mathrm{i}\boldsymbol{P}\boldsymbol{Y}} \psi'_{\boldsymbol{K}}(\zeta(\boldsymbol{Y})). \quad (16)$$

Thus, equation (13) can be written as

$$0 = W_{\boldsymbol{R}} A_{\boldsymbol{R}} (2\pi)^2 \delta(\boldsymbol{K}) + \int \frac{\mathrm{d}^2 P}{(2\pi)^2} g_{\boldsymbol{K}+\boldsymbol{R};\boldsymbol{K}-\boldsymbol{P}}^{(-)} \tilde{\psi}_{\boldsymbol{R};\boldsymbol{P}} . \quad (17)$$

Given a random quantity f, we can write it as the sum of its mean $\bar{f}$ and its fluctuation Δf ,

$$\bar{f} \equiv \langle f \rangle \qquad \Delta f \equiv f - \bar{f} \quad (18)$$

where $\langle \cdots \rangle$ denote the average over the assembly of surface roughness functions characterized by the same RMS roughness amplitude and lateral correlation length. On the other hand, we find from (15) that

$$\langle g_{\boldsymbol{K};\boldsymbol{P}}^{(\pm)} \rangle = (2\pi)^2 \delta(\boldsymbol{P}) \bar{g}_{\boldsymbol{K}}^{(\pm)} \quad (19)$$

where

$$\bar{g}_{\boldsymbol{K}}^{(\pm)} = \langle \phi_{\boldsymbol{K}}^{(\pm)}(\zeta(\boldsymbol{Y})) \rangle . \quad (20)$$

Thus we can write (17) in the convenient form of a Fredholm integral equation

$$\tilde{\psi}_{\boldsymbol{R};\boldsymbol{K}} = \tilde{\psi}_{\boldsymbol{K};\boldsymbol{P}}^{(0)} + \int \frac{\mathrm{d}^2 P}{(2\pi)^2} \mathcal{K}_{\boldsymbol{R};\boldsymbol{K},\boldsymbol{P}} \tilde{\psi}_{\boldsymbol{R};\boldsymbol{P}} \quad (21)$$

where

$$\tilde{\psi}_{\boldsymbol{R};\boldsymbol{K}}^{(0)} \equiv -(W_{\boldsymbol{R}} A_{\boldsymbol{R}} / \bar{g}_{\boldsymbol{R}}^{(-)}) (2\pi)^2 \delta(\boldsymbol{K}) \quad (22)$$

and

$$\mathcal{K}_{R;K,P} \equiv \Delta g^{(-)}_{K+R;K-P} / \bar{g}^{(-)}_{K+R}. \tag{23}$$

This integral equation can be effectively solved by means of the 'smoothing method' (Maradudin 1986). Thus we can write, instead of (21),

$$\tilde{\psi}_{R;K} = \tilde{\psi}^{(0)}_{K;P} + \int \frac{d^2 P}{(2\pi)^2} \mathcal{M}_{R;K,P} \langle \tilde{\psi}_{R;P} \rangle \tag{24}$$

where the new kernel $\mathcal{M}$ is itself a solution of another integral equation, namely

$$\mathcal{M}_{R;K,P} = \mathcal{K}_{R;K,P} + \int \frac{d^2 Q}{(2\pi)^2} \mathcal{M}_{R;K,Q} \Delta \mathcal{M}_{R;Q,P}. \tag{25}$$

At first sight it may appear that nothing has been gained by this procedure. A complicated integral equation has been replaced by two other still more involved integral equations. But in fact two decisive simplifications have been achieved. First, equation (24) gives rise to another equation which is algebraic rather than integral and easily soluble. Furthermore, if one solves equation (25) perturbatively to some finite order (by retaining, for instance, only the first non-vanishing term in the iterated kernel approximation) this is equivalent to an *infinite* order perturbation schema applied to the original equation (21).

4. The average wavefunction

We begin by calculating the average wavefunction. Averaging both sides of equation (24) we have

$$\langle \tilde{\psi}_{R;K} \rangle = \tilde{\psi}^{(0)}_{K;P} + \int \frac{d^2 P}{(2\pi)^2} \bar{\mathcal{M}}_{R;K,P} \langle \tilde{\psi}_{R;P} \rangle \tag{26}$$

where the average kernel is

$$\bar{\mathcal{M}}_{R;K,P} \equiv \langle \mathcal{M}_{R;K,P} \rangle = (\langle \mathcal{K} \rangle + \langle \mathcal{K} \Delta \mathcal{K} \rangle + \langle \mathcal{K}(\Delta(\mathcal{K}\Delta\mathcal{K})) \rangle + \cdots)_{R;K,P} \tag{27}$$

by (24). We note that $\langle \mathcal{K} \rangle = 0$. Thus, the first non-zero term in the expansion (27) is $\bar{\mathcal{M}} \simeq \langle \mathcal{K} \Delta \mathcal{K} \rangle = \langle \Delta g^{(-)}_{K+R;K-S} \Delta g^{(-)}_{S+R;S-P} \rangle$, that is

$$\bar{\mathcal{M}}_{R;K,P} \simeq \int \frac{d^2 S}{(2\pi)^2} \frac{\langle \Delta g^{(-)}_{K+R;K-S} \Delta g^{(-)}_{S+R;S-P} \rangle}{\bar{g}^{(-)}_{K+R} \bar{g}^{(-)}_{S+R}}. \tag{28}$$

The precise form of the right-hand side of equation (28) cannot, in general, be calculated, because it depends on the correlation of a wavefunction at two different points of the surface and this depends, in turn, on the specific physical situation. (For the present case, the appropriate functions are calculated in the appendix.) In order to proceed further, let us define a new function H by

$$H^{(a,b)}_{K,K'}(Y - Y') \equiv \langle \phi^{(a)}_{K}(\zeta(Y)) \phi^{(b)}_{K'}(\zeta(Y')) \rangle / \bar{g}^{(a)}_{K} \bar{g}^{(b)}_{K'} \tag{29}$$

where $a, b = \pm$. This function depends on the difference $\boldsymbol{Y} - \boldsymbol{Y}'$, because the operation of taking averages re-establishes the translational invariance in the x–y plane. Thus, we immediately obtain

$$\langle \Delta g^{(a)}_{\boldsymbol{K};\boldsymbol{Q}} \Delta g^{(b)}_{\boldsymbol{K}';\boldsymbol{Q}'} \rangle = (2\pi)^2 \delta(\boldsymbol{Q} + \boldsymbol{Q}') \bar{g}^{(a)}_{\boldsymbol{K}} \bar{g}^{(b)}_{\boldsymbol{K}'} F^{(a,b)}_{\boldsymbol{K};\boldsymbol{K}'}(\boldsymbol{Q}) \tag{30}$$

where the function F is given by the Fourier transform

$$F^{(a,b)}_{\boldsymbol{K};\boldsymbol{K}'}(\boldsymbol{Q}) \equiv \int \mathrm{d}^2 Z \, \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\boldsymbol{Z}} \left(H^{(a,b)}_{\boldsymbol{K},\boldsymbol{K}'}(\boldsymbol{Z}) - 1 \right). \tag{31}$$

The translational invariance of averages implies furthermore that the kernel $\bar{\mathcal{M}}$ is diagonal in its two last indices

$$\bar{\mathcal{M}}_{\boldsymbol{R};\boldsymbol{K},\boldsymbol{P}} = (2\pi)^2 \delta(\boldsymbol{K} - \boldsymbol{P}) \Sigma_{\boldsymbol{R};\boldsymbol{K}} \tag{32}$$

defining the quantity Σ, analogous to a self-energy function . We note that, as anticipated, the equation (26) is thus algebraic rather than integral, with solution

$$\langle \tilde{\psi}_{\boldsymbol{R};\boldsymbol{K}} \rangle = \frac{\tilde{\psi}^{(0)}_{\boldsymbol{R};\boldsymbol{K}}}{1 - \Sigma_{\boldsymbol{R};\boldsymbol{K}}} = -\frac{W_{\boldsymbol{R}} A_{\boldsymbol{R}}}{\bar{g}^{(-)}_{\boldsymbol{R}} (1 - \Sigma_{\boldsymbol{R};\mathbf{o}})} (2\pi)^2 \delta(\boldsymbol{K}) \tag{33}$$

using (22). We note, lastly, that in the approximation in which (28) is valid,

$$\Sigma_{\boldsymbol{R};\boldsymbol{K}} = \int \frac{\mathrm{d}^S}{(2\pi)^2} F^{(-,-)}_{\boldsymbol{K}+\boldsymbol{R};\boldsymbol{S}+\boldsymbol{R}}(\boldsymbol{K} - \boldsymbol{S}). \tag{34}$$

In this way we have computed the average of the only unknown of (2), i.e. the quantity $\langle \psi'_{\boldsymbol{K}}(\zeta) \rangle$. Thus, this same equation allows us to calculate the average wavefunction of a conduction electron anywhere inside the metal. On the other hand, it is not apparent that an average wavefunction is an interesting (or even meaningful) quantity. In order to compute the reflectivity of the randomly rough surface, for instance, we need instead the average particle currents which, on account of spatial correlations, clearly cannot be expressed simply as products of average wavefunctions and their derivatives.

5. The quantum reflectivity of a rough surface

We now take the asymptotic limit $z \ll -\delta$ in equation (2), i.e. we consider a position well below the mean excursion of the surface roughness. It is seen that the wavefunction for a conduction electron in the metal is

$$\psi(\boldsymbol{x}) = \int \frac{\mathrm{d}^2 K}{(2\pi)^2} \left[A_{\boldsymbol{K}} \mathrm{e}^{\mathrm{i}\boldsymbol{K}\boldsymbol{X}} \phi^{(+)}_{\boldsymbol{K}}(z) + \int \frac{\mathrm{d}^2 Q}{(2\pi)^2} R_{\boldsymbol{K},\boldsymbol{Q}} \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\boldsymbol{X}} \phi^{(-)}_{\boldsymbol{Q}}(z) \right] \tag{35}$$

where the reflection amplitude $R_{\boldsymbol{K},\boldsymbol{Q}}$ is given by

$$R_{\boldsymbol{K},\boldsymbol{Q}} = \frac{1}{W_{\boldsymbol{Q}}} \int \mathrm{d}^2 Y \, \mathrm{e}^{\mathrm{i}\boldsymbol{Y}(\boldsymbol{K}-\boldsymbol{Q})} \phi^{(+)}_{\boldsymbol{Q}}(\zeta(\boldsymbol{Y})) \psi'_{\boldsymbol{R}}(\zeta(\boldsymbol{Y})). \tag{36}$$

By the Fourier transform formulae (15) and (16),

$$R_{K,Q} = \frac{1}{W_K} \int \frac{\mathrm{d}^2 S}{(2\pi)^2} g^{(+)}_{Q;Q-K-S} \tilde{\psi}_{K;S} \,. \tag{37}$$

We note that for the case of a perfectly smooth surface the corresponding reflection amplitude $R^{(0)}$ is

$$R^{(0)}_{K,Q} = -A_K \frac{\phi^{(+)}_K(0)}{\phi^{(-)}_K(0)} (2\pi)^2 \delta(K - Q). \tag{38}$$

The average scattered current involves not only $\langle R \rangle$ but the average $\langle R^* R \rangle$, given by

$$\begin{aligned}\langle R^*_{K,Q} R_{K,P} \rangle &= \frac{1}{W^*_Q W_P} \int \mathrm{d}^2 Y \, \mathrm{d}^2 Y' \, \mathrm{e}^{\mathrm{i}[-(K-Q)Y+(K-P)Y']} C_{K;Q,P}(Y - Y') \\ &= (2\pi)^2 \delta(Q - P) r_{K,Q}\end{aligned} \tag{39}$$

where

$$r_{K,Q} = \frac{1}{|W_Q|^2} \int \mathrm{d}^2 Z \, \mathrm{e}^{-\mathrm{i}(K-Q)Z} C_{K;Q,Q}(Z) \tag{40}$$

and

$$\begin{aligned}C_{K;Q,P}(Z) &= \langle \phi^{(+)*}_Q(\zeta(Y)) \psi'^*_K(\zeta(Y)) \phi^{(+)}_P(\zeta(Y - Z)) \psi'_K(\zeta(Y - Z)) \rangle \\ &= f^*_{K,Q} f_{K,P} [L_{K;Q,P}(Z) + 1]\end{aligned} \tag{41}$$

by the properties of averages, where

$$L_{K;Q,P}(Z) = \frac{\langle \Delta[\phi^{(+)*}_Q(\zeta(Y)) \psi'^*_K(\zeta(Y))] \Delta[\phi^{(+)}_P(\zeta(Y - Z)) \psi'_K(\zeta(Y - Z))] \rangle}{f^*_{K,Q} f_{K,P}} \tag{42}$$

and

$$f_{K,Q} = \langle \phi^{(+)}_Q(\zeta(Y)) \psi'_K(\zeta(Y)) \rangle. \tag{43}$$

Thus, the function r separates naturally into *specular* and *diffuse* contributions $r^{(\mathrm{s})}$ and $r^{(\mathrm{d})}$, which combine additively

$$r_{K,Q} = r^{(\mathrm{s})}_K (2\pi)^2 \delta(K - Q) + r^{(\mathrm{d})}_{K,Q} \tag{44}$$

where, according to (40) and (41)

$$r^{(\mathrm{s})}_K = |f_{K,K}|^2 / |W_K|^2 \tag{45}$$

and

$$r^{(\mathrm{d})}_{K,Q} = \frac{|f_{K,Q}|^2}{|W_Q|^2} \int \mathrm{d}^2 Z \, \mathrm{e}^{-\mathrm{i}(K-Q)Z} L_{K;Q,Q}(Z). \tag{46}$$

According to (38), we see that a perfectly smooth surface can produce only specular reflections.

In an earlier treatment of this scattering problem one of us, following Shen and Maradudin (1980), performed a separation of the scattered intensity into specular and diffuse contributions which was similar in form, although different in principle from the present one (Moraga 1987). Its purpose was, however, the same. Given a current incident with a certain direction $\boldsymbol{K}$, the second term in the RHS of (35) allows us to compute the particle current scattered by the randomly rough surface. According to (44) this scattered current divides naturally into a specular and a diffuse contribution, which we identify with the specular and diffuse parts of the distribution function. Thus, the specularity parameter appearing in the boundary conditions for the Boltzmann transport equation is taken here to be identical with the specular part of the quantum reflectivity function; i.e. the ratio of the average specularly scattered current to the incident current.

This procedure can be justified in general terms by making use of microscopic considerations. As is well known, the quantum transport theory proceeds not from a transport equation, but by identifying the distribution function with certain one-particle Green function (Kadanoff and Baym 1962, Rammer and Smith 1986). Thus, the problem of the spatial boundary conditions appropriate for this distribution function can be related to the corresponding problem for the Green function, which is in turn related to that of the wavefunction by a well known prescription.

In the present case, this average is computed as follows. First, from (15) and (16)—or, rather, their inverses—we see that

$$f_{\boldsymbol{K},\boldsymbol{Q}} = \int \frac{\mathrm{d}^2 S\, \mathrm{d}^2 S'}{(2\pi)^4} \mathrm{e}^{\mathrm{i}(\boldsymbol{S}+\boldsymbol{S}')\mathrm{Y}} \langle g^{(+)}_{\boldsymbol{Q};\boldsymbol{S}} \tilde{\psi}_{\boldsymbol{K};\boldsymbol{S}'} \rangle . \tag{47}$$

Furthermore, we have from (24)

$$\begin{aligned} \langle g^{(+)}_{\boldsymbol{Q};\boldsymbol{S}} \tilde{\psi}_{\boldsymbol{K};\boldsymbol{S}'} \rangle &= \bar{g}^{(+)}_{\boldsymbol{Q}} \tilde{\psi}^{(0)}_{\boldsymbol{K}} (2\pi)^4 \delta(\boldsymbol{S})\delta(\boldsymbol{S}') + \int \frac{\mathrm{d}^2 S''}{(2\pi)^2} \langle g^{(+)}_{\boldsymbol{Q};\boldsymbol{S}} \mathcal{M}_{\boldsymbol{K};\boldsymbol{S}',\boldsymbol{S}''} \rangle \langle \tilde{\psi}_{\boldsymbol{K};\boldsymbol{S}''} \rangle \\ &= \bar{g}^{(+)}_{\boldsymbol{Q}} \tilde{\psi}^{(0)}_{\boldsymbol{K}} \left[(2\pi)^4 \delta(\boldsymbol{S})\delta(\boldsymbol{S}') + \frac{\langle g^{(+)}_{\boldsymbol{Q};\boldsymbol{S}} \mathcal{M}_{\boldsymbol{K};\boldsymbol{S}',\boldsymbol{0}} \rangle}{\bar{g}^{(+)}_{\boldsymbol{Q}} (1 - \Sigma_{\boldsymbol{K},\boldsymbol{0}})} \right] \end{aligned} \tag{48}$$

by (33). On the other hand, the lowest non-zero contribution to the average of the second term in the RHS of this equation is

$$\begin{aligned} \frac{\langle g^{(+)}_{\boldsymbol{Q};\boldsymbol{S}} \mathcal{M}_{\boldsymbol{K};\boldsymbol{S}',\boldsymbol{0}} \rangle}{\bar{g}^{(+)}_{\boldsymbol{Q}}} &\simeq \frac{\langle g^{(+)}_{\boldsymbol{Q};\boldsymbol{S}} \mathcal{K}_{\boldsymbol{K};\boldsymbol{S}',\boldsymbol{0}} \rangle}{\bar{g}^{(+)}_{\boldsymbol{Q}}} = -\frac{\langle g^{(+)}_{\boldsymbol{Q};\boldsymbol{S}} \Delta g^{(-)}_{\boldsymbol{S}'+\boldsymbol{K};\boldsymbol{S}'} \rangle}{\bar{g}^{(+)}_{\boldsymbol{Q}} \bar{g}^{(-)}_{\boldsymbol{S}'+\boldsymbol{K}}} \\ &= -(2\pi)^2 \delta(\boldsymbol{S}+\boldsymbol{S}') F^{(+,-)}_{\boldsymbol{Q},\boldsymbol{K}-\boldsymbol{S}}(\boldsymbol{S}) \end{aligned} \tag{49}$$

by (25), (23) and (31). Thus, by (47)

$$f_{\boldsymbol{K},\boldsymbol{Q}} = \bar{g}^{(+)}_{\boldsymbol{Q}} \tilde{\psi}^{(0)}_{\boldsymbol{K}} \left[1 - (1 - \Sigma_{\boldsymbol{K},\boldsymbol{0}})^{-1} \int \frac{\mathrm{d}^2 S}{(2\pi)^2} F^{(+,-)}_{\boldsymbol{Q};\boldsymbol{K}-\boldsymbol{S}}(\boldsymbol{S}) \right] \tag{50}$$

and, in the approximation in which (34) is valid

$$r_K^{(s)} = \frac{|\bar{g}_Q^{(+)} \tilde{\psi}_K^{(0)}|^2}{|W_K|^2} \left| 1 - \left[1 - \int \frac{d^2 S}{(2\pi)^2} F_{K;K+S}^{(-,-)}(-S) \right]^{-1} \int \frac{d^2 S}{(2\pi)^2} F_{K;K-S}^{(+,-)}(S) \right|^2 . \tag{51}$$

In order that this reflected intensity can be properly interpreted in terms of a quantum reflectivity function, it is necessary that the wavefunctions have correct asymptotic properties. In our case we ought to take, for instance, as wavefunction $U(\alpha, \pm x) + \mathrm{i}\Gamma(\frac{1}{2} - \alpha)V(\alpha, \pm x)$ in (7) instead of just $U(\alpha, \pm x)$, and calculate the reflected intensity in the limit in which these functions resemble plane waves (Abramowitz and Stegun 1965) . Alternatively, we can proceed by calculating the ratio of the intensity reflected by the rough surface to the intensity reflected by a perfectly smooth surface. Thus, as by (22) the first factor of the RHS of (51) is just $|\bar{g}_K^{(+)}/\bar{g}_K^{(-)}|^2$, the reflectivity function is obtained from it by a further division by $r_K^{(0)} = |\phi^{(+)}(0)|^2/|\phi^{(-)}(0)|^2$.

The quantum reflectivity function p is thus

$$p_K = \frac{|\bar{g}_K^{(+)} \phi^{(-)}(0)|^2}{|\bar{g}_K^{(-)} \phi^{(+)}(0)|^2} \left| 1 - \left[1 - \int \frac{d^2 S}{(2\pi)^2} F_{K;K+S}^{(-,-)}(-S) \right]^{-1} \int \frac{d^2 S}{(2\pi)^2} F_{K;K-S}^{(+,-)}(S) \right|^2 \tag{52}$$

accurate up to terms of order F.

6. The specularity function

For practical purposes, a simplified form of the reflectivity function (52) can be used. We note first that $\bar{g}_K^{(\pm)} = \phi^{(\pm)}(0) + O(\delta^2)$. Furthermore, the rational function on the RHS of (52) can be replaced by an exponential function of the appropriate variables, maintaining the accuracy in F. Thus we can write

$$p_K = \exp\left\{ 2 \,\mathrm{Re} \int \frac{d^2 Q}{(2\pi)^2} \left[F_{K;Q+K}^{(-,-)}(Q) - F_{K;Q+K}^{(+,-)}(Q) \right] \right\} \tag{53}$$

also exact up to terms of order F. As the wavevector of a conduction electron has necessarily a fixed length k_F, the subindex K in (53) denotes in fact the direction in which the electron arrives at the rough surface. In the semiclassical formulations which start from the Boltzmann transport equation, this dependence is important because the transport coefficients turn out to be integrals over the angles defining this direction.

The semiclassical and quantum formulation are related as follows. Under a magnetic field applied in the x-direction the wavevector of the electron as a function of time t is

$$\begin{aligned} k_x(t) &= k_F \cos\theta \\ k_y(t) &= k_F \cos(\omega t + \phi) \sin\theta \\ k_z(t) &= -k_F \sin(\omega t + \phi) \sin\theta \end{aligned} \tag{54}$$

where ω is the same as before. Thus, the orbit of an electron passing at $t = 0$ throughout the point $x = 0$, $y = r\sin\phi\sin\theta$ and $z = 0$ is

$$\begin{aligned} x(t) &= \omega r t\cos\theta \qquad y(t) = r\sin(\omega t+\phi)\sin\theta \\ z &= r[\cos(\omega t+\phi) - \cos\phi]\sin\theta. \end{aligned} \tag{55}$$

The projection of this orbit on the y–z plane is a circle of radius $r = \hbar k_F/m\omega = \hbar k_F c/eB$ centred at $z_0 = \hbar k_y(t=0)/m\omega$, in accordance with equation (7). We note that this radius r is related to the parameter α of (8) by

$$r = \left(\frac{-2\hbar\alpha}{m\omega}\right)^{1/2} \tag{56}$$

that θ is the angle between the trajectory at $t = 0$ and the magnetic field, and that the angle of incidence Θ is given by

$$\cos\Theta = -\sin\phi\sin\theta. \tag{57}$$

We note that formula (53) has contributions of all orders on the RMS amplitude of the surface roughness δ and the lateral correlation length a and that it further depends on the strength and direction of the applied magnetic field. The latter is, of course, the main advantage of the present treatment over earlier formulations. Formerly, experimental data were interpreted in terms of a phenomenological parameter p or of the specularity function of Soffer (1967), both entirely independent of the magnitude and direction of the magnetic field. In the present case, the appropriate wavefunctions are, by (7), parabolic cylinder functions. Fortunately, the average of a parabolic cylinder function is another parabolic cylinder function, and the correlation of two such functions can be written as a series of products of two other parabolic cylinder functions (see the appendix). This makes it possible to calculate analytic formulae for the specularity function in this case.

In figures 2–5 we have plotted the values of this specularity as a function of the angle of incidence Θ in which the electron, following a classical trajectory, would arrive at the average surface, and θ, which is the angle made by this trajectory at the point of incidence with the direction of the magnetic field. All figures correspond to values of $ak_F = 0.5$, $\delta k_F = 0.25$, while the strength of the magnetic field B (in units of $\hbar c k_F^2/2e$) varies from 2 to 4. It is seen that, at low fields, the specularity function shows a considerable angular anisotropy although exhibiting a certain region in which the surface appears to be nearly specular. When the magnetic field is increased, these extremes of behaviour diminish, and the specularity becomes a much smoother function of the angles. We note that the minimum of the specularity occurs at intermediate values of θ, suggesting the interest of performing magnetoresistance measurements in thin films as a function of the angle between the magnetic and electric fields.

7. The longitudinal magnetoresistance of thin films

The longitudinal conductivity σ of a thin metal film, i.e. E parallel to B and to the plane of the film) in units of the bulk conductivity σ_∞, was calculated by Koenisberg

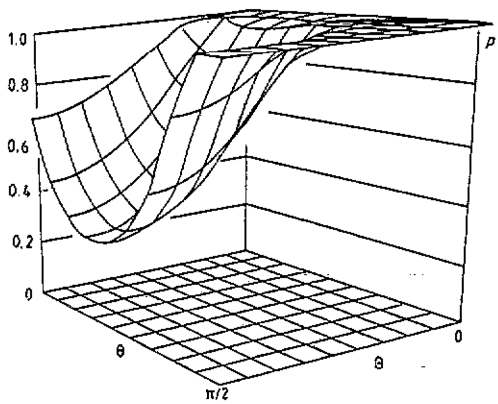

Figure 2. The specularity function of a randomly rough surface as a function of Θ and θ, which are the angles that the classical trajectory makes with the average surface and the magnetic field, respectively, at the point of incidence. Here $a\,k_F = 0.5$, $\delta k_F = 0.25$ and $B = 2$ (B in units of $\hbar c k_F^2/2e$).

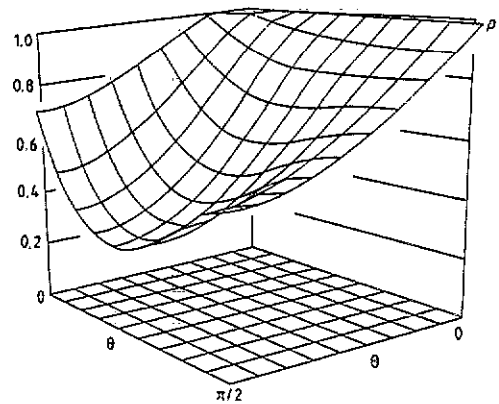

Figure 3. As in figure 2, except that $B = 2.5$.

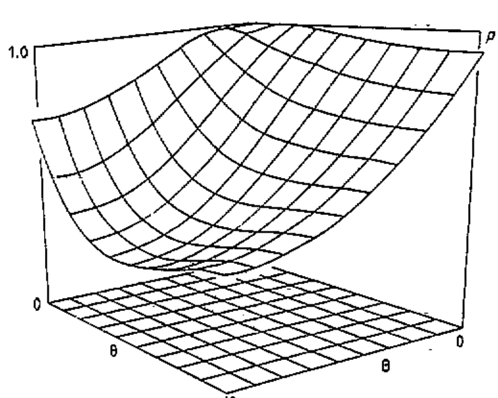

Figure 4. As in figure 2, except that $B = 3$.

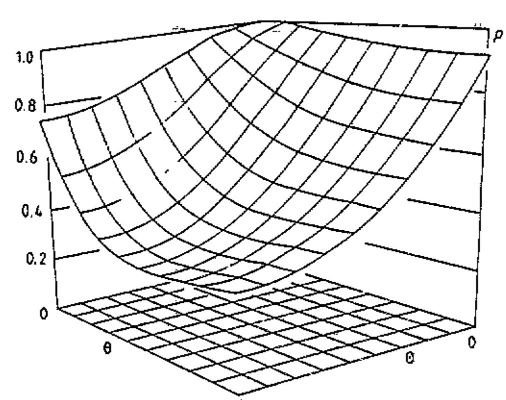

Figure 5. As in figure 2, except that $B = 4$.

(1953), Kao (1965), Ditlefsen and Lothe (1966), McGill (1968) and Way and Kao (1972). All these authors assumed, besides the validity of the Boltzmann transport equation, a spherically symmetrical mean-free path and Fermi surface, and that the boundary scattering could be described by a specularity parameter. In the notation of the present paper, this conductivity is

$$\frac{\sigma}{\sigma_\infty} = 1 - \frac{3}{4\pi d}\int \mathrm{d}\theta\,\sin\theta\cos^2\theta \int \mathrm{d}z \int \mathrm{d}\phi\,(1-p)\frac{\exp(-\psi/\eta)}{1-p\exp(-\Psi/\eta)} \tag{58}$$

where d is the thickness of the film, $\eta = l/r\sin\theta$ (l is the mean-free path), ψ is the angle traversed by an electron on its classical path from a point on the surface to a generic point in the bulk and Ψ is the angle traversed along the same orbit if it were extended until the electron hits a boundary again. These angles can be expressed in terms of θ, ϕ and z (Way and Kao 1972). The specularity function p is given by (53), where the parallel component of the wavevector K is related to the angles by (54) evaluated at $t = 0$.

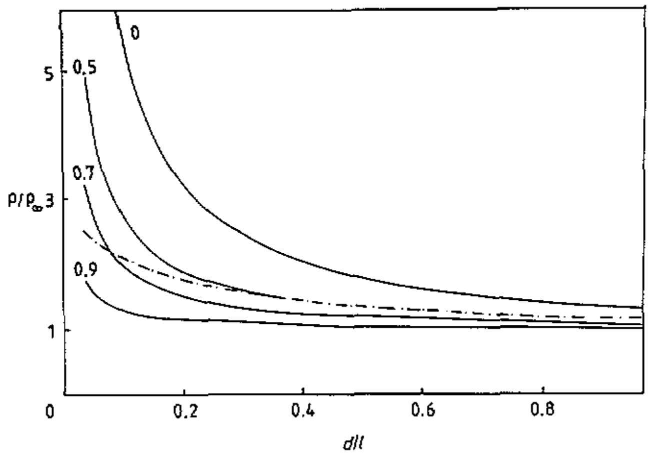

Figure 6. The resistivity ρ (in units of the bulk resistivity ρ_∞) of a thin metallic film of thickness d (in units of the mean-free path l) for the case when the electric and magnetic fields are both longitudinal and parallel. Here $ak_F = 0.5$, $l = 5$, $\delta k_F = 0.25$ and $B = 2$. The discontinuous line is the magnetoresistance calculated according to the theory of this paper; the continuous lines are calculated for $p =$ a constant having the values shown.

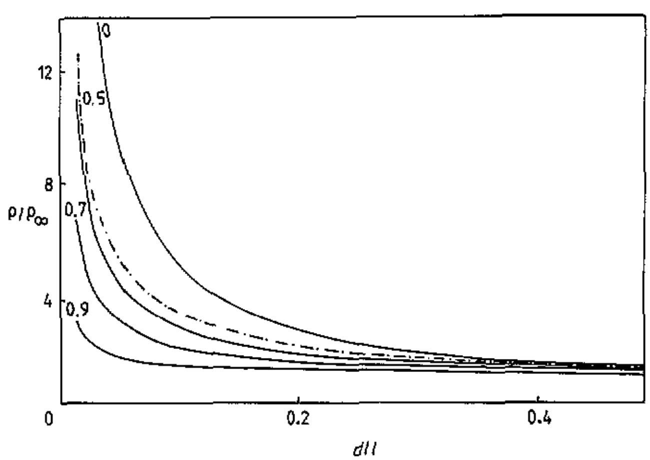

Figure 7. As in figure 6, except that $\delta k_F = 0.125$ and $B = 5.5$.

In figures 6 and 7 we show calculations of this longitudinal magnetoresistance of thin metallic films as a function of thickness d in units of the mean-free path l. In both figures, $ak_F = 0.5$ and $l = 5$; in figure 6 $\delta k_F = 0.25$ and $B = 5$, and in figure 7, $\delta k_F = 0.125$ and $B = 5.5$. The curves calculated using the present approach are compared with curves computed from the usual theory in which p is a constant (Way and Kao 1972). It is apparent that for high enough values of the magnetic field, the magnetoresistence computed according to the present theory is similar in shape to one of those obtained from the usual formalism (figure 7). On the contrary, for a somewhat smaller field, the behaviour predicted by the theory presented here is qualitatively different from the magnetoresistence calculated according to the older formalism (figure 6); corresponding in appearance to surfaces which become smoother as the thickness of the film is diminished. Of course if the magnetic field is decreased further the magnetoresistance itself also decreases, and the new results tend to conform again with those obtained by the usual method.

8. Conclusions

A priori, one should not expect much of a transport theory based on the Boltzmann equation. In fact, this treatment gives surprisingly correct results about the electrical resistivity of solids. In a well known classical paper, for instance, Prange and Kadanoff (1964) derived a transport equation for the case of phonons and electrons using the formulation of Kadanoff and Baym (1962). They wrote that their results 'lead one to believe that there is nothing to worry about the use of the Boltzmann equation throughout the entire temperature range. With the Landau correction, ordinary transport properties should be capable of description to a very high accuracy'. They also concluded that the DC resistivity 'is unaffected by many-body effects'. In recent years, the transport properties of solids have been further and extensively explored by means of quantum field-theoretical methods (Rammer and Smith 1986, Mahan 1987). The use of these methods has provided additional microscopic justification for the use of the Boltzmann equation, and has shown how this approach should be generalized in order to take into account renormalization and lifetime effects.

When the treatment based on the Boltzmann equation is extended to the case of small samples, however, the results have not been so good. Sambles and a number of collaborators (Sambles and Elsom 1980, Sambles and Preist 1982, Preist and Sambles 1986) have analysed the discrepancies between theory and experiment in this case, and have shown that they originate not from the Boltzmann equation itself, but from the use of inadequate boundary conditions. When the correct conditions are used, however, surprisingly good agreements are obtained, even in the case of metals with quite complicated Fermi surfaces.

This paper has been concerned with setting up just these boundary conditions for the case of scattering by a random surface in the presence of a magnetic field. The new boundary conditions, in the form of an angle-dependent and field-dependent specularity function p, have been obtained by solving the Schrödinger equation appropriate for this situation approximately. Besides its dependence on the strength and direction of the magnetic field, this p is a function of the RMS average of the departure of the surface from flatness and of the lateral correlation length. By exploiting the properties of the parabolic cylinder functions (the wavefunctions of the electrons in this case), we have computed explicit formulae for the correlation functions, whose Fourier transforms determine the value of p.

In view of these considerations, it appears reasonable to suppose that the electrical resistivities of thin films and wires computed using these improved boundary conditions will be in good accord with experience in this case too. For instance, we have found that the spatial anisotropy of the new specularity parameter results in significant differences between the longitudinal magnetoresistance of thin films predicted by the new and the old formulations at intermediate values of the magnetic field strength. Thus, one should be able to distinguish between these two theories by means of resistivity measurements made on films whose surface characteristics have been independently determined.

Appendix

Let $U(\alpha, x)$ denote the parabolic cylinder function of argument x and parameter α (Abramowitz and Stegun 1965). If ζ is a Gaussian random variable with zero mean and standard deviation δ, and $\langle\cdots\rangle$ denotes the average taken over this probability distribution, then

$$\langle U[\alpha, \beta(\zeta + z_0)]\rangle = \frac{(1+\beta^2\delta^2/2)^{\alpha/2-1/4}}{(1-\beta^2\delta^2/2)^{\alpha/2+1/4}} \exp\left[\frac{z_0^2\beta^4\delta^2}{8(1-\beta^4\delta^4/4)}\right] U\left(\alpha, \frac{\beta z_0}{\sqrt{1-\beta^4\delta^4/4}}\right).$$

This can be most easily proved proceeding from the integral representation of U. By making use of its asymptotic expansion, one can see that for $\beta z_0 > 0$—in spite of appearances—this average is regular at the point $\beta^2\delta^2 = 2$.

If, furthermore, ζ_1 and ζ_2 are two such random variables with correlation $\delta^2 W$, it can also be shown that

$$\begin{aligned}\langle U[\alpha_1, \beta_1(\zeta_1+z_{01})]U[\alpha_2, \beta_2(\zeta_2+z_{02})]\rangle &= \exp\left\{\frac{1}{d}\left[\frac{b_1^2}{4a_{11}} + \frac{b_2^2}{4a_{22}} + c\right]\right\} d^{(\alpha_1+\alpha_2)/2} \\ &\quad\times \sum_{n=0}^{\infty} \frac{(a_{12})^n}{(a_{11})^{(\alpha_1+1/2+n)/2}(a_{22})^{(\alpha_2+1/2+n)/2}} \frac{(\alpha_1-\frac{1}{2})_n(\alpha_2-\frac{1}{2})_n}{n!} \\ &\quad\times U(\alpha_1+n, \tilde{z}_1)U(\alpha_2+n, \tilde{z}_2)\end{aligned}$$

where

$$z_1 = b_1/(a_{11})^{1/2} \qquad \tilde{z}_2 = b_2/(a_{22})^{1/2}$$

$$a_{11} = d_1d_2 - \alpha_1^2\delta^2 d_2 + \beta_1^2\beta_2^2\delta^4 W^2/4$$

$$a_{22} = d_1d_2 - \alpha_2^2\delta^2 d_1 + \beta_1^2\beta_2^2\delta^4 W^2/4$$

$$a_{12} = \beta_1\beta_2\delta^2 W$$

$$b_1 = d_1d_2\beta_1 z_{01} - \beta_1^3 z_{01}\delta^2 d_2/2 - \beta_1\beta_2^2\delta^2 z_{02}W/2$$

$$b_2 = d_1d_2\beta_2 z_{02} - \beta_2^3 z_{02}\delta^2 d_1/2 - \beta_1^2\beta_2\delta^2 z_{01}W/2$$

$$c = \beta_2^4\delta^2 z_{02}^2 d_1/8 + \beta_1^4\delta^2 z_{01}^2 d_2/8 - d_1d_2(\beta_1^2 z_{01}^2 + \beta_2^2 z_{02}^2)/4 + \beta_1^2\beta_2^2\delta^2 z_{01}z_{02}W/4$$

$$d_1 = 1 + \beta_1^2\delta^2/2 \qquad d_2 = 1 + \beta_2^2\delta^2/2$$

and

$$d = d_1d_2 - \beta_1^2\beta_2^2\delta^4 W^2/4.$$

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