Resistance of planar barriers

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The resistance of planar barriers is discussed for a variety of situations in which different sources of scattering act incoherently, allowing a semiclassical approach. This includes single barriers, a sequence of identical parallel barriers, and identical barriers at random angles simulating grain boundaries. Existing results are related, and only limited extension of these is provided. The case of a single barrier embedded in a uniformly resistive medium has been treated by Kunze and others. Kunze's analysis is validated and interpreted via a considerably simplified version of his model.

I. INTRODUCTION

A number of analyses have dealt with the resistance of planar barriers by themselves, as part of a sequence of similar barriers, or embedded in a medium with spatially homogeneous scattering by lattice vibrations.

This author, in 1957,[1] investigated the case of a sequence of incoherent and identical barriers. Sorbello[2] has examined the case of single barriers, as well as barriers in a homogeneous medium providing additional scattering. Laikhtman and Luryi[3] also treated the case of a single localized barrier embedded in a uniform resistive medium. A sequence of papers from the Chemnitz group[4–6] cites additional papers beyond those we have listed. This note is intended to provide some comments on this field and the relationships among existing results, without necessarily adding much to the list of available results.

We concentrate on the case where different sources of scattering act incoherently, allowing a semiclassical treatment. We will emphasize two-dimensional barriers in a three-dimensional medium. The case of linear barriers in a two-dimensional medium differs only in trivial ways and the modification applicable to that case will be described for some results. Magnetic field effects will be ignored. The barriers will be assumed to be homogeneous and translationally invariant, causing specular reflection and transmission depending on the angle θ relative to the normal to the plane.

II. SINGLE BARRIERS WITHOUT BULK SCATTERING

Mesoscopic physics has invoked two principal results for the case of a single quantum mechanical scatterer.[7–10] If the potential is measured in reservoirs that are wide compared to the leads leading to the obstacle and the reservoirs connected in a nonreflective way to the leads leading to the scatterer, then

$$\mathcal{G} = \frac{e^2}{\pi\hbar}\mathrm{Tr}(t^\dagger t), \tag{2.1}$$

where t is the transmission matrix of the scattering element, defined in terms of the transverse modes in the leads. Equation (2.1) allows for a twofold spin degeneracy for each transverse mode. Alternatively if the potential difference is measured in the leads, and averaged over a region large enough to eliminate quantum oscillations we find[7–11]

$$\mathcal{G} = \frac{e^2}{\pi\hbar}\frac{\left(\sum_i T_i\right)\left(\sum v_i^{-1}\right)}{\sum_i v_i^{-1}(1+R_i-T_i)}. \tag{2.2}$$

T_i measures the total transmission probability into the ith channel, if all the incident channels on the other side are occupied. Similarly R_i denotes the total reflection probability into channel i, if all the incident channels on the same side are occupied. v_i is the longitudinal velocity of the ith channel. The results in Eqs. (2.1) and (2.2) become identical in the small transmission limit.

Sorbello[2] has applied Eqs. (2.1) and (2.2) to the plane barrier. Equation (2.1) for the conductance of a planar barrier, per unit area, yields

$$\sigma = \frac{e^2k_F^2}{8\pi^3\hbar}\int T(\theta)\mid\cos\theta\mid d\Omega, \tag{2.3}$$

where the integration extends over the whole 4π range of possible directions of motion. $T(\theta)$ is the transmission probability for carriers incident at an angle θ with respect to the normal to the scattering plane. k_F is the wave vector at the Fermi surface. In the case of a two-dimensional medium with a linear barrier the integral extends over the 2π range of available directions. The prefactor in front of the integral becomes $e^2k_F/4\pi^2\hbar$, in that case.

Sorbello's corresponding result for Eq. (2.2) applied to the plane barrier is

$$\sigma = \frac{e^2k_F^2}{2\pi^2\hbar}\frac{\int T(\theta)\mid\cos\theta\mid d\Omega}{\int R(\theta)d\Omega}. \tag{2.4}$$

The conductance, per unit width, of the linear barrier in a two-dimensional medium has the prefactor $e^2k_F/2\pi\hbar$, instead.

The case of the plane barrier with leads whose cross-sectional area is less than that of the barrier has also been treated,[9] but will not be taken up here. McLennan, Lee, and Datta[12] have analyzed a number of tunneling problems numerically, via a Kadanoff-Baym-Keldysh formalism. They exhibit the detailed spatial variation of the electrochemical potential and of the electrostatic potential near the barrier. These results, while conveying important insight, are not easily relatable to the analytical results presented in this paper. There is also a huge body of literature motivated by resonant tunneling devices, and we cite only two examples.[13,14] Papers in this category typically emphasize nonlinearity, numerical simulation, and Wigner distributions, and do not allow easy comparison to analytical results. The highly localized voltage drop expected for a planar barrier has been studied with scanning tunneling potentiometry.[15]

III. INCOHERENT SUCCESSIVE BARRIERS

This author showed[1] that the conductance per unit volume for a series of parallel barriers is

$$\sigma = \frac{e^2k^2}{8\pi^3\mathcal{N}\hbar}\int d\Omega \mid \cos\theta \mid \frac{1-R(\theta)}{R(\theta)}. \tag{3.1}$$

Here $\mathcal{N}$ is the linear density of barriers. In the two-dimensional medium the prefactor becomes modified as described in connection with Eq. (2.3). Equation (3.1) corresponds to a resistance for a single unit area barrier

$$\mathcal{R} = \frac{8\pi^3\hbar}{e^2k^2} \Big/ \int \frac{1-R(\theta)}{R(\theta)} \mid \cos\theta \mid d\Omega. \tag{3.2}$$

The derivation of Eq. (3.1) invoked the fact that in the case of many barriers we could expect the carrier velocity distribution to be uniform along most of the chain. (To avoid the need for a subsidiary explanation consider the case where the screening length is short compared to the typical carrier spacing. Furthermore, assume that the uniformity of velocity distribution applies to spaces which are a few screening lengths away from any barrier.)

The fact that a long sequence of identical barriers should establish a space-independent velocity distribution is plausible. But it is, perhaps, in 1995, after a great deal of contact with disordered and mesoscopic systems not as compelling as it seemed in 1957. The reflecting barriers only couple motion along two directions to each other. That leaves many uncoupled channels, related to each other only through Poisson's equation, i.e., through the requirement for neutrality. We may question whether that is enough to maintain a spatially uniform relationship between all the velocity classes. One way out: Add a little random thermal background scattering. This can be small enough to have relatively little influence on the resistance, but decouples the behavior in far-apart portions of the system. Thus the spatial uniformity in the velocity distribution becomes justified.

We do not, however, need to rely on this indirect sort of reasoning. Let us return to the original problem without added background scattering. Consider a typical mode, confined by guiding walls with a transverse wave function, say

$$\psi = \cos k_x x \; \sin k_y y, \tag{3.3}$$

for a rectangular guide. This can be considered a superposition of traveling waves

$$\exp(\pm ik_x x) \; \exp(\pm ik_y y). \tag{3.4}$$

The mode in Eq. (3.3) propagating in the z direction with wave vector k_z, will be transmitted and reflected according to the respective probabilities $T(\theta)$ and $R(\theta)$, where θ is defined by the orientation of the vector (k_x, k_y, k_z). The transport along this one-dimensional quantum channel is uncoupled to other channels. We have an electrochemical potential μ_L at the left end of the chain and μ_R at its right end, with μ_L and μ_R the same for all of the parallel channels.

Two barriers in series, scattering incoherently, yield an effective ratio of R/T for the combined set;[4,16]

$$\frac{R}{T} = \frac{R_1}{T_1} + \frac{R_2}{T_2}. \tag{3.5}$$

For a series of n identical barriers, each with the same value of R_0/T_0 we have

$$R/T = n(R_0/T_0), \tag{3.6}$$

reflecting the addition of identical series resistances expected in the incoherent case. The drop in electrochemical potential in *each* channel corresponding to a transverse mode of Eq. (3.3), and across *each* barrier, is $(\mu_L - \mu_R)/n$. If we think of the current in each of the uncoupled channels as comprised of an excess density in the carriers moving to the right and a deficit density in the left moving population, those deviations from equilibrium must be constant along the chain. Furthermore, for that distribution each channel is self-screening. No further Coulomb coupling between channels is needed. That justifies the assumed departure point for the derivation of Eq. (3.1).

The result in Eq. (3.1) need not be derived by the route discussed above, but can be viewed as a consequence of Eq. (2.4). For a long chain of barriers $R(\theta)$ approaches unity. Then the integral in the denominator of Eq. (2.4) becomes 4π. In the same approximation Eq. (3.5) becomes $T(\theta) \cong T(\theta)/R(\theta) = [T_0(\theta)/R_0(\theta)]/n$. If these results are entered into Eq. (2.4), it reduces to Eq. (3.1). Laikhtman and Luryi[3] compare their results for the resistance of a barrier embedded in a uniformly conducting medium to the resistance of a single barrier as given by Eq. (3.2). They imply that this was derived[1] as the resistance of a single barrier exposed to flux from two reservoirs. But that would lead us to Eq. (2.3) or Eq. (2.4), applied to a single barrier. Those results are not equivalent to Eq. (3.2).

IV. BARRIERS AT RANDOM ANGLES

Section III dealt with a series of parallel barriers. What if the planes are angled at random, approximating a series of highly resistive grain boundaries? One approach would be simply to average the resistance per boundary and for a unit area R_b, as specified in Eq. (3.2), over all possible angles for the boundaries relative to the direction of current flow. Assume a current i flows in the z direction. For plane boundaries whose normal is at an angle θ to the z direction the current flow component perpendicular to these boundaries will be $i\cos\theta$. This produces a voltage drop $iR_b\cos\theta$ across that boundary. If there are n of these boundaries per unit length, in the direction separating them, we will encounter $n\cos\theta$ of them, per unit length, moving in the z direction. Thus the electric field in the z direction will be $iR_b n\cos^2\theta$. Averaging over all directions yields $\frac{1}{3}iR_b n$, or a resistivity $\frac{1}{3}R_b n$. Note that n is also the grain boundary area per unit volume and we can thus write the resistivity as $\frac{1}{3}R_b A$, where A is the grain boundary area per unit volume. We now continue to provide an alternative derivation for this result, which makes the approximation involved more explicit.

A set of well conducting volumes separated by highly resistive boundaries can be considered to be a two-phase medium, frequently treated by effective medium theory and related approaches.[17] In our case the grain boundary material is continuous and the disjoint grain volumes are embedded in that. The approximation particularly suitable for that is the Clausius-Mossotti approximation of dielectric theory. In the heterogeneous media field it is often ascribed to a nonexistent Maxwell-Garnett field. The history of that erroneous terminology has been discussed.[17,18]

In the Clausius-Mossotti approximation[17]

$$\frac{\sigma-\sigma_0}{\sigma+2\sigma_0}=\eta_1\,\frac{\sigma_1-\sigma_0}{\sigma_1+2\sigma_0}. \tag{4.1}$$

Here σ is the effective conductivity, σ_1 the conductivity of the material taken to be discontinuous and σ_0 that of the continuous material. η_1 is the volume fraction of the discontinuous component. σ_1 will be taken to be infinite. Therefore

$$\frac{\sigma-\sigma_0}{\sigma_0+2\sigma_0}=\eta_1=1-\epsilon, \tag{4.2}$$

where ϵ is the fraction of grain boundary volume. Equation (4.2) is equivalent to

$$\sigma=\frac{3+2\epsilon}{\epsilon}\,\sigma_0, \tag{4.3}$$

which for $\epsilon\ll 1$ becomes

$$\sigma=3\sigma_0/\epsilon. \tag{4.4}$$

Equation (4.4) can also be written in terms of resistivities as $\rho=\rho_0\epsilon/3$. The volume fraction ϵ can be replaced by tA where t is the thickness of the layer and A the area per unit volume. Thus $\rho=\rho_0 tA/3$. But $\rho_0 t$ is the resistance R_b per unit area. Thus $\rho=R_bA/3$, as derived by the earlier procedure, averaging over angles.

Our second approach allows us to understand the nature of the approximation involved. The interior of the grains is represented by a macroscopic infinite conductivity that permits the current flow to be incident normally on the high resistance boundaries. The necessary change of direction in current flow, within the interior of the grains, is presumed to come free of charge; no electric field is required for that. Actually fields have to be there and the condition of normal incidence on the boundary may not be satisfied. If the boundary of the region is a tunneling barrier and if its transmission probability depends critically on the incident angle of the carrier (as is often the case), then the representation of the barrier by a simple conductance becomes a poor approximation. But that approximation, though potentially important, is a secondary consequence of the fact that the incident velocity distribution depends on the detailed kinetics within the grain volume.

V. BARRIERS IN RESISTIVE MEDIUM

We now come to the case where the barrier is embedded in a medium whose scattering behavior gives us a flux incident on the barrier differing from that presumed in Eqs. (2.3) and (2.4). These equations assume that all the carriers incident on one side of the barrier are characterized by the same electrochemical potential. This differs, for example, from the typical shifted Fermi sphere found in a lead characterized by a relaxation time for carrier scattering. The resulting complications have been stressed by Lenk[4] and by this author.[19] The one-dimensional case[17] of a barrier in a resistive medium was treated long ago. This case is particularly simple because the question of velocity distribution for incident carriers over a Fermi half sphere does not arise in that case. In one dimension the magnitude of the incident current defines the velocity distribution completely. As a result the resistance of the extended medium and that given by Eq. (2.2), for the barrier, just add to yield the total resistance. The one-dimensional case was revisited by Eränen and Sinkkonen,[20] with an extension to the nonlinear case.

In general, when we have current flow past successive obstacles of differing character, the current has to be partially transferred from the velocities best transmitted by one obstacle to those best transmitted by the other obstacle. This transfer is an irreversible event, typically manifested by a contribution to the overall resistance. It is very similar to a spreading resistance that occurs when a narrow conductor impinges onto the flat end of a wider conductor. It is also similar to *vertical transport*, i.e., the situation where carriers have to be shifted to a different energy[7,9,19,21] to be transmitted most effectively.

The total additional resistance due to a planar barrier, in a medium characterized by a relaxation time τ, has been evaluated by several investigators[2,3,5,6] in a way that does justice to the effects we have just discussed. Kunze[6] presents a particularly detailed physical picture of the spatial distribution of the electrochemical potential in the vicinity of the barrier. I will go on to discuss a very simplified *toy* model of Kunze's analysis, which will contain most of its essential physical ingredients, without the need for computer analysis. The toy model is also closely related to concepts in Sec. II of Lenk's[4] discussion.

Our toy model will consist of carriers in n parallel and identical one-dimensional channels. Carriers can be scattered between these channels. The population moving in a given direction, in a particular channel, will be assumed to relax with a relaxation time τ towards the average population for all $2n$ combinations of direction and channel, at that point in space. A barrier will be presumed at $x = 0$, which totally blocks $n-1$ of the channels. The remaining channel, designated by the subscript 0 hereafter, will have a transmission probability T at the barrier. Thus, far from the barrier, the current will be distributed uniformly among all n channels, but will have to be funneled toward the distinguished channel, near the barrier. We will proceed by considering the diffusion of uncharged carriers and then employ self-consistent screening, or the Einstein relation,[1] to yield a conductance.

Let $\rho_+(x)$ be the total carrier density, summed over all channels, moving to the right, and $\rho_-(x)$ to be the density for left moving carriers. The relaxation time approximation, applicable as long as we are not at the barrier, yields

$$\tau \frac{d\rho_+}{dt} = \frac{\rho_+ + \rho_-}{2} - \rho_+ . \tag{5.1}$$

Let v be the carrier velocity. Then, in the steady state, we can invoke

$$\tau(d\rho_+/dt) = \tau v(\partial\rho_+/\partial x). \tag{5.2}$$

Equation (5.2) inserted into Eq. (5.1), and using $\lambda = v\tau$, yields

$$\frac{\partial\rho_+}{\partial x} = \frac{1}{2\lambda}(\rho_- - \rho_+). \tag{5.3}$$

Similarly we find

$$\frac{\partial\rho_-}{\partial x} = \frac{1}{2\lambda}(\rho_- - \rho_+). \tag{5.4}$$

Equations (5.3) and (5.4) show that ρ_+ and ρ_- change in the same way with position. That is necessary if current flow, proportional to $\rho_+ - \rho_-$, is to be conserved.

Let the right and left moving densities in the preferred channel be ρ_{0+} and ρ_{0-}, respectively. Relaxation toward the average density, $(\rho_+ + \rho_-)/2n$, then yields via similar reasoning as above

$$\frac{\partial\rho_{0+}}{\partial x} = \frac{\rho_+ + \rho_-}{2n\lambda} - \frac{\rho_{0+}}{\lambda}, \tag{5.5}$$

$$\frac{\partial\rho_{0-}}{\partial x} = -\frac{\rho_+ + \rho_-}{2n\lambda} + \frac{\rho_{0-}}{\lambda}. \tag{5.6}$$

Equations (5.3)–(5.6) are a set of four coupled first-order linear differential equations. On each side of the barrier they can readily be shown to have the following four elementary solutions, which can be superimposed to yield all others. (I) A spatially uniform density change, the same for all channels, and without current flow. (II) A uniform current flow, equally distributed over all channels. It satisfies

$$\rho_{0+} = \rho_+/n, \quad \rho_{0-} = \rho_-/n,$$
$$\rho_+ = \frac{j}{2v}\left(1 - \frac{x}{\lambda}\right), \quad \rho_- = \frac{j}{2v}\left(-1 - \frac{x}{\lambda}\right). \tag{5.7}$$

j is the resulting particle flux that satisfies

$$j = v(\rho_+ - \rho_-). \tag{5.8}$$

(III) A redistribution between unequally populated channels, with their difference decaying to the right. In that case $\rho_{0+} = \delta_+ \exp(-x/\lambda)$, and $\rho_+ = \rho_- = \rho_{0-} = 0$. For $\delta_+ > 0$ this puts excess right moving carriers into the distinguished channel, compensated by a negative density in all other right moving carrier populations. (IV) A similar unequal occupation decaying to the left with $\rho_{0-} = \delta_- \exp(x/\lambda)$, and $\rho_+ = \rho_- = \rho_{0+} = 0$.

Clearly solution (III) remains unbounded only on the right side of the barrier and solution (IV) only on the left side. (III) and (IV) can only be invoked where they remain bounded. We must now find a superposition of (I), (II), and (III) on the right side, and (I), (II), and (IV) on the left, which satisfy the following: (A) The same particle flux j, uniformly distributed over all channels, exists on the far right and the far left. (B) The flow in all of the $n-1$ undistinguished channels vanishes at the barrier at $x = 0$. (C) The flow away from the barrier in the distinguished channel, on each side, is related to the incident flow in that same channel through the reflection and transmission probability for that channel.

No physical insight is gained through the elementary algebra represented by (A), (B), and (C). We do note, however, without further analysis, that the total carrier density varies, in space on each side, only through solution (II). The redistribution between channels given by (III) and (IV) does not affect that. Therefore the net concentration gradient is spatially uniform. After invoking space charge neutrality, that means the electric field is uniform, except within a few screening lengths of the barrier. The additional voltage drop resulting from the insertion of the barrier, including that attributable to the redistribution between channels, *all* occurs at the barrier. The results of Sorbello[2] and Kunze[6] are more complex than that because they do not assume identical channels, as we do, away from the barrier. Sorbello[2] and Kunze[6] can get transport fields near the barrier that can be larger or smaller than those far away, depending on their choice for $R(\theta)$. Our actual voltage drop, resulting from insertion of the barrier, arises entirely from the discontinuity in solution (I) at the barrier. With the omitted algebra we find an additional resistance, due to barrier insertion:

$$\mathcal{R} = \frac{\hbar\pi}{e^2}\left(\frac{1}{T} - \frac{1}{n}\right). \tag{5.9}$$

It is the simplicity of this result, discussed in the next section, which warrants our crude model.

VI. INTERPRETATION OF RESULTS

For $n = 1$ the above analysis reduces to the one-dimensional case. Equation (5.9) becomes

$$\mathcal{R} = \frac{\hbar\pi}{e^2}\frac{R}{T}. \tag{6.1}$$

This is the well-known result of Eq. (2.2) applied to a one-dimensional scatterer. Thus, the extra resistance due to insertion of the barrier into the resistive medium is just the resistance of that barrier in an otherwise ideal one-dimensional conductor, confirming earlier results.[17]

In the limit of large n Eq. (5.9) becomes

$$\mathcal{R} = \frac{\hbar\pi}{e^2}\frac{1}{T}, \tag{6.2}$$

which is the single channel version of Eq. (2.1). That agreement, however, is fortuitous. After all, Eq. (2.1) is derived from a model where the reservoirs widen and allow geometrical dilution of carriers entering it, before appreciable scattering associated with the reservoir takes place. Equation (6.2), however, has carriers going into other channels because of the assumed background scattering.

Equation (5.9) gives a resistance that increases monotonically with n. The resistance, for $n > 1$, is larger than the result of Eq. (6.1). To discuss that, we will refer to the electrochemical potential, in a channel, or for all channels taken together, at a given position of space. The electrochemical potential, defined here for simplicity only for the diffusing noninteracting particle case, is simply the Fermi level that in equilibrium would give the same number of carriers. The drop in electrochemical potential, in the preferred channel, at the barrier will be given by the resistance of Eq. (6.1), multiplied by the total current. As the barrier is approached and the current transferred into the preferred channel the electrochemical potential gradient in that preferred channel has to increase above the value it has far from the barrier. The electrochemical potential for *all* the channels has a constant gradient as the barrier is approached, reflecting the diminishing gradient in the blocked channels.

The increase in the preferred channel *exactly* balances the decrease in the blocked channels only in our *very simple* model and is not characteristic of other treatments.[2,5,6] The fact that the resistance increase in Eq. (5.9) exceeds that of Eq. (6.1) for the barrier resistance in the preferred channel implies that there is a contribution to the total resistance which comes from the need to transfer carriers between channels. This difference, in our model, depends only on barrier properties, and not on scattering rates. That is again a result of the simplicity of the model that has only one parameter τ for the resistive background. It can be contrasted, for example, with the more complex results[19] for the case where *vertical* flow (i.e., in energy) is required and where the rates for transition in energy can be independent of the transition rates that determine spatial flow.

Knäbchen[5] points out that his result, expressed in his Eq. (16), consists of the background resistance plus a contribution that only depends on the barrier, as in our Eq. (5.9). He then goes on to state that this additivity verifies Matthiessen's rule. That seems to be an unfortunate choice of words. The term that depends only on the barrier is *not* the resistance of the barrier by itself, as given in Eqs. (2.3) or (2.4), but includes a funneling resistance whose value is independent of the value of the background scattering.

We have to add a note of caution to this discussion. On the basis of our model one might assume that immersing any obstacle in a medium with background scattering will give us a resistance that exceeds the sum of the separately calculated resistances. That is not always correct; adding background scattering can *reduce* the total resistance. Consider a compound obstacle in which a left-hand barrier permits good transmission only in a narrow range of incident angles. This is followed at some distance by a second layer, which has a similar narrow angular window, not overlapping the range of the first window. Adding scattering between the two barriers, and thereby allowing conversion from one angle to the other, will increase the net transmission.

Note added in proof. Recent experiments[22] have utilized the two-dimensional version of Eq. (3.1) to interpret the resistance of misfit dislocations in a high-mobility heterostructure layer.

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