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The minimal principle for the current distribution in microstructures and the resistance in long incoherently coupled chains

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Abstract. As in the Landauer–Büttiker approach to transport, a transmitter is, at fixed energy, characterized by its reflection and transmission coefficients. Generalizing a prior approach, we establish a variational principle to determine, without magnetic field, the distribution of the current over the different channels if the transmitter is coupled incoherently to its surroundings. For transmitters coupled with each other, a general demand of additivity defines the form of the variational functional. Contacts are treated as special transmitters, and, as a test, the results of the standard model are reproduced.

A typical serial resistance is defined as the resistance within a long incoherently coupled chain, with no regard to contacts and reservoirs. This resistance is strictly additive. It is shown that well within the chain a relaxed current and density distribution is established that is independent of the conditions at the ends of the chain. This distribution coincides with the optimal distribution that minimizes the resistance of each of the single transmitters that are the building blocks of the chain. For a sufficiently long chain, the serial resistance is determined by the linear dependence of the inverse total transmission on the number of single transmitters.

The relaxational behaviour of a long chain implies corresponding features of the reflection and transmission matrices in the asymptotic regime, especially a factorization of the transmission matrix, expressing memory loss with respect to the ingoing and outgoing channels.

1. Introduction

In a previous paper [1], we addressed anew an old question: what is the resistance of an elastic transmitter between two probes? In the spirit of Landauer—cf. [2] for example—we have replaced the usually assumed ideal leads by resistive leads. In such leads the carriers can, via channel–channel transitions, adapt their channel distribution in such a manner as to facilitate transport through a given transmitter, i.e. to populate transparent channels and to avoid the others. Far from the perturbing transmitter, an unperturbed current and density distribution is established, also due to channel–channel transitions, where a local chemical potential (or its on-energy-shell precursor) is well defined. This allows a sound definition of a resistance. The transport within the leads has been treated within a rather simple semi-classical kinetic method. As a by-product of this approach, we found that the solution for the coupled system of a transmitter and the resistive leads attached to it can be found by minimizing a certain variational functional. This functional is strictly additive in parts corresponding to each of the two leads and to the transmitter, each part separately is positive

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definite, and the simple mathematical form of the lead functional points to the interpretation in terms of dissipated power.

In [1], the needs to represent the lead kinetics, and to couple it with the reflection–transmission properties of the transmitter and—mainly—the rather cumbersome procedure to prove the existence of the variational functional and to express it, at least for special cases, explicitly as a functional of the currents themselves has tended to mask the generality of the approach. In this paper we take, in a somewhat axiomatic manner, the variational principle as the starting point. In this context, it is quite natural to consider, instead of the special two-probe case, a general network of transmitters, connected with each other in parallel or in series and with the ‘external world’ via any number of leads. In this paper, resistive leads are not revisited.

We note that the concept of carriers that adapt their distribution over channels or directions to a given obstacle has been successfully applied recently by Kunze to similar problems, i.e. to a localized obstacle in a quantum film [3] or in the 3d bulk [4] and to a planar defect of grain boundary type [5]; cf. also [13]. All of these results, some of them belonging in full to classical transport theory, are beyond perturbational approaches.

We state now the main conceptual points of our paper.

(a) We study, without magnetic field and without inelastic processes, dc transport of non-interacting particles. The current is driven by density differences or gradients, respectively, i.e. there is no driving force (no electric field). Because for an ensemble of many electrons this situation cannot be realized, the results must be translated, at the end, to the force case. This can be, as usual, achieved via the Einstein equivalence between differences in voltage and chemical potential. This equivalence only works if a chemical potential can be really defined, at least locally. This is the case in reservoirs or in resistive leads far away from the transmitter.

(b) Quantities like resistance or conductance cannot be defined for a subsystem if there are coherent interactions with others. Only if these effects are either destroyed or can be neglected, i.e. if the subsystem is coupled incoherently to its surroundings, can it be considered in the classical sense as a subunit of the whole system. The incoherence is maintained especially in the standard model [6] due to the very concept of reservoirs. Between transmitters we could also imagine connecting leads where weak phase-breaking processes destroy coherence without contributing appreciably to the resistance. In other cases the subdivision of a larger system into incoherently coupled parts is sensible in order to mimic phase-breaking processes that really occur within them. If (and only if!) the incoherence condition is fulfilled, classical combination rules should hold. For transmitters in series this means additivity of their resistances.

For a general network of incoherently coupled transmitters, the corresponding additive physical quantity is interpreted as the dissipated power. We will show in section 2 that the general demand of additivity is very stringent; in fact it defines the form of the functional wanted.

(c) Apart from in the simplest one-channel case, a transmitter is a much more complicated object than a classical ‘resistor’ where the situation is completely defined if the total current is given. For a typical transmitter, the resistance depends on the specific distribution of the given total current over the channels (lateral modes) that are defined for all leads. This means that a transmitter cannot be described simply by a single ‘resistance’ or ‘conductance’ but must necessarily be defined by a functional that determines this quantity *for all possible* current distributions. Depending on the coupling with others and with external leads and/or reservoirs, a specific current distribution is finally established.

(d) The dissipation functional is employed to establish a variational principle: the correct current distribution yields minimal dissipation. This is in accord with the principle of minimal entropy production [7] that rules, in the framework of the thermodynamics of irreversible processes, a stationary non-equilibrium state. Nevertheless it seems to be not quite the same because the physical transport situation in microstructures cannot be fully described with the concept of local thermodynamic equilibrium states.

The dissipated power has to be minimized under the constraint of given total currents in all external leads, varying the distribution over the channels for each external lead. For internal leads, connecting different transmitters, not only the total currents but even their distribution over all of the channels are precisely determined by the given transition coefficients of the transmitters forming the network if the external current distribution is completely specified. The complexity of a network is reflected in the difficulty of solving this question. Another variant, followed in sections 2 and 3, is to consider formally the whole network as a single transmitter. The task is then to construct the transition coefficients for this complex from those of its constituents. This remains also to be done if necessary—cf. [8] for the calculation of the corresponding amplitudes.

There is no general proof for the validity of the variational principle stated above. In the present paper, we only show, generalizing the discussion in [1], that it correctly reproduces the standard model where ideal leads couple via contacts to reservoirs.

The specific problem in the present paper is, for transmitters in series, the behaviour of the current distribution and the corresponding resistance in a (long) chain. A single transmitter within the chain is neither in the situation modelled in the standard model nor in that where resistive leads are attached to it. Whereas a huge amount of work has been done on calculating the properties of complex single transmitters with all internal interference effects, this problem has been scarcely studied. The current distribution in a long chain should be mainly a property of the chain itself, nearly independent of the external leads and reservoirs for the chain as a whole. For a single transmitter as a constituent of a long chain, we envisage a certain kind of embedding, and a definite resistance should correspond to this situation. We call it typical serial resistance.

The relaxational mechanism that produces the well-defined ‘chain distribution’ is also responsible for the dependence of the chain reflection and transmission matrices on the number of constituting single blocks. In the present paper, this problem is only briefly considered in the asymptotic regime where the transmission matrix for sufficiently long chain segments factorizes.

This paper is organized as follows. In section 2 the variational principle is restated and generalized. We prove that the functional is positive definite. In section 3 the variational principle is used to reproduce the well-known results of the standard model. This allows one to treat the contacts to the reservoirs as special transmitters. In section 4 it is shown that in a long chain, sufficiently far from its ends, just that channel distribution evolves that is optimal for each of the single blocks. Finally, in section 5, the asymptotic reflection and transmission properties of a chain are discussed.

2. The variational functional

Consider an arbitrary elastic transmitter (often called a block in the following) coupled to its surroundings via a set of channels n . These channels can be realized by lateral modes of quantum wires but, allowing for continuous spectra, other situations are possible too. In each channel the resulting current may flow towards or away from the transmitter, depending

on the specific situation. The transitions between the channels via the block are described by a set of normalized transition probabilities T_{nm} from m to n , $\sum_n T_{nm} = 1$. Without any magnetic field, reciprocity holds in the form $T_{nm} = T_{mn}$, and the transition probabilities form a symmetrical matrix.

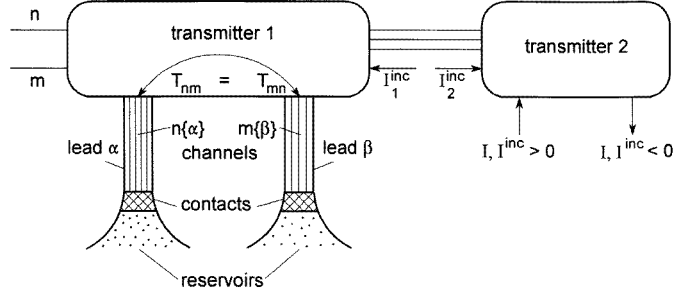


Figure 1. Some basic notation used in sections 2 and 3.

For each channel, we define currents as positive if they flow to the transmitter just considered. Current balance means then that $\sum I_n = 0$. The currents can be considered as the result of incident currents I_n^{inc} ; cf. figure 1 for notation. The total incident currents are positive by definition. They comprise, however, a part $I_n^{inc} = \text{constant}$ that characterizes the current-free equilibrium state. Therefore $I_n^{inc} < 0$ becomes possible for the only relevant current-proportional part. I_n^{inc} in all channels being given, the resulting currents are

$$I_n = I_n^{inc} - \sum_m T_{nm} I_m^{inc}. \quad (1)$$

For a general network of incoherently coupled scatterers, the dissipated power P_B must be additive with respect to the subsystems. Because all of the single channels n can contribute, alone or grouped in any way to form leads, an additive form $P_B = \sum P_n$ should exist. If channel n , within an ideal lead, couples two blocks, this channel disappears as an external one for the combined system. This means that $P_n^{(1)} + P_n^{(2)} = 0$ if 1 and 2 denote the two blocks. This relation must be the mathematical consequence of a simple and general linear relationship between them. There is only one such relation, namely

$$I_n^{(1)} = -I_n^{(2)} = [I_n^{(1)} - I_n^{(2)}]^{inc}. \quad (2)$$

One easily confirms that

$$P_n = I_n(2I_n^{inc} - I_n) \quad (3)$$

fulfils the requirement of additivity; thus

$$P_B = \sum_s P_B^{(s)} \quad P_B^{(s)} = \sum_n^{(s)} P_n^{(s)} \quad (4)$$

holds for any network of subblocks s . Note that the arbitrariness $I_n^{inc} \rightarrow I_n^{inc} + \text{constant}$ of the incident currents does not affect P_B . For the special case of two leads, the equivalent formula has been derived as equation (58) in [1]. (Unfortunately there is a printing error in this formula: the last sign should read '+'.)

Because all interference effects outside the transmitter are neglected, we can decompose these currents and carrier densities according to the two possible directions of motion in

each channel, i.e.

$$\rho_n = \rho_n^+ + \rho_n^- \quad I_n = v_n(\rho_n^+ - \rho_n^-). \quad (5)$$

We have then

$$I_n^{inc} = v_n \rho_n^+ = \frac{1}{2}(v_n \rho_n + I_n) \quad (6)$$

and

$$P_B = \sum_n I_n v_n \rho_n. \quad (7)$$

v_n are the channel-specific velocities. In the form (7), the internal compensation for connected blocks and thus the additivity (4) are obvious because the density is the same for both blocks.

Because $I_n^{inc} = \text{constant}$ yields no net currents I_n , the incident currents cannot be reconstructed unambiguously from the currents. Therefore we consider P_B as a functional of the incident currents alone:

$$P_B = \tilde{I}(2\mathbf{I}_{inc} - \mathbf{I}) = \tilde{I}_{inc}(1 - \mathbf{T})(1 + \mathbf{T})\mathbf{I}_{inc} = \tilde{I}_{inc}(1 - \mathbf{T}^2)\mathbf{I}_{inc}. \quad (8)$$

Here we have introduced vector and matrix notation for all of the currents and transition probabilities. Whenever convenient, it will be also used in the following.

If the interpretation in terms of dissipated power is correct, $P_B \geq 0$ must hold. This is true if the real eigenvalues t_i of the (symmetrical) matrix \mathbf{T} obey

$$-1 \leq t_i \leq 1 \quad t_i^2 \leq 1. \quad (9)$$

This is indeed fulfilled for matrices with non-negative elements and a normalized sum for each line or row; cf. [9]. We present a simple argument. Together with \mathbf{T} all \mathbf{T}^m , $m > 1$ integer, are matrices of the same kind, representing a possible set of transition probabilities. The eigenvalues of such a matrix are clearly restricted in absolute value, and this property remains valid for \mathbf{T}^m if (9) holds.

3. Contacts and the standard model

In accordance with typical experimental situations, we combine subsets of channels $\{n(\alpha)\}$ in groups α to represent leads. Within such a group, transitions from $n(\alpha)$ to $n'(\alpha)$ are reflections with respect to the lead α ; all others are transmissions between different leads.

We consider now a transmitter which joins a given number of leads α, β, \dots . We further assume that all of the transition coefficients are simply given by $T_{nm} = N^{-1}$ where N is the total number of channels; see below, however. This implies that all of the channels are coupled very smoothly to the block, for example by an adiabatic widening of the leads. Otherwise some ‘direct reflection’ at the ‘entrance’ to the block would appear. Relation (1) gives now $I_n = I_n^{inc} + \text{constant}$. Such a constant term, however, reflects just the arbitrariness of the incident currents, corresponding to the always-present current-free solution. Thus we can simply ignore that term, and get

$$P_B \rightarrow P_C = \sum_n I_n^2 = \tilde{I}\mathbf{I} \quad (10)$$

As indicated by the notation, this is a model of a contact (a soldered joint) where different channels (leads) are connected. With a slight modification of the model, we have already used [1] this expression to describe the contacts between leads and reservoirs. If the present model of contacts is correct, the simple expression (10) can be used for all kinds of contacts

acting as couplers, splitters or mixers that are characterized by sufficient complexity to ensure the assumed memory loss and by smoothness to avoid direct reflections. To each channel where the current enters or leaves such a contact a, ‘resistance’ of value 1 is attributed, independently of the number of channels and their grouping to form leads.

The simple relation $T_{nm} = N^{-1}$ may strictly hold only on average with respect to the configuration of the contact; fluctuation problems remain open to question. Also elastic enhancement due to anomalous backscattering [10] is beyond the simple contact model.

What we really need in the present context is a description of contacts between leads and (large) reservoirs. For this special but most important case, the result (10) can be reproduced quite generally. At first, due to the very large number N_R of channels on the reservoir side R , the term $\tilde{\mathbf{I}}^R \mathbf{I}^R \propto N_R^{-1}$ can be neglected. The incident currents there are those of an equilibrium state, i.e. $I_m^{inc}|_R = A = \text{constant}$, and this gives $P_C^R \rightarrow 2A \sum I_m^R$ for the reservoir side of the contact. There are no reflections on the lead side; the contact acts like a black body. Thus we have

$$I_{n(L)} = I_{n(L)}^{inc} - \sum_m T_{n(L), m(R)} I_m^{inc} = I_{n(L)}^{inc} - A \quad (11)$$

where the normalization of the transition elements, now without reflection on the lead side L , is employed. Equation (11) allows us to eliminate the incident currents on the lead side of the contact with the result

$$P_C = P_C^L + P_C^R = \sum_n^{(L)} I_n^2 + 2A \left[\sum_n^{(L)} I_n + \sum_m^{(R)} I_m \right] = \sum_n^{(L)} I_n^2. \quad (12)$$

The square bracket is zero due to the overall current balance. Thus we arrive again at the form (10), but now applied to the lead side of the contact only.

Note that the second term in (11) is just the current injected from the reservoir into the lead. Its equipartition over all of the lead channels follows from the absence of reflections. With a magnetic field \mathbf{B} applied, we get $T_n(-B)$ for the sum of transmission coefficients appearing in (11); thus $T_n = 1$ again because this relation does not depend on B at all and especially not on its sign.

In contrast to the considerations leading to the formally equivalent relation (10), the treatment of the lead–reservoir contact is not burdened by fluctuation problems. Equation (12) remains correct for fluctuating currents, even if the internal properties of the contact should fluctuate.

We denote as ‘standard’ the model [6] where a transmitter is connected via ideal leads and contacts to reservoirs that feed all channels of a given lead with the same incident current, but channels in different leads with different currents according to the specific chemical potentials of the reservoirs.

For the two-probe case [1] we have already demonstrated that the dissipated power P can be used as a variational functional: the correct distribution of the current over the channels minimizes P . Now we generalize this variational principle to the case of a block, connected with any number of reservoirs via ideal more-channel leads and contacts. For the standard model, the functional P_{st} consists of the block term P_B and the contact term P_C . The contacts (10) just compensate the corresponding term in the block functional (3), (4). This is essential for the simplicity of the standard result. We get

$$P_{st} = P_B + P_C = 2 \sum_n I_n^{inc} I_n = 2 \tilde{\mathbf{I}}_{inc} \mathbf{I}. \quad (13)$$

Due to the equivalence of all channels for the construction of P_B as well of P_C , P_{st} itself does not depend on the α -grouping of channels to form leads.

Now the leads come into play because the total currents I_α in the different leads can be fixed independently. Their specific values are not determined by the variational principle that only rules the distribution of the current over *coupled* channels. Given values of I_α are restrictive conditions for the variational principle. We define Θ_α as a vector whose components are 1 for each channel belonging to lead α and zero otherwise. Then we have

$$I_\alpha = \tilde{\Theta}_\alpha I = \tilde{\Theta}_\alpha (1 - \mathbf{T}) I_{inc}. \quad (14)$$

With Lagrangian multipliers $2\lambda_\alpha$ the incident currents can be varied independently with the result

$$I = \frac{1}{2} (1 - \mathbf{T}) \sum_\alpha \lambda_\alpha \Theta_\alpha. \quad (15)$$

Comparison with (1) shows that $I_{n(\alpha)}^{inc} = \lambda_\alpha/2$.

The currents in all channels for all leads are now uniquely determined. The equal-feeding rule is a consequence of the variational principle and the properties of a contact. This does not come as a surprise because this feature of the injection process had already been found when the functional P_C of a contact was constructed; cf. the text after (12).

The minimal value of P_{st} is

$$\text{Min } P_{st} = \sum_\alpha I_\alpha \lambda_\alpha. \quad (16)$$

Obviously the parameters λ_α are determined only up to a common constant; remember that $\sum I_\alpha = 0$. λ_α is closely related to the chemical potential μ_α in the reservoir α . In fact, at zero temperature at least, $\lambda_\alpha = (g/\pi\hbar)\mu_\alpha$ with spin factor $g = 2$ for electrons yields Büttiker's formulation [6] of the standard model. The parameters λ_α determine the currents I_α ; for given I_α they have to be adjusted so as to produce these. We find from (15)

$$I_\alpha = \frac{1}{2} (N_\alpha - R_\alpha) \lambda_\alpha - \frac{1}{2} \sum_{\beta \neq \alpha} T_{\alpha\beta} \lambda_\beta \quad (17)$$

where N_α is the number of channels in lead α , and, as usual, R_α and $T_{\alpha\beta}$ gather together all reflection or transmission coefficients that correspond to the given lead grouping of channels. Equation (17) is the basic equation in Büttiker's formulation [6].

4. Optimal current distribution and resistance in a chain

The resistance of a given transmitter is not an intrinsic property; rather it is defined only with respect to a specific kind of embedding that inevitably influences the current distribution at the transmitter interface and thus its resistance. This may not be a serious problem for small probes where the standard model applies. It becomes a problem, however, if one wants to describe bulk properties, especially in localization theory where at the end, with a certain temperature-dependent phase-breaking length, blocks of that length scale are coupled incoherently, i.e. according to the classical rules. Then each of these 'coherence blocks' is generally not in a position like a microprobe between, for example, reservoirs. Instead its environment is composed of all of the other coherence blocks, all more or less the same. Here we will discuss only the serial problem for identical transmitters. In a long chain of such transmitters, one expects a current distribution that only at the outermost blocks is strongly influenced by external leads and/or contacts. Well within the chain, the distribution should characterize the chain itself, and, in the sense of being its constituents, the single blocks, too.

There are two different questions. The first one is very simple: what distribution of current and density minimizes the resistance of a single transmitter and what is the corresponding minimal value of the resistance? The second one is more involved: is there really a relaxational mechanism for establishing a certain distribution that is specific for the chain, and how are this distribution and the corresponding value of the resistance specified? We will prove that this distribution is exactly the optimal single-block distribution. There is thus complete serial compatibility, and the minimal resistance is realized in a long chain of identical transmitters.

Employing the variational principle, it is easy to find the optimal current distribution for a single transmitter. For simplicity, we restrict the discussion to a transmitter with equivalent left- and right-hand sides, $\mathbf{R}_l = \mathbf{R}_r = \mathbf{R} = \tilde{\mathbf{R}}$, and a left–right symmetrical transmission matrix \mathbf{T} . On symmetry grounds, the minimum of P_B is attained for $\mathbf{I}_l = \mathbf{I}_r = \mathbf{I}$. (Unlike for the general case—sections 2 and 3—the currents are now counted as positive if they flow from the left to the right, i.e. we have a change in the sign convention for \mathbf{I}_r .) The functional (3) takes the simplified form

$$P_B = I^2 \mathcal{R} = 2\tilde{\mathbf{I}}(\mathbf{I}_l^{inc} - \mathbf{I}_r^{inc} - \mathbf{I}) = \frac{1}{2}(\tilde{\mathbf{I}}_l - \tilde{\mathbf{I}}_r)^{inc} (1 - \mathbf{R} + \mathbf{T})(1 + \mathbf{R} - \mathbf{T})(\mathbf{I}_l - \mathbf{I}_r)^{inc} \quad (18)$$

which defines the resistance \mathcal{R} . Varying the difference of the incident currents under the constraint $I = \text{constant}$, we find the optimal distribution

$$\mathbf{I}^o \propto (1 + \mathbf{R} - \mathbf{T})^{-1}(1 - \mathbf{R} + \mathbf{T})\mathbf{1} \quad (19)$$

and the minimal resistance

$$\frac{1}{2}\mathcal{R}^o = \left[\tilde{\mathbf{1}}(1 + \mathbf{R} - \mathbf{T})^{-1}(1 - \mathbf{R} + \mathbf{T})\mathbf{1} \right]^{-1}. \quad (20)$$

The current distribution (19) on both sides corresponds to a density distribution $\mathbf{v}\rho \propto \mathbf{1}$ there. This can be seen from the relations (24); cf. below. It means that the lateral density distribution is the same as in the equilibrium state.

The resistance formula (20) is obviously of the Landauer type, i.e. $\mathcal{R}^o = 0$ without reflections. It yields $\mathcal{R}^o = 2R/T$ in the one-channel case, of course. In the limit of small transmission, $(1 + \mathbf{R} - \mathbf{T})\mathbf{1} \approx (1 + \mathbf{R} + \mathbf{T})\mathbf{1} = 2 \times \mathbf{1}$, one finds again the standard result $\mathcal{R}^o \approx 2T_{tot}^{-1}$. If all of the channels are equivalent, $\mathbf{R}\mathbf{1} \propto \mathbf{T}\mathbf{1} \propto \mathbf{1}$, we get

$$\frac{1}{2}\mathcal{R}^o = T_{tot}^{-1} - N_c^{-1} \quad (21)$$

with N_c as the number of channels; cf. equation (32) in [1] for the case of different channel numbers on the two sides, and also a recent paper [13] of Landauer for a discussion of a simplified model.

For the special case of only two channels (on either side), we have calculated \mathcal{R}^o numerically for a large number of transmitters with randomly chosen parameters. The results (figure 2) show that \mathcal{R}^o is close to the reference value (21) in most cases. For strong inequivalence of channels, however, it can be significantly lower. Such a change is promoted by reflective and hindered by transmittive channel coupling.

Of some interest—cf. also the next section—is a transmitter with factorized transmission matrix $\mathbf{T} \propto \mathbf{t} \circ \tilde{\mathbf{t}}$. Employing the matrix inversion formula

$$[\mathbf{A} + c\mathbf{u} \circ \tilde{\mathbf{u}}]^{-1} = \mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{u} \circ \tilde{\mathbf{u}}\mathbf{A}^{-1}}{\tilde{\mathbf{u}}\mathbf{A}^{-1}\mathbf{u} + c^{-1}} \quad (22)$$

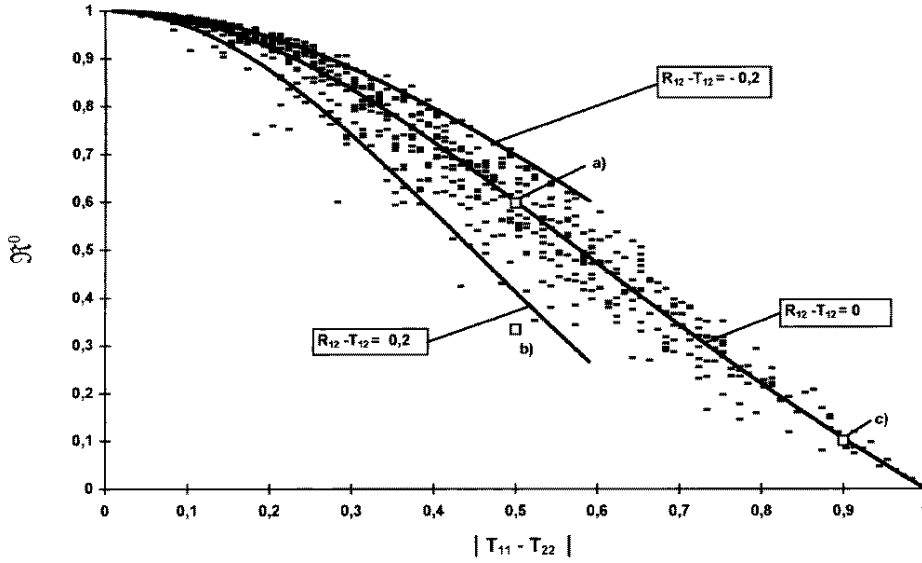


Figure 2. Minimal resistance for randomly chosen transmitters with two channels each. The total transmission is fixed at $T_{tot} = 1$, i.e. at half its maximal value. The resistance (21) for two equivalent channels, suited as a reference value, is thus 1. For the meaning of the three points marked by (a), (b), (c), see figure 4.

we get from the general expressions (19), (20)

$$I^o \propto (1 + \mathbf{R})^{-1}(1 - \mathbf{R})\mathbf{1}$$

$$\frac{1}{2}\mathcal{R}^o = T_{tot}^{-1} - \left\{ 2 \left[\tilde{\mathbf{1}}(1 - \mathbf{R})\mathbf{1} \right]^{-1} - \left[\tilde{\mathbf{1}}(1 + \mathbf{R})^{-1}(1 - \mathbf{R})\mathbf{1} \right]^{-1} \right\}. \quad (23)$$

Due to the reflection-transmission balance, the reflection matrix \mathbf{R} must obey $(1 - \mathbf{R})\mathbf{1} \propto t$, in other respects it remains unspecified here.

The first term in (23) is the resistance within the well-known standard model [6], i.e. it corresponds, in the general case at least, to a current distribution that differs from I^o and comprises in any case both contact resistances. Therefore the term in the curly bracket has to be positive to yield $\mathcal{R}^o < 2T_{tot}^{-1}$. The expression in (23) meets this condition. This can be easily shown to follow from the property $-1 \leq r_i \leq 1$ of the (real) eigenvalues of \mathbf{R} ; cf. [9], p 55.

Now, independently of the minimal principle, we ask: is it possible to maintain a characteristic current (and corresponding density) distribution that remains *constant* along a chain of identical, incoherently coupled transmitters? The answer is ‘yes’, and the ‘chain distribution’ is just the optimal ‘single-block distribution’ (19). The latter statement is simple but a bit strange, for it means that it is not necessary to effect a compromise where a non-minimal resistance is accepted in order to achieve self-consistency along the chain.

For a proof, we eliminate in the basic reflection–transmission equations the incident currents in favour of the densities; cf. (5) and (6). The results are relations between the currents and densities; on the two sides of a transmitter. They read

$$I_l + I_r = (1 + \mathbf{R} - \mathbf{T})^{-1}(1 - \mathbf{R} + \mathbf{T})(\mathbf{v}\rho_l - \mathbf{v}\rho_r) \equiv \mathbf{M}_1\mathbf{v}(\rho_l - \rho_r)$$

$$I_l - I_r = (1 + \mathbf{R} + \mathbf{T})^{-1}(1 - \mathbf{R} - \mathbf{T})(\mathbf{v}\rho_l + \mathbf{v}\rho_r) \equiv \mathbf{M}_2\mathbf{v}(\rho_l + \rho_r). \quad (24)$$

As is seen merely by inspection, $I_l = I_r = I^o$ and $\mathbf{v}\rho_{l,r} \propto \mathbf{1}$ solves (24). More important for the chain problem, $I_r = I^o$ and $\mathbf{v}\rho_r \propto \mathbf{1}$ follows from the same relations for the left-hand side. Indeed, with $\mathbf{M}_1^{-1}I_l \propto \mathbf{1}$ and $\mathbf{M}_2\mathbf{v}\rho_l = 0$ we find, combining the two lines of (24), $(1 - \mathbf{M}_1^{-1}\mathbf{M}_2)\mathbf{v}\rho_r \propto \mathbf{1}$ with

$$1 - \mathbf{M}_1^{-1}\mathbf{M}_2 = 4(1 - \mathbf{R} + \mathbf{T})^{-1}\mathbf{T}(1 + \mathbf{R} + \mathbf{T})^{-1} \quad (1 - \mathbf{M}_1^{-1}\mathbf{M}_2)\mathbf{1} \propto \mathbf{1}. \quad (25)$$

This yields $\mathbf{v}\rho_r \propto \mathbf{1}$ and thus $I_l = I_r$ according to the second line of (24)—i.e. it proves the statement above: if the optimal ‘single-block distribution’ is reached in a chain, it transforms itself to the neighbour intervals.

The real physical question is more challenging. We should show that any distribution, corresponding to an arbitrarily given situation at the ends of the chain, relaxes to the optimal distribution well within. To study this problem, we decouple the equation system (24) to find equations for the current or the density separately. This is achieved by going from the first-order differences of currents and densities in (24) to second-order differences, involving three neighbouring intervals along the chain. We find

$$\Delta_2 I_m \equiv I_{m+1} - 2I_m + I_{m-1} = \mathbf{M}(I_{m+1} + 2I_m + I_{m-1}) \quad \text{with} \quad \mathbf{M} \equiv \mathbf{M}_2\mathbf{M}_1^{-1} \quad (26)$$

and a similar relation for $\mathbf{v} \Delta_2 \rho$ where \mathbf{M} is replaced by the transposed matrix $\tilde{\mathbf{M}} = \mathbf{M}_1^{-1}\mathbf{M}_2$. The two matrices have the same eigenvalues m_λ but different eigenfunctions:

$$\begin{aligned} \mathbf{M}\mathbf{u}_\lambda &= m_\lambda \mathbf{u}_\lambda & \tilde{\mathbf{M}}\mathbf{v}_\lambda &= m_\lambda \mathbf{v}_\lambda \\ \tilde{\mathbf{u}}_\lambda \mathbf{v}_\lambda &= \delta_{\lambda\lambda} \end{aligned} \quad (27)$$

that are related with each other via

$$\mathbf{u}_\lambda \propto \mathbf{M}_1 \mathbf{v}_\lambda. \quad (28)$$

The eigenvalues can be represented in the form

$$m_\lambda = \frac{\tilde{\mathbf{v}}_\lambda \mathbf{M} \mathbf{u}_\lambda}{\tilde{\mathbf{v}}_\lambda \mathbf{u}_\lambda} = \frac{\tilde{\mathbf{v}}_\lambda \mathbf{M}_2 \mathbf{v}_\lambda}{\tilde{\mathbf{v}}_\lambda \mathbf{M}_1 \mathbf{v}_\lambda}. \quad (29)$$

See (24) for the definition of \mathbf{M}_1 and \mathbf{M}_2 .

As usual, the eigenvalues determine the essential properties of the relaxation process. The eigenvalue $m_0 = 0$ yields the stationary solution $\mathbf{v}\rho_0 = v_0 \propto \mathbf{1}$ and $I_0 \propto \mathbf{M}_1 \mathbf{1} \propto I^o$. In contrast to \mathbf{M} or $\tilde{\mathbf{M}}$, the $\mathbf{M}_{1,2}$ are symmetric. Thus they have real eigenvalues. These are generally positive, with the zero eigenvalue of \mathbf{M}_2 as a trivial exception. This important property follows from $P_B \geq 0$; see (8) and (9) for the general proof. Specializing to the case of a transmitter with only two leads, as studied now, one gets the form given in equation (60) of [1]. If the transmitter is left–right symmetric and the incident currents from the left and from the right are equal we find that $1 - (\mathbf{R} + \mathbf{T})^2 = (1 + \mathbf{R} + \mathbf{T})(1 - \mathbf{R} - \mathbf{T})$ is a positive semi-definite operator; if they differ only in sign this statement follows for $1 - (\mathbf{R} - \mathbf{T})^2 = (1 + \mathbf{R} - \mathbf{T})(1 - \mathbf{R} + \mathbf{T})$. This proves that also \mathbf{M}_1 and \mathbf{M}_2 are positive (semi-)definite.

Going back to the eigenvalue problem (27), this property of $\mathbf{M}_{1,2}$ renders it possible to symmetrize the equations (27) by using $U_\lambda = \mathbf{M}_1^{1/2} \mathbf{u}_\lambda$ or $V_\lambda = \mathbf{M}_2^{1/2} \mathbf{v}_\lambda$ within the scheme of real matrices. Therefore not only $\mathbf{M}_{1,2}$ but also \mathbf{M} and $\tilde{\mathbf{M}}$ have only real eigenvalues and thus real eigenfunctions. Thus the representation (29) can be used with the restriction to a real vector space that the v_λ belong to, and this shows finally that

$$m_\lambda \geq 0. \quad (30)$$

As a consequence of the fact that $P_B \geq 0$, the matrices \mathbf{M} , $\tilde{\mathbf{M}}$ have only real and positive eigenvalues.

With the eigenvalue problem (27) solved, the solutions of the second-order differential equations for \mathbf{I}_m and $\mathbf{v}\rho_m$ —see (26) and the nearby text—are easily found as

$$\mathbf{I}_{\lambda,m} \propto \alpha_\lambda^m \mathbf{u}_\lambda \quad \mathbf{v}\rho_{\lambda,m} \propto \alpha_\lambda^m \mathbf{v}_\lambda \quad (31)$$

with

$$\frac{1}{2}(\alpha_\lambda + \alpha_\lambda^{-1}) = \frac{1 + m_\lambda}{1 - m_\lambda} \quad \left(\frac{1 - \alpha_\lambda}{1 + \alpha_\lambda}\right)^2 = m_\lambda.$$

With $m_\lambda \geq 0$, the latter relation is always solved by two real values of α_λ , and their product equals 1. α_λ and α_λ^{-1} correspond to relaxation in either direction along the chain. $m_0 = 0$ gives $\alpha_0 = \alpha_0^{-1} = 1$, where in the density case a constant *difference* $\mathbf{v}\Delta\rho \propto \mathbf{1}$ is the correct solution of the coupled system (24). For $m_\lambda < 1$, α_λ and α_λ^{-1} are positive, and the relaxation (in the corresponding mode) is monotonic then. For $m_\lambda > 1$, α_λ and α_λ^{-1} are negative which yields an alternating relaxation behaviour.

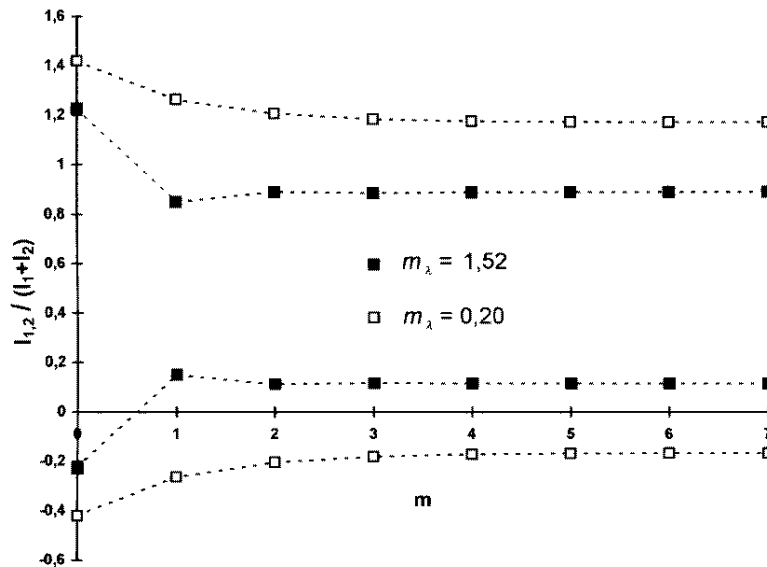


Figure 3. Relaxational behaviour of the channel currents for two transmitters with two channels each. For $m_\lambda = 1.52$ the relaxation is alternating and very quick; for $m_\lambda = 0.20$ it is monotonic and a bit slower. The numerical calculation is done for a chain with $M = 20$ transmitters totally. $m = 0$ means outside the chain; the partial currents there depend strongly on the currents incident from the left.

The considerations of this section show that the minimal resistance (20) of a single transmitter is not a mere mathematical lower bound but a value that attains physical significance as the serial resistance in a sufficiently long chain. This is by no means self-evident. On the contrary, it is rather unexpected because simple examples, e.g. with two channels only, show that the optimal current distribution may be characterized by back-currents in channels of lower transmittivity if the channel–channel coupling is effective enough. The tendency to minimize the resistance is strong enough to establish such distributions in the physical reality of a chain.

In figure 3 two examples for the current relaxation are shown, including alternating behaviour and the occurrence of back-currents. The numerical data result from a direct treatment of the coupled-chain problem with arbitrarily chosen incident currents on the left and/or right. The analytical theory of the relaxation process is not employed.

5. Transmission and reflection for long chains

The very fact that the current and density distributions relax to the stationary distributions I^o and $\mathbf{v}\rho^o \propto \mathbf{1}$, independently of the incident currents at the ends of the chain, implies that, as the mathematical formulation of memory loss, the transmission matrices of sufficiently long chain segments must factorize with the total transmission T_M^{tot} as the only parameter that depends on the number of single blocks in the segment. The reflection matrix for $M \gg 1$ comprises a factor term of the same kind and a non-factorized term $\hat{\mathbf{R}}$, too:

$$M \gg 1: \quad \mathbf{T}_M \cong A_M \mathbf{t} \circ \tilde{\mathbf{t}} \quad \mathbf{R}_M \cong \hat{\mathbf{R}} + B_M \mathbf{t} \circ \tilde{\mathbf{t}}. \quad (32)$$

Only the coefficients A_M and B_M depend on M , in contrast to \mathbf{t} and $\hat{\mathbf{R}}$. The values of A_M, B_M depend on the chosen normalization of \mathbf{t} that can remain unspecified in the present context. The form (32) has been shown to be asymptotically correct for a resistive wire [11], and is established in generality in a recent paper by Tartakovski [12].

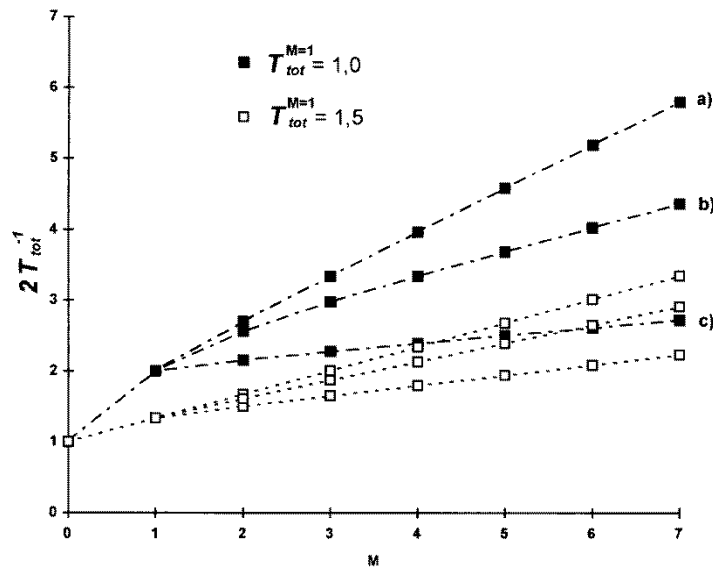


Figure 4. The inverse total transmission for a chain composed of M equal transmitters with two channels each. Two groups with different total single-block transmissions are shown. For the group with $T_{tot} = 1$ for the single block, the minimal resistance values for the same transmitters are also marked in figure 2 by (a), (b), (c) as in the present figure.

For given incident currents at the chain ends, the current and density distributions for any interval within the chain are uniquely determined by the transmission and reflection properties of the two segments. If we consider an interval sufficiently distant from the chain ends, the expressions (32) can be used, with the result

$$I \propto (1 - \hat{\mathbf{R}})^{-1} (1 + \hat{\mathbf{R}}) \mathbf{1} \quad \mathbf{v}\rho \propto \mathbf{1}. \quad (33)$$

A proof is sketched in the appendix. This current distribution must be identical with the optimal single-block distribution \mathbf{I}^o .

The minimal resistance for a chain segment with any length $M \geq 1$ is $M\mathcal{R}^o$ according to the results of the preceding section. For $M \gg 1$, the resistance formula in (23) applies for $\mathcal{R}_M^o = M\mathcal{R}^o$ with T_{tot} replaced by T_M^{tot} and \mathbf{R} by $\hat{\mathbf{R}}$. This relation can be read as a statement on the asymptotic behaviour of T_M^{tot} :

$$(T_M^{tot})^{-1} \cong \frac{1}{2}M\mathcal{R}^o + \text{constant} \quad (34)$$

where the constant term has been given in (23), but now with $\hat{\mathbf{R}}$ instead of \mathbf{R} . This is a very appealing result: the linear term in the inverse total transmission of a long chain defines the serial resistance of a single block; cf. figure 4. This result corresponds nicely with the standard model. Note, however, that this model is not employed at all, that an additional constant term appears in (34), and that the coefficient $\mathcal{R}^o/2$ is not equal to T_{tot}^{-1} for a single block.

In this paper, we will not discuss further the properties of $\hat{\mathbf{R}}$. There is only one simple special case: if already each single block, with reflection matrix \mathbf{R}_0 , shows factorized transmission, we get simply $\hat{\mathbf{R}} = \mathbf{R}_0$. In this case equation (34) holds not only asymptotically but also for any $M \geq 1$. Therefore the right-hand side of (23) defines a strictly additive quantity for the serial combination of factor blocks that are either identical or only equivalent in the sense of $\hat{\mathbf{R}}_0 \rightarrow \mathbf{R}_0 + \text{constant} \times t \circ \tilde{t}$ —see below.

In any case $\hat{\mathbf{R}}$ is only defined up to a ‘gauge’ transformation $\hat{\mathbf{R}} \rightarrow \hat{\mathbf{R}} + \alpha t \circ \tilde{t}$ —cf. (32). All physically relevant quantities, especially the constant term in (23) and (34), are ‘gauge invariant’.

6. Concluding remarks

A short summary of the content is given in the abstract. Finally we only wish to accentuate certain aspects.

The formulation given can be considered as a generalization of the well-known Landauer–Büttiker approach that is reproduced correctly as a special case. As a by-product it is shown that the usual equal-feeding rule (for all channels in an ideal lead from a given reservoir) is a direct consequence of the absence of reflections on the lead side of the contacts.

The basic aspect of the model is the incoherent coupling of subsystems. Contacts and reservoirs are special subsystems. Incoherence yields additivity in the classical sense. This means additivity of dissipated power for a general network and additivity of resistance for the special serial case. The demand of additivity is strong enough to determine these additive quantities as functionals of the currents in all of the ingoing and outgoing channels. A proof of positive definiteness is given, substantiating the general reasoning.

A scheme is established that allows one to consider new kinds of incoherent embedding for a given transmitter. This possibility is demonstrated explicitly for a long chain composed of identical transmitters. The results demonstrate that the resistance of a given subsystem can be very sensitive to the specific kind of embedding. At the same time, for a long chain as a whole, the dominant role of the total transmission is confirmed anew, and a plausible rule for extracting the single-block resistance from the total chain transmission is validated.

The chain problem studied is just the probably simplest example. Generalizations, e.g. to chains with inhomogeneities or disorder, to coupled chains or to two- and three-dimensional space-filling block arrangements, can be considered along the same lines.

Independently of the variational approach, a method has been invented to study the relaxational process in a chain with its discrete block structure. This approach can be applied for constructing the resulting reflection–transmission behaviour of the chain from those of its constituents—especially the asymptotic behaviour for long chains. Also in this respect, generalizations to more complex arrangements can be studied.

Appendix. Distribution between blocks with factorized transmission

Consider the interval between two arbitrary blocks 1 and 2, each of them left–right symmetric and with factorized transmission as in equation (32). Externally, on both sides, we have incident currents $I_{1,2}^{inc}$. Then we get between these two blocks the currents

$$\begin{aligned} I'_+ &= (1 - \mathbf{R}_1 \mathbf{R}_2)^{-1} (\alpha_1 t_1 + \alpha_2 \mathbf{R}_1 t_2) \\ I'_- &= (1 - \mathbf{R}_2 \mathbf{R}_1)^{-1} (\alpha_2 t_2 + \alpha_1 \mathbf{R}_2 t_1) \end{aligned} \quad (\text{A1})$$

with $\alpha_i \propto t_i I_i^{inc}$.

Employing the inverse of

$$1 - \mathbf{R}_1 \mathbf{R}_2 = (1 - \mathbf{R}_1) + (1 - \mathbf{R}_2) - (1 - \mathbf{R}_1)(1 - \mathbf{R}_2) \quad (\text{A2})$$

we find

$$I' = I'_+ - I'_- = (\alpha_1 - \alpha_2) [(1 - \mathbf{R}_1)^{-1} + (1 - \mathbf{R}_2)^{-1} - 1]^{-1} \mathbf{1} \quad (\text{A3})$$

and

$$\mathbf{v}\rho' = I'_+ + I'_- = \alpha_1 (1 + \mathbf{R}_2)(1 - \mathbf{R}_2)^{-1} [\dots]^{-1} \mathbf{1} + \alpha_2 (1 + \mathbf{R}_1)(1 - \mathbf{R}_1)^{-1} [\dots]^{-1} \mathbf{1} \quad (\text{A4})$$

where $[\dots]^{-1}$ denotes the same matrix as in (A3).

Now we specialize the two factor blocks as long chain segments, i.e. $t_1 \propto t_2$, and $\mathbf{R}_{1,2}$ are both of the form (32). Then, applying the matrix inversion formula (22), we find

$$(1 - \mathbf{R}_i)^{-1} = (1 - \hat{\mathbf{R}})^{-1} + \text{constant} \times \mathbf{1} \circ \tilde{\mathbf{1}} \quad (\text{A5})$$

and

$$I' \propto [(1 - \mathbf{R}_1)^{-1} + (1 - \mathbf{R}_2)^{-1}]^{-1} \mathbf{1} \propto (1 + \hat{\mathbf{R}})^{-1} (1 - \hat{\mathbf{R}}) \mathbf{1}. \quad (\text{A6})$$

According to section 4, this asymptotic distribution must coincide with I^o for a single block.

This is a condition for $\hat{\mathbf{R}}$ that remains to be studied.

The density distribution (A4) is the sum of two similar terms. With

$$(1 + \mathbf{R}_i)(1 - \mathbf{R}_i)^{-1} = 2(1 - \mathbf{R}_i)^{-1} - 1 \quad (\text{A7})$$

and with equations (A5) and (A6), each of them is seen to be of the form

$$\alpha_i [(1 - \hat{\mathbf{R}})^{-1} (1 + \hat{\mathbf{R}}) + \text{constant} \times \mathbf{1} \circ \tilde{\mathbf{1}}] (1 + \hat{\mathbf{R}})^{-1} (1 - \hat{\mathbf{R}}) \mathbf{1} \propto \mathbf{1}. \quad (\text{A8})$$

Thus the simple and general result $\mathbf{v}\rho' \propto \mathbf{1}$ —cf. section 4—is confirmed.

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