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An obstacle in a quantum film: the density dipole and extra resistance

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Abstract. The additional resistivity of a quantum film due to an obstacle is investigated. The film is treated by a semi-classical formalism whilst the obstacle is characterized by its quantum mechanical scattering cross-section. The film intrinsic scattering mechanism allows for the adaptation of an arbitrary density distribution to a characteristic 'ideal' distribution over the channels. Special attention is paid to the multiple-scattering cycles between the obstacle and its surroundings, i.e., the scattering background of the film. The analysis of these backscattering processes leads to a self-consistent equation for the current density incident on the scatterer. For the general case of an arbitrarily strong obstacle and many conducting channels, this equation system can be solved only numerically. However, the formalism becomes handy if the obstacle scatters only weakly. A condition is found for the obstacle to be considered as weak. On the other hand, if one considers only one conducting channel it is possible to solve the transport problem analytically even for a strong obstacle. In this case, we find an expression for the resistivity which contains the scattering cross-section in a non-linear manner. This non-linearity was already predicted in 1957 by Landauer.

1. Introduction

Electronic transport through very thin films is a field which still attracts great interest among experimental as well as theoretical physicists. One of the first but nevertheless very successful attempts to describe the electronic transport in thin films with rough surfaces was the Fuchs theory [1] and its extensions and generalizations [2, 3]. Fuchs' theory rests on the description of the rough surface with a single 'specularity' parameter, and even very sophisticated non-classical theories re-cover its results in the thick-film limit. Whereas this theory was basically classical, quantum mechanical approaches [4, 5, 6, 7, 8, 9] have been developed. A quantum mechanical treatment of transport in thin films reveals quantum size effects which are particularly strong in the presence of surface roughness. The most remarkable feature is a roughness-induced d^{-6} dependency of the resistivity if the film thickness d tends to zero [10, 6, 11, 8, 9].

On the experimental side, recent film growth techniques have made it possible to manufacture ultra-thin films with a nanometre scale thickness [12, 13, 14, 15, 16] and even with atomically sharp interfaces [17]. Is has been noticed by many authors [18, 19, 20, 21, 22] that these films show a bimodal roughness spectrum composed of a micro-roughness on the atomic scale and large terraces of approximately constant height.

The influence of the micro-roughness on the resistance of thin films seems to be well-investigated. The underlying model of micro-roughness is mostly that of a statistically corrugated surface with a correlation length and an RMS, both small compared to the Fermi wavelength of the electrons [8]. In a scattering picture using bumps randomly distributed over the surface [9, 23] this means that the extension R_{ob} of the bosses forming the roughness is much smaller than λ_F. For a broad review on this topic see [24, 25].

On the other hand, a question still to be solved is that of how terraces with an extension comparable to or even larger than λ_F act on the electronic transport in quantum films. For such terraces the simple s-scatterer picture definitely fails, and one is forced to look for a well-suited method to handle the quasi-two-dimensional scattering problem. We will show here that it is possible, in a semi-classical approach, to express the additional resistivity of an obstacle in an otherwise homogeneous resistive quantum film as a function of its scattering cross-section $\sigma_{nn'}(\varphi, \varphi')$.

In order to have an appropriate tool to investigate this problem we take advantage of a recently developed theory [26]. There, the influence of an obstacle on the transport through a resistive quantum wire is the major objective. We have extended the theory to a quasi-two-dimensional system (quantum film), retaining the same assumptions as made in [26]. We only recall them here. More details and the underlying physical concept, however, can be found in [26].

(i) The system is filled with a uniform background of randomly distributed weak isotropic scatterers. The finite mean free path (MFP) gives rise to a certain intrinsic film resistivity.

(ii) The de Broglie wavelength of the particles is much smaller than the MFP. The condition $\lambda_F/l \ll 1$ is the basic condition that renders the quasi-classical treatment of the in-plane motion possible at all.

(iii) As the MFP is much larger than the film thickness, the lateral quantization is conserved. The in-plane motion, however, is described in classical terms as a diffusion problem, neglecting all interference effects that would occur in a consequent quantum mechanical treatment.

(iv) In our model, the current is driven by a density gradient which takes a constant value far from the obstacle. After having solved the diffusion problem we transform the results to the usual field-driven case using the Einstein relation.

(v) The results for the resistivity are given at zero temperature. In this limit, all problems concerning ensemble averages disappear since only particles with the Fermi energy contribute to the transport. Both density and current density are taken at the Fermi level. All scattering processes do not change the particle energy.

The scattering background allows for transitions between different lateral modes and different directions of motion. In the homogeneous film, this leads to a distribution where the density of each individual channel is proportional to the channel-specific local density of states (LDOS). In the quasi-two-dimensional case, the channel LDOS does not depend on energy, and hence all channel densities are equal in the homogeneous film. If this distribution is disturbed (e.g., by scattering at an obstacle), the film background relaxes the densities in a way that the deviation from the 'ideal' distribution decays with increasing distance from that obstacle. Because of its ability to equilibrate disturbed density distributions, such a system is called 'adaptive' [26].

An approach similar to the present one was demonstrated by Chu and Sorbello [27] where much emphasis was laid on the effects of multiple quantum mechanical scattering between the walls and the obstacle. Here we assume the obstacle scattering cross-section comprising all those effects to be given. As in [27], we calculate a long-range density dipole around the obstacle which gives rise to the additional resistance wanted. This is the so-called residual resistivity dipole (RRD) first introduced by Landauer in his seminal 1957 paper [28] (see below). In the calculation of the RRD, the angle- and channel-dependent current density $j_n^{\mathrm{inc}}(\varphi)$ incident on the obstacle holds a key position. In [27] it is assumed, within a Boltzmann model, that $j_n^{\mathrm{inc}}(\varphi)$ is a shifted Fermi circle. Here we show that this can be justified only if the obstacle scatters weakly. We will see that the incident currents are in general very involved quantities that are to be determined self-consistently: particles once scattered by the obstacle can also be scattered by the film background and return to the obstacle again, thus forming anew an incident current. Therefore also the near density field is generally influenced by the relaxation mechanism of the film, in contrast to what is indicated by some remarks in [27]. From a detailed analysis of these repeated scattering relaxation processes we can derive a criterion for the applicability of the said approximation as used in [27].

If we restrict ourselves to a two-dimensional system (which is practically done by taking only one conducting lateral mode), we can solve the self-consistency problem for the incident currents analytically, without restriction to weak scatterers. We get a very simple expression for the resistivity due to an obstacle. Its scattering cross-section σ enters the extra film resistivity in a non-linear form, $\delta\rho_{\mathrm{film}} \sim \sigma/(1-\alpha\sigma)$ where the product $\alpha\sigma$ is a quantity comprising the effect of repeated scattering from the obstacle into the film medium and back to the obstacle. Summing up all these backscattering cycles, one finds the value of the enhancement factor to be $(1-\alpha\sigma)^{-1}$. Based on the same multiple-scattering arguments, Landauer predicted such a non-linear behaviour already in his very first works on the RRD concept [28, 29]. Even though Landauer addressed systems with arbitrary dimensionality ($d = 1$–3) in his general considerations, it seems that only the result for one-dimensional systems became widely recognized in transport theory. He found that the extra resistance of an obstacle with reflection coefficient r is proportional to $r/(1-r)$ showing a pronounced non-linear dependence on the scattering behaviour. It is clear that in higher dimensions the non-linearity is not as strong as in the one-dimensional case for the particles can circumvent the obstacle. To our best, but restricted, knowledge, we have derived for the first time an analytical formula for the resistance which takes into account these multiple-backscattering processes for $d = 2$. This can be viewed as a generalization of the one-dimensional Landauer formula.

In multi-channel wires, the mathematical expressions become more complicated. This prevents us from solving the problem for the general case. However, one could find the solution of the equation system arising in the form of a perturbational series.

There are, throughout the paper two restrictions to the obstacle:

(i) its extension R_{ob} is small compared with the film MFP;
(ii) its scattering cross-section obeys the symmetry relation $\sigma_{nn'}(\varphi,\varphi') = \sigma_{nn'}(\varphi-\varphi')$.

The first condition ensures that it is possible to treat the density near field and the far field separately. The second restriction is not of principal nature, but it helps substantially to simplify the formulae.

The organization of this paper is as follows: in section 2, we will formulate the basic equations for the kinetics in the homogeneous film and find their long-range and relaxation solutions, respectively. We will show how to calculate the RRD from the scattering behaviour of the obstacle. Section 3 will make contact between the RRD and the additional resistivity. Section 4 then illustrates the application of our method to some well-investigated models and shows that the results obtained are sensible. Final conclusions are given in section 5. Appendix A shows how to obtain the basic differential equation used throughout the paper from the kinetic equation for the film. In appendix B, the mathematical procedure for calculating incident currents from densities around the obstacle is sketched. There, we will derive the condition for a scatterer to be considered as weak.

2. Densities and currents in the film

2.1. Kinetics of a quantum film

Assume a film of thickness d where particles move in N channels labelled n. We decompose both the 2D current density $j_n(r)$ and the 2D particle density $\varrho_n(r)$ of each lateral mode according to particles moving into all possible directions φ:

$$\varrho_n(r) = \int \mathrm{d}\varphi \; \varrho_n(r, \varphi) \tag{1}$$

$$j_n(r) = \int \mathrm{d}\varphi \; \hat{e}_\varphi j_n(r, \varphi) \tag{2}$$

where $\hat{e}_\varphi$ is the unit vector in the φ direction. Density and current density are connected by the relation $j_n(r, \varphi) = v_n \, \varrho_n(r, \varphi)$. This decomposition implies the neglect of all quantum mechanical interference. Here and in the following, angular integrations are performed in the interval $(0, 2\pi)$. Note that all densities and currents throughout this paper are related to particles at the Fermi energy (refer to section 1). In the diffusion problem to be solved here, a constant equilibrium density can always be added without changing the results.

There are transitions between different modes and angles, respectively, due to the resistive background. We introduce rates γ_{nm} for the transition from mode m into mode n. The transition rates are proportional to the LDOS of the channel the particle is scattered into. This means in a two-dimensional model where the LDOS of each channel is independent of the energy that

$$\gamma_{nm} = \gamma_{mn}. \tag{3}$$

The scattering mechanism is assumed to be isotropic; thus no angles occur in γ_{nm}, and it is assumed to be strictly local, which allows us to state the simple kinetic equation

$$\hat{e}_\varphi \frac{\partial}{\partial r} j_n(r, \varphi) = \frac{1}{2\pi} \sum_m \gamma_{nm} \varrho_m(r) - \gamma_n \varrho_n(r, \varphi) \tag{4}$$

where $\hat{e}_\varphi \; \partial / \partial r$ is the derivative in the φ direction, and

$$\gamma_n = \sum_m \gamma_{mn}.$$

Here and in the following, the sums are taken over all conducting channels. After an integration of the kinetic equation over all angles we get

$$\frac{\partial}{\partial r} j_n(r) = \sum_m \left[\gamma_{nm} \varrho_m(r) - \gamma_{mn} \varrho_n(r) \right]. \tag{5}$$

The total current

$$\sum_n j_n$$

is stationary, of course, whilst the channel currents are source-free only if the density is the same for all channels. This is what we called in section 1 the 'ideal', i.e. unperturbed, density distribution.

From the kinetic equation we can derive a non-local relation between the current $j_n(r)$ and the density gradient at all points of the film. Details are shown in appendix A. We repeat the result equation (A2) found there:

$$j_n(r) = -\frac{v_n}{2\pi\gamma_n}\int \mathrm{d}\varphi\ \hat{e}_\varphi \int_0^\infty \mathrm{d}\tilde{r}\exp\left(-\frac{\tilde{r}\gamma_n}{v_n}\right)\sum_m \gamma_{nm}\left(\hat{e}_\varphi\frac{\partial}{\partial r}\right)\varrho_m(r-\hat{e}_\varphi\tilde{r}). \tag{6}$$

We note that the currents are generally determined not only by the local density gradient but also by contributions from a region around r which is of order γ_n/v_n. If the density gradient is constant within this range we find the usual two-dimensional diffusion law

$$j_n(r) = -\frac{l_n v_n}{2}\frac{\partial}{\partial r}\varrho_n(r) \tag{7}$$

with $l_n = v_n/\gamma_n$. Furthermore, we find from equation (6) that the current distribution over the channels in the case of an ideal, i.e., relaxed, density distribution is $j_n \sim v_n l_n$.

Introducing equation (6) into (5) (see appendix A for a major simplification) gives the linear differential equation system

$$l_n v_n \frac{\partial^2}{\partial r^2}\varrho_n(r) = \sum_m \left[\gamma_{mn}\varrho_n(r) - \gamma_{nm}\varrho_m(r)\right]. \tag{8}$$

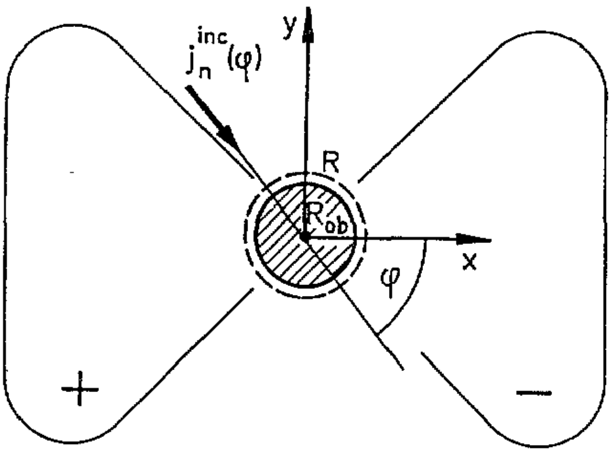

Figure 1. The obstacle (hatched) centred at the origin is entirely enclosed by the auxiliary circle (dashed) with radius R. One possible direction of an incident current is sketched. The asymptotic current flows in the x direction ($\varphi = 0$). The current-induced density dipole is indicated by the large regions labelled + for the excess density and − for the deficit, respectively.

Now we look for solutions of equation (8). We will restrict ourselves to solutions outside a circle $\{R\}$ with radius R where they obey a Dirichlet boundary condition $\varrho_n(R) = \varrho_n^c(R)$. ($\varrho^c$ itself will be obtained from the scattering behaviour of the obstacle in section 2.3.)

There are two kinds of solutions, detailed below.

(i) We make the *ansatz*

$$\varrho_{\lambda pn}(r) = \hat{\varrho}_{\lambda n}\cos p\varphi\frac{H_p^{(1)}(\mathrm{i}\kappa_\lambda r)}{H_p^{(1)}(\mathrm{i}\kappa_\lambda R)} \tag{9}$$

where the division by $H_p^{(1)}(\mathrm{i}\kappa_\lambda R)$ is only for later convenience. The $H_p^{(1)}(\mathrm{i}x)$ are the Hankel functions of purely imaginary argument which are often called modified Hankel functions denoted by $K_p(x)$ [30]. Introducing this *ansatz* into equation (8) leads to the linear eigenvalue problem

$$l_n\, v_n\, \kappa_\lambda^2\, \hat{\varrho}_{\lambda n} = \sum_m \left[\gamma_{mn}\hat{\varrho}_{\lambda n} - \gamma_{nm}\hat{\varrho}_{\lambda m}\right] \tag{10}$$

where the meaning of the indices becomes clear: the integers $\lambda = 1, \ldots, N-1$ label the eigensolution $\hat{\varrho}_{\lambda n}$ belonging to the inverse decay lengths κ_λ. The integer index $p = 0, \ldots, \infty$ denotes the angular dependency of the solutions. The decay lengths k_λ^{-1} are generally of the order of the film MFP.

(ii) One solution of the Laplace equation for the case where all channel densities are equal (see the remarks after equation (5))is thus

$$\frac{\partial^2}{\partial r^2}\varrho_n(r) = 0. \tag{11}$$

The solution for the Dirichlet problem mentioned above can be found by means of the so-called inversion method outlined in [31] from where we take

$$\varrho_{0pn}(r) = \hat{\varrho}_{0n}\cos p\varphi \int \frac{\mathrm{d}\Phi}{2\pi}\cos p\Phi \frac{r^2 - R^2}{r^2 + R^2 - 2Rr\cos\Phi}. \tag{12}$$

For formal completeness, we attribute an index $\lambda = 0$ to this solution as well as an index n although ϱ_{0pn} is the same for all channels.

The boundary condition can be fulfilled by an appropriate superposition of all N solutions $\varrho_{\lambda pn}(\boldsymbol{R})$, i.e.,

$$\varrho_n^{\mathrm{c}}(\boldsymbol{R}) = \sum_{\lambda=0}^{N-1}\sum_{p=0}^{\infty} B_{p\lambda}\cdot\varrho_{\lambda pn}(\boldsymbol{R}) \tag{13}$$

From the symmetry of equation (8) we find the relation

$$\sum_n \hat{\varrho}_{\lambda n} v_n l_n \hat{\varrho}_{\lambda' n} = \delta_{\lambda\lambda'} \qquad \lambda, \lambda' = 0,\ \ldots,\ N-1 \tag{14}$$

where the normalization of the $\hat{\varrho}_{\lambda n}$ has been properly fixed. This orthogonality relation will be used below in order to calculate the coefficients $B_{p\lambda}$.

2.2. *The far field and the density dipole*

The superposition

$$\varrho_n(\boldsymbol{r}) = \sum_{\lambda=0}^{N-1} B_{p\lambda}\varrho_{\lambda pn}(\boldsymbol{r}) \tag{15}$$

gives the density distribution, spatially as well as over the lateral modes, which arises from a given $\varrho_n^{\mathrm{c}}(\boldsymbol{R})$ if $\varrho_n(\boldsymbol{r})$ reproduces $\varrho_n^{\mathrm{c}}(\boldsymbol{R})$ for $\boldsymbol{r} \to \boldsymbol{R}$. Now we will calculate the coefficients $B_{p\lambda}$. On the circle, equation (15) takes the simple form

$$\varrho_n^{\mathrm{c}}(\boldsymbol{R}) = \sum_\lambda \sum_p B_{p\lambda}\hat{\varrho}_{\lambda n}\cos p\varphi \tag{16}$$

if we use the representations (9) and (12). The coefficients $B_{p\lambda}$ can be extracted from (16) by a two-step procedure. The first step eliminates the sum over p by projecting $\varrho_n^{\mathrm{c}}(\boldsymbol{R})$ onto $\cos p\varphi$, the second step uses the orthogonality relation (14) of the eigensolutions. This gives

$$B_{p\lambda} = \frac{1}{\pi}\sum_n \hat{\varrho}_{\lambda n} v_n l_n \int \mathrm{d}\varphi_R\ \varrho_n^{\mathrm{c}}(\boldsymbol{R})\cos p\varphi_R \tag{17}$$

where the integration is performed on the circle $\{R\}$. Consider now the long-range behaviour of the density distribution resulting from a given $\varrho_n^c(R)$. Obviously only the term with $\lambda = 0$ in (15) gives rise to a long-range change in the density. This change will lead to an additional resistance; see section 3. Apart from an uninteresting rotationally symmetric part originating from the equilibrium particle density, the leading angle-dependent term of equation (12) is the dipole field

$$|r| \to \infty : \qquad \varrho_{0n}(r) = \varrho_0(r) \approx p_d \frac{\cos\varphi}{r} \tag{18}$$

with the dipole moment

$$p_d \equiv B_{10} R \Big/ \sqrt{\sum_m l_m v_m}.$$

This just represents the residual resistivity dipole introduced by Landauer [28]; see also [27]. Thus we need only the coefficient B_{10} which is found from equation (17) to be

$$B_{10} = \left(1 \Big/ \sqrt{\sum_m v_m l_m}\right) \sum_n v_n l_n \int \frac{d\varphi_R}{\pi}\, \varrho_n^c(R) \cos\varphi_R \tag{19}$$

2.3. The near field of the density

Now we are going to calculate the density near field $\varrho_n^c(R)$ from the scattering behaviour of an obstacle. The obstacle is centred in the origin and entirely enclosed by the circle $\{R\}$. We characterize the obstacle by its quasi-2D differential cross section $\sigma_{nn'}(\varphi, \varphi')$. We assume the scattering cross-section to obey the symmetry relation $\sigma_{nn'}(\varphi, \varphi') = \sigma_{nn'}(\varphi - \varphi')$. Moreover, its extension R_{ob} is assumed to be small compared to the film MFP. Apart from the reason already mentioned in section 1, this condition also ensures that the mathematical procedure which leads to equation (A6) in appendix A and to equation (8) remains applicable in the presence of the obstacle. In appendix A, the integrations $\int d\varphi \int d\tilde{r}\ (\ldots)$ were performed assuming the film itself as homogeneous. The error now introduced remains small if the obstacle region is small compared to the total region where the main contributions to the integral come from.

If currents $j_n^{inc}(\varphi)$ are incident on the obstacle, the total current density outgoing radially through the circle $\{R\}$ is

$$j_n(\varphi_R) = j_n^{inc}(\varphi_R) + \delta j_n(\varphi_R) \tag{20}$$

$$\delta j_n(\varphi_R) = \frac{1}{R} \sum_{n'} \int d\varphi' \ \left\{\sigma_{nn'}(\varphi - \varphi') - \delta_{nn'}\delta(\varphi - \varphi')\sigma_{n'}\right\} j_{n'}^{inc}(\varphi')$$

where

$$\sigma_n = \sum_m \int d\Phi\ \sigma_{mn}(\Phi).$$

The second term in the curly brackets takes into account that the current in the forward direction is diminished by the total scattered current.

Thus the change of the density on $\{R\}$ due to the presence of the obstacle is simply $\delta\varrho_n^c(R) = v_n^{-1}\,\delta j_n(\varphi_R)$ We explicitly note that this relation is correct only in the quantum mechanical far-field region. Therefore, the radius R of the circle enclosing the obstacle must be larger by some wavelengths than the obstacle itself. For $R_{ob} \gg \lambda_F$, $R \approx R_{ob}$ is a good approximation whereas for the opposite case R must be of the order of some wavelengths. In other words, we omit all density contributions from the quantum mechanical near field.

We believe this approximation to be justified because the quantum mechanical length scale is much smaller than the length scale of the diffusion and relaxation processes which is of the order of the film MFP. The relaxation due to the film background is noticeable only in a region where the density can be well-described by using the scattering far field.

For the additional resistance it is sufficient to consider only the density change $\delta\varrho_n^c(\boldsymbol{R})$ due to the obstacle instead of the total density on $\{\boldsymbol{R}\}$.

Equation (20) contains the incident current densities as essential ingredients. They are very involved quantities as they comprise not only the primarily incident current distribution, i.e., that of the homogeneous film far from the perturbation (see our remarks after equation (6)), namely

$$j_n^0(\varphi) = \text{constant} + |j^0| \cos\varphi \; v_n l_n \Big/ \left(\pi \sum_m v_m l_m\right) \qquad (21)$$

but also a contribution $\delta j_n^{\text{inc}}(\varphi)$ that originates from the relaxation mechanism of the film: particles scattered by the obstacle are allowed to return to it and thus to form anew an incident current which, on its turn, undergoes the same scattering-relaxation mechanism. The $\delta j_n^{\text{inc}}(\varphi)$ are thus determined self-consistently via an equation of the form

$$j_{n,1}^{\text{inc}}(\varphi) = j_{n,1}^0(\varphi) + \hat{A}_{n,1}\left[j_{n',1}^{\text{inc}}(\varphi')\right](\varphi) \qquad (22)$$

where $\hat{A}$ is a linear operator which will be derived in appendix B, and the index 1 indicates the restriction to terms with $p = 1$ which are the only contributions of importance here.

It seems impossible to determine $\delta j_{n,1}^{\text{inc}}(\varphi)$ analytically for the general case. However, if we make the simplifying assumption that the obstacle scatters only weakly, j_n^{inc} can be replaced by the unperturbed current density distribution (21) which would be present in the absence of the obstacle.

From appendix B, equation (B2), we take the condition of validity for this approximation:

$$\frac{\sigma_n}{l} \ln\frac{l}{R} \ll 1. \qquad (23)$$

This can be roughly understood in the following way. For the resistance, only terms belonging to the dipolar term with $p = 1$ are of importance. Contributions to δj^{inc} come mainly from a region of order l around the obstacle. Since the $p = 1$ density terms under consideration here behave there like $(j^{\text{inc}}\sigma)\,R/r$, the resulting integral for the current density is proportional to $(j^{\text{inc}}\sigma/l)\,\ln(l/R)$ where the factor l^{-1} accounts for the effectiveness of background scattering.

Normally, a sufficiently small scattering cross-section can be achieved by a sufficiently small extension R of the obstacle. There are, however, special resonance cases [32, 23, 27] where σ_n sharply rises. In these cases, care is needed. On the other hand, the condition of a sufficiently small quantity (23) can always be satisfied if the film MFP is sufficiently large.

Introducing Eqs.(21) and (20) into the dipole moment gives

$$p_{\text{d}} = |j^0| \sum_{nn'} v_{n'} l_{n'} \int \mathrm{d}\Phi \,\{l_n \cos\Phi - l_{n'}\}\,\sigma_{nn'}(\Phi) \Big/ \left[2\pi^2 \left(\sum_m v_m l_m\right)^2\right]. \qquad (24)$$

From equation (24) we have derived a formula that allows us to calculate the RRD dipole from the scattering cross section of an arbitrary but, in the above sense, weakly scattering obstacle. Note that the scattering cross section entering p_{d} in equation (24) is related to 2d current densities and therefore has the dimension of a length.

3. Resistivity

In this section we show the connection between the RRD and the additional resistivity due to the scatterer in the limit $T = 0$.

Note that all densities and current densities used in the preceding section are two-dimensional quantities. In order to make contact with real films with thickness d in z direction, we now take the usual 3d density $\varrho_n^{(3D)}(z) = \varrho_n\,|\chi_n(z)|^2$ and $j_n^{(3D)}(z) = j_n\,|\chi_n(z)|^2$. The $\chi_n(z)$ are the lateral eigenfunctions of the film. In the case of hard film boundary conditions, they are of the form $\chi_n(z) = \sqrt{2/d}\,\sin(n\pi z/d)$.

Instead of the particle density itself we will in the following use the quantity $u(x, y) \equiv \varrho^{(3D)}(x, y, z)/n(E, z)$ where

$$n(E, z) = \pi^{-1}\Im m\, G = \frac{m}{2\pi\hbar^2}\sum_n |\chi_n(z)|^2$$

is the quasi-two-dimensional LDOS, and m is the electron mass. Note that u does not depend on the lateral coordinate z. Now we assume that independently acting obstacles are distributed with a mean volume density $\mathcal{N}$ over the entire film. We chose two arbitrary points (x_1, y, z_1) and (x_2, y, z_2) in the film. Then the difference $\delta u(x_1, y) - \delta u(x_2, y)$ additionally introduced by this random distribution of obstacles is

$$\delta u(x_1, y) - \delta u(x_2, y) = \frac{2\pi\hbar^2}{m}\sum_s(\varrho_d(x_1, y|\boldsymbol{r}_s) - \varrho_d(x_2, y|\boldsymbol{r}_s)) \tag{25}$$

where $\varrho_d(x, y|\boldsymbol{r}_s)$ means the density dipole field from equation (18) at (x, y) due to an obstacle at position $\boldsymbol{r}_s$. Configurationally averaging over all obstacle positions gives

$$\langle\delta u(x_1, y) - \delta u(x_2, y)\rangle = \frac{4\pi^2\hbar^2\mathcal{N}\langle|p_d|\rangle\,(x_2 - x_1)\,d}{m}. \tag{26}$$

This difference does not depend on y. Now it makes sense to identify $\langle\delta u(x_1, y) - \delta u(x_2, y)\rangle$ with an additional potential drop $e\,\delta U$ along the x direction.

Thus the additional resistivity $\delta\rho_{\mathrm{film}}$ reads (in terms of $\hbar/e^2$)

$$\delta\rho_{\mathrm{film}} = \frac{\pi^2 d^2\mathcal{N}\langle|p_d|\rangle\hbar}{m|j^0|}. \tag{27}$$

In order to avoid any confusion of the particle density $\varrho(\boldsymbol{r})$ and the resistivity we write for the latter ρ_{film}.

4. Examples

It is illustrative to take as a first example a two-dimensional system by restricting our calculations to only one channel. In this case, no interchannel relaxation occurs, of course, and we can calculate self-consistently the incident current density without restriction to weak scatterers. First we calculate the coefficient B_{10} which enters equation (B3) and represents the main constituent of the dipole moment. Using equation (20) we have

$$B_{10} = \sqrt{\frac{l}{vR^2}}\,\sigma_T\,\tilde{j}^{\mathrm{inc}} \tag{28}$$

where we have used the abbreviations

$$\sigma_T \equiv \int d\Phi\,(1 - \cos\Phi)\,\sigma(\Phi)$$

$$\bar{j}^{\text{inc}} \equiv \int \mathrm{d}\Phi \ \cos\Phi \ j^{\text{inc}}(\Phi).$$

Inserting B_{10} into equation (B5) gives

$$\delta\bar{j}^{\text{inc}} = \ln\left(\frac{l}{R}\right) \ \frac{\sigma_{\mathrm{T}}}{l} \ \bar{j}^{\text{inc}} \tag{29}$$

and thus

$$\delta\rho_{\text{film}} = \frac{\hbar}{2mv} \ \frac{\mathcal{N}^{(2\mathrm{D})} \ \sigma_{\mathrm{T}}}{1 - \ln(l/R) \ \sigma_{\mathrm{T}}/l}. \tag{30}$$

This formula and the preceding one can be interpreted as follows. The primarily incident carrier flux causes a density excess of particles reflected by the obstacle and a density deficit behind the obstacle. Those particles which are scattered by the surrounding film medium have the chance to reach the obstacle again and to give a correction to the incident current. The angular dependence of this correction corresponds to the dipole of the primary scattering process at the obstacle. An infinte repetition of these processes results in the geometrical series found in equation (30).

We want to point out a subtlety of the result (30) concerning the choice of the radius R. For obstacles large compared to the wavelength, the enhancement factor is simply $(1 - \ln(l/R_{\text{ob}})\,(\sigma_{\mathrm{T}}/l))^{-1}$. However, for the opposite limit of an obstacle small compared to λ_{F}, R is of the order of λ_{F}, and the enhancement factor becomes approximately $(1 - \ln(l/\lambda_{\mathrm{F}})\,(\sigma_{\mathrm{T}}/l))^{-1}$. Even for resonant point-like scatterers, σ_{T} is maximally of order λ_{F}. This means that for point-like scatterers the smallness of the correction goes definitely beyond the limits of our quasi-classical model where λ_{F}/l is *a priori* negligible.

The same kind of a non-linear relation between resistance and scattering properties of the obstacle as found here shows up in the one-dimensional Landauer formula where the additional resistance is proportional to $r/(1-r)$ where r is the reflection coefficient; see for example [33]. From the very beginning of the RRD concept, such a non-linear relation has also been predicted to exist in two- and three-dimensional systems, repectively [28, 29]. However, the non-linear effect was expected to be less pronounced in higher dimensions as the current can bypass the obstacle. This is what we have found in equation (30).

Next we investigate point-like ($R_{\text{ob}} \ll \lambda_{\mathrm{F}}$) obstacles in a multi-channel film. We take s scatterers, each with scattering amplitude f, which are randomly distributed with a volume density $\mathcal{N}$. Far from backscattering resonances due to the film wall, [27, 32], $\sigma_{nn'}$ for each individual scatterer reads [32]

$$\sigma_{nn'} = \frac{|f|^2}{2k_{n'}d^2}\sin^2(z\pi n/d)\sin^2(z\pi n'/d) \tag{31}$$

with $k_n = (m/\hbar)v_n = \left(k_{\mathrm{F}}^2 - n^2\pi^2/d^2\right)^{-1/2}$ and k_{F} the Fermi wavenumber. $\sigma_{nn'}$ depends on the lateral position z of the scatterer but not on any angular arguments. The channel MFP l_n is assumed to be proportional to the channel velocity v_n. Averaging $\sigma_{nn'}$ over the film thickness and inserting $\langle\sigma_{nn'}\rangle$ into the general formula (27) gives the well-known result [4, 9]

$$\delta\rho_{\text{film}} = 2\pi\mathcal{N}|f|^2\left(N + \frac{1}{2}\right)\Bigg/\left(\sum_{m=1}^{N} k_m^2\right). \tag{32}$$

Finally, we consider short-ranged surface bumps that are randomly distributed with a mean surface density $\mathcal{N}^{(2\mathrm{D})}$ and have a scattering amplitude f_s. They serve as a model for surface micro-roughness [9, 23]. The scattering theory for such surface imperfections has been shown to be similar to that of volume scatterers in [23] and [9]. From there we take

$$\langle \sigma_{nn'} \rangle = \frac{\pi^3 n^2 n'^2}{2d^6 k_F^4 k_{n'}} |f_s|^2. \tag{33}$$

This results in the additional resistivity

$$\delta\rho_{\text{film}} = \mathcal{N}_s |f_s|^2 \sum_{n=1}^{N} n^2 \sum_{m=1}^{N} k_m^2 m^2 \Bigg/ \left[\left(\sum_{m=1}^{N} k_m^2 \right)^2 k_F^4 d^5 \right]. \tag{34}$$

In the limit of very thin films (i.e., $N \sim 1$), $\delta\rho$ exhibits the pronounced d^{-6} behaviour [10, 6, 8, 9] (note that k_n itself depends on d). In the limit of thick films, $N \gg 1$, the Fuchs result [1, 27, 9] is recovered. The typical quantity $\mathcal{N}_s |f_s|^2$ corresponds, up to a factor of the order of unity, to the fraction $(1 - p)$ of diffusely scattered particles where p is Fuchs' specularity parameter.

These three examples that served as a test of the present theory show that the semi-classical approach gives reasonable results for well-investigated situations in the case of weak scatterers. This encourages us to apply our method to more complicated obstacles such as shallow terraces with an extension R comparable to or even larger than λ_F but again small against l.

5. Summary

It was our goal here to find, within a semi-classical framework, the additional resistivity due to an obstacle which is characterized by its scattering cross-section $\sigma_{nn'}(\varphi, \varphi')$. The intrinsic film resistivity is caused by a background of randomly distributed weak scatterers which allow for transitions between different lateral modes and directions of planar motion.

Our method rests on a recently developed semi-classical theory [26] for transport in quantum wires. We have demonstrated how this theory can be re-formulated for the quasi-two-dimensional case.

Starting from a local kinetic equation we have derived second-order differential equations that describe the relaxation of an arbitrary density distribution given along a closed contour. Two qualitatively different solutions have been found, one of them giving rise to a long-range density dipole. This is the so-called residual resisitivity dipole (RRD) introduced by Landauer [28].

The current density incident onto the obstacle plays an essential role in our theory. We have shown that and how it can be calculated self-consistently. The condition has been derived under which one can treat an obstacle as weak. In this case, the formulae are strongly simplified, and one gets an analytical expression for the additional resistance. The said condition can be satisfied either by sufficiently small and non-resonant scatterers at a given film MFP, or by a sufficiently large MFP.

For only one conducting lateral mode, however, we were able to solve analyically the self-consistency problem of the incident currents for arbitrarily strong obstacles. As a result, we have derived an expression where the resistance depends on the scattering cross-section in a non-linear manner. This agrees with the prediction by Landauer [28, 29] that the multiple-scattering processes between the obstacle and surrounding medium should result in a resistance formula of the form $\delta\rho_{\text{film}} \sim \sigma/(1 - \alpha\sigma)$. The enhancement factor turned out to be negligible, within our quasi-classical framework, for obstacles small compared to the wavelength.

Furthermore, we have considered some well-investigated examples of obstacles in multi-channel wires (i.e., volume and surface scatterers) in order to check our method.

With the formalism developed in the present paper, it is possible to calculate the additional resistivity due to obstacles which are embedded in a multi-channel resisitive quantum film treated semi-classically. The only restrictions on them are that they are much smaller than the film MFP and that they are rotationally symmetric. The whole formalism becomes very handy if we deal only with weakly scattering obstacles. Then, the incident current density can be replaced by the current density distribution of the unperturbed film.

One possible example for future investigations could be extended perturbations of the film such as large terraces on the film surfaces discussed in the context of bimodal roughness spectra [18, 20, 19, 21] or even holes in the film. They possess a fairly complicated $\sigma_{nn'}(\varphi - \varphi')$ which will be discussed elsewhere.

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Appendix A.

The kinetic equation in its integral form reads

$$\varrho_n(\boldsymbol{r}, \varphi) = \frac{1}{2\pi v_n} \int_0^\infty \mathrm{d}\tilde{r} \exp\left(-\frac{\tilde{r}\gamma_n}{v_n}\right) \sum_m \gamma_{nm} \varrho_m(\boldsymbol{r} - \hat{\mathrm{e}}_\varphi \tilde{r}). \tag{A1}$$

Inserting this form into equations (2) and integrating partially with repect to $\tilde{r}$ we find

$$\boldsymbol{j}_n(\boldsymbol{r}) = -\frac{v_n}{2\pi\gamma_n} \int \mathrm{d}\varphi\ \hat{\mathrm{e}}_\varphi \int_0^\infty \mathrm{d}\tilde{r} \exp\left(-\frac{\tilde{r}\gamma_n}{v_n}\right) \sum_m \gamma_{nm} \left(\hat{\mathrm{e}}_\varphi \frac{\partial}{\partial \boldsymbol{r}}\right) \varrho_m(\boldsymbol{r} - \hat{\mathrm{e}}_\varphi \tilde{r}). \tag{A2}$$

Hence the source density of the current is

$$\begin{aligned}\frac{\partial}{\partial \boldsymbol{r}} \boldsymbol{j}_n(\boldsymbol{r}) = &-\frac{v_n}{2\pi\gamma_n} \int \mathrm{d}\varphi \int_0^\infty \mathrm{d}\tilde{r} \exp\left(-\frac{\tilde{r}\gamma_n}{v_n}\right) \\ &\times \sum_m \gamma_{nm} \left[\left(\hat{\mathrm{e}}_\varphi \frac{\partial}{\tilde{r}\partial \boldsymbol{r}}\right) + \left(\hat{\mathrm{e}}_\varphi \frac{\partial}{\partial \boldsymbol{r}}\right)^2\right] \varrho_m(\boldsymbol{r} - \hat{\mathrm{e}}_\varphi \tilde{r}).\end{aligned} \tag{A3}$$

On the other hand, if we insert equation (A1) into equation (2), and apply the Laplace operator to the expression arising we find

$$\frac{\partial^2}{\partial \boldsymbol{r}^2} \varrho_n(\boldsymbol{r}) = \frac{1}{2\pi v_n} \int \mathrm{d}\varphi \int_0^\infty \mathrm{d}\tilde{r} \exp\left(-\frac{\tilde{r}\gamma_n}{v_n}\right) \sum_m \gamma_{nm} \left(\frac{\partial^2}{\partial \boldsymbol{r}^2}\right) \varrho_m(\boldsymbol{r} - \hat{\mathrm{e}}_\varphi \tilde{r}). \tag{A4}$$

We can decompose the Laplace operator into its tangential and a radial components, respectively, i.e.

$$\int \mathrm{d}\varphi \left(\frac{\partial^2}{\partial \boldsymbol{r}^2}\right) \varrho(\boldsymbol{r} - \hat{\mathrm{e}}_\varphi \tilde{r}) = \int \mathrm{d}\varphi \left[\left(\hat{\mathrm{e}}_\varphi \frac{\partial}{\tilde{r}\partial \boldsymbol{r}}\right) + \left(\hat{\mathrm{e}}_\varphi \frac{\partial}{\partial \boldsymbol{r}}\right)^2 + \left(\hat{\mathrm{e}}_t \frac{\partial}{\partial \boldsymbol{r}}\right)^2\right] \varrho(\boldsymbol{r} - \hat{\mathrm{e}}_\varphi \tilde{r}). \tag{A5}$$

The third term on the right-hand side vanishes as the integration is performed over a full circle. Using this in equation (A4) and comparing (A4) with (A3) we are left with the relation

$$\frac{\partial}{\partial r} j_n(r) = -\frac{v_n^2}{\gamma_n} \frac{\partial^2}{\partial r^2} \varrho_n(r). \tag{A6}$$

Having in mind the generally non-local relation between current and density gradient, equation (A6) is surprisingly simple. Combining this with equation (5), we find the differential equation system (8).

Appendix B

Here we will calculate the quantity $\delta j_n^{\mathrm{inc}}(\varphi)$. Inserting the density from equations (12) and (9) explicitly into the kinetic equation in its integral form,

$$\delta j_n^{\mathrm{inc}}(\varphi) = \frac{1}{2\pi} \int_0^\infty \mathrm{d}\tilde{r} \exp\left(-\frac{\tilde{r}\gamma_n}{v_n}\right) \sum_m \gamma_{nm} \delta\varrho_m(\boldsymbol{R} - \hat{\boldsymbol{e}}_\varphi \tilde{r}) \tag{B1}$$

we get

$$\delta j_n^{\mathrm{inc}}(\varphi) = \frac{R}{2\pi} \int_1^\infty \mathrm{d}c\ \mathrm{e}^{-\beta_n(c-1)} \sum_{mp} \cos p\varphi\ \gamma_{nm} \times \left[\hat{\varrho}_{0m} B_{p0} \int \mathrm{d}\Phi\ \frac{\cos p\Phi\ (c^2-1)}{2\pi(1+c^2-2c\cos\Phi)} + \sum_{\lambda\neq 0} \hat{\varrho}_{\lambda m} B_{p\lambda} \frac{H_p^{(1)}(\mathrm{i}\alpha_\lambda c)}{H_p^{(1)}(\mathrm{i}\alpha_\lambda)} \right] \tag{B2}$$

where $\alpha_\lambda = R\kappa_\lambda$, $\beta_n = R/l_n$, and $c = r/R$. For our purpose, only the coefficient B_{10} is of importance. Therefore, we will consider in the following only the terms which belong to $p = 1$ and denote them by an index 1. One easily convinces oneself that all other terms are of no influence on B_{10}. Performing the integration $\int \mathrm{d}c\ (\ldots)$ of the two corresponding contributions in the angular brackets of equation (B2) gives [30]

$$\lambda = 0: \qquad \frac{-v_n}{2\pi} \cos\varphi\ \hat{\varrho}_{0n}\beta_n\ \ln\beta_n\ B_{10} \tag{B3}$$

and

$$\lambda \neq 0: \qquad \frac{-v_n}{2\pi} \cos\varphi \sum_{\lambda\neq 0} \hat{\varrho}_{\lambda n} \left[1 - \frac{l_n^2\kappa_\lambda^2}{4}\right] \beta_n \ln\beta_n B_{1\lambda}. \tag{B4}$$

Combining the two contributions, we get

$$\delta j_{n,1}^{\mathrm{inc}}(\varphi) = \frac{-v_n \ln\beta_n}{2\pi} \cos\varphi \sum_\lambda \hat{\varrho}_{\lambda n} \left[1 - \frac{l_n^2\kappa_\lambda^2}{4}\right] \beta_n B_{1\lambda}. \tag{B5}$$

With $B_{1\lambda}$ from equation (17), and $\delta\varrho_n^{\mathrm{c}}(\boldsymbol{R})$ from equation (20) we can write the $p = 1$ term of $j_n^{\mathrm{inc}}(\varphi)$ in the very compact form

$$j_{n,1}^{\mathrm{inc}}(\varphi) = j_n^0(\varphi) + \hat{A}\left[j_{n',1}^{\mathrm{inc}}(\varphi')\right](\varphi) \tag{B6}$$

where

$$\hat{A}\left[j_{n',1}^{\mathrm{inc}}(\varphi')\right](\varphi) = \frac{-v_n \ln\beta_n}{(2\pi)^2} \cos\varphi \sum_\lambda \hat{\varrho}_{\lambda n} \left[1 - \frac{l_n^2\kappa_\lambda^2}{4}\right] \beta_n \times \sum_{n'n''} \hat{\varrho}_{\lambda n''} \beta_{n''}^{-1} \left\{ \int \mathrm{d}\Phi \cos\Phi\ \sigma_{n''n'}(\Phi) - \delta_{n''n'}\sigma_{n'} \right\} \int \mathrm{d}\varphi' \cos\varphi'\ j_{n',1}^{\mathrm{inc}}(\varphi'). \tag{B7}$$

Using this equation, one could in principle calculate the dipole moment and thus the additional resistivity up to any order by a perturbational series.

Finally we can derive a condition under which the approximation $j_n^{\mathrm{inc}}(\varphi) \approx j_n^0(\varphi)$ is justified. With equation (14) we find

$$-\frac{\sigma_n}{l} \ln \beta_n \ll 1 \tag{B8}$$

which must hold for all n.

References

[1] Fuchs K 1938 *Proc. Camb. Phil. Soc.* **34** 100
[2] Tellier C R and Tosser A J 1982 *Size Effects in Thin Films* (Amsterdam: Elsevier)
[3] Lenk R and Knäbchen A 1993 *J. Phys.: Condens. Matter* **5** 6563
[4] Sandomirskij V B. 1967 *Zh. Eksp. Teor. Phys.* **52** 158
[5] Leung K M 1984 *Phys. Rev.* B **30** 647
[6] Sakaki H, Noda T, Hirakawa K, Tanaka M and Matsusue T 1987 *Appl. Phys. Lett.* **51** 1934
[7] Tešanović Z, Jarić M V and Maekava S 1986 *Phys. Rev. Lett.* **57** 2760
[8] Fishman G and Calecki D 1989 *Phys. Rev. Lett.* **62** 1302
[9] Kunze C 1993 *Solid State Commun* **87** 359
[10] Gold A 1986 *Solid State Commun* **60** 531
[11] Hirakawa K, Noda T and Sakaki H 1988 *Surf. Sci.* **196** 365
[12] Badoz P A, Briggs A, Rosencher E and Arnaud d'Avitaya F 1987 *Appl. Phys. Lett.* **51** 169
[13] Henz J, von Känel H, Ospelt M and Wachter P 1987 *Surf. Sci.* **189/190** 1055
[14] Palevski A, Beltram F, Capasso F, Pfeiffer L and West K W 1990 *Phys. Rev. Lett.* **65** 1929
[15] Jalochovski M, Bauer E, Knoppe H and Lilienkamp G 1992 *Phys. Rev.* B **45** 13607
[16] Jalochovski M, Knoppe H, Lilienkamp G and Bauer E 1992 *Phys. Rev.* B **46** 4693
[17] Gerar J-M and LeRoux G 1993 *Appl. Phys. Lett.* **62** 3452
[18] Warwick C A, Jan W J, Ourmazd A and Harris T D 1990 *Appl. Phys. Lett.* **56** 2666
[19] Gammon D, Shanabrook B V and Katzer D S 1991 *Phys. Rev. Lett.* **67** 1547
[20] Warwick C A and Kopf R F 1992 *Appl. Phys. Lett.* **60** 386
[21] Orschel B, Oelgart G and Houdré R 1993 *Appl. Phys. Lett.* **62** 843
[22] Jalochovski M, private communication
[23] Kunze C 1993 *Phys. Rev.* B **48** 14338
[24] Bass F G and Fuks I M 1979 *Wave Scattering by Statistically Rough Surfaces* (Oxford: Pergamon)
[25] Ogilvy J A 1991 *Theory of Wave Scattering from Random Rough Surfaces* (Bristol: Institute of Physics)
[26] Lenk R 1994 *Z. Phys.* B at press
[27] Chu C S and Sorbello R S 1988 *Phys. Rev.* B **38** 7260
[28] Landauer R 1957 *IBM J. Res. Dev.* **1** 223
[29] Landauer R and Woo J W F 1972 *Phys. Rev.* B **5** 1189
[30] Gradshteyn I S and Ryzhik I M 1971 *Tablizy Integralov, Summ, Ryadov i Proizvedenij* (Moscow: Nauka)
[31] Sommerfeld A 1949 *Partial Differential Equations in Physics* (New York: Academic)
[32] Kunze C and Lenk R 1992 *Solid State Commun* **84** 457
[33] Landauer R 1989 *J. Phys.: Condens. Matter* **1** 8099