Classical transport within the scattering formalism

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The quantum composition rule for two multichannel scatterers (i.e., two pieces of a wire) in series is used to derive classical scaling (Ohm's law). Scattering processes leading to the classical behavior are identified and separated from quantum interference processes, which are responsible for quantum localization and anomalous conductance fluctuations.

To study transport phenomena with rigor and precision one needs an expression for the macroscopic transport coefficients, e.g., the electric conductance, in terms of the microscopic Hamiltonian of the system. The two major approaches providing such expressions are the linear response theory[1] (Kubo formalism) and the scattering approach pioneered by Landauer.[2,3] The latter approach is particularly suitable for studying finite-size systems, e.g., a piece of a wire, and it relates the conductance of the system (sandwiched between two perfect current leads) to its scattering S matrix.[2-8]

Usually, except for some trivial cases, neither the linear-response Kubo formula nor the S matrix in the scattering approach can be evaluated exactly, and various approximations are introduced. In particular, it is important to identify the approximation which produces the results of the standard (also called "classical") transport theory, based on the Boltzmann equation. Such an approximation, in addition to having conceptual significance, represents the first step of a systematic perturbative calculation, with respect to disorder.

There are various derivations of the classical transport results using the Kubo formula of the linear-response theory.[9] Also within the scattering formalism (which, after all, should be equivalent to the Kubo formula[4,7]) it is known that a properly defined conductance, at zero temperature, scales classically when the system (a wire) is short compared to the localization length[3,5,6,10] (for a long wire quantum localization effects take over[11]). In this Brief Report classical transport will be derived, within the scattering approach, starting from the composition rule for two pieces of a wire in series. The main purpose, however, is to identify the scattering processes leading to classical behavior and to separate them from processes responsible for quantum interference effects, such as weak localization[12,13] or quantum conductance fluctuations.[14-16] It will thus become clear what kind of approximation, or rather neglect of which scattering processes, produces classical behavior. The approach taken in this paper may pave the way to a systematic perturbation expansion, in weak disorder, within the scattering formalism.

Thus, I consider a disordered electronic system of a finite size (a piece of wire), connected via perfect leads to two particle reservoirs, on the left and the right. Eigenstates in the leads, at the Fermi energy[17] define the channels, for noninteracting electrons. Each channel can carry two waves, propagating in opposite directions. For instance, an electron impinging on the system from the left, in channel α, can be reflected into some channel β or transmitted into some channel to the right. Amplitudes for corresponding scattering processes are denoted by $r_{\beta\alpha}$ and $t_{\beta\alpha}$, which are, respectively, elements of the reflection matrix on the left, $\underline{r}$, and the transmission matrix from left to right, $\underline{t}$. Similarly, one defines matrices $\underline{r}'$ and $\underline{t}'$ on the right. Together these four matrices define the $2N\times 2N$ S matrix, where $N\simeq Ak_F^2$ is the number of channels (A and k_F are the wire cross section and the Fermi wave number, respectively). This S matrix contains all the information needed to determine the zero-temperature dc conductance of the system. For the multichannel case ($N\gg 1$) and when the sample length L is greater than the mean free path l, the dimensionless (in units $e^2/\pi\hbar$) conductance g is given approximately by[4-8,18]

$$g=\mathrm{Tr}\,\underline{t}\,\underline{t}^{\dagger}=\sum_{\alpha,\beta}T_{\alpha\beta}=N-\sum_{\alpha,\beta}R_{\alpha\beta}\ , \tag{1}$$

where $T_{\alpha\beta}\equiv|t_{\alpha\beta}|^2$ is the transmission probability from channel β on the left into channel α on the right, $R_{\alpha\beta}\equiv|r_{\alpha\beta}|^2$ is the reflection probability, and the last equality in Eq. (1) follows from unitarity (current conservation).

In order to understand the scaling properties of the conductance,[19] i.e., how g scales with sample length, one needs rules for combining $\underline{t}$ and $\underline{r}$ matrices of two segments of a wire in series. These rules are easily derived. For instance, the combined t matrix is

$$\underline{t}=\underline{t}_2\underline{t}_1+\underline{t}_2\underline{r}'_1\underline{r}_2\underline{t}_1+\cdots=\underline{t}_2(1-\underline{r}'_1\underline{r}_2)^{-1}\underline{t}_1\ , \tag{2}$$

which is just the composition rule given, e.g., in Ref. 5 (with $\underline{t}_1$ and $\underline{t}_2$ interchanged). The first term in the series describes direct transmission through both segments, 1 and 2, the second term describes transmission with one scattering back and forth between the two segments, etc. Similarly, the combined reflection matrix, on the left, $\underline{r}$, is given by

$$\begin{aligned}\underline{r}&=\underline{r}_1+\underline{t}'_1\underline{r}_2\underline{t}_1+\underline{t}'_1\underline{r}_2\underline{r}'_1\underline{r}_2\underline{t}_1+\cdots\\&=\underline{r}_1+\underline{t}'_1\underline{r}_2(1-\underline{r}'_1\underline{r}_2)^{-1}\underline{t}_1\ .\end{aligned} \tag{3}$$

Below, a small bit of wire, δL, is taken as segment 2

and it is added to a wire of arbitrary length L (segment 1). δL is chosen to be much smaller than the mean free path l, which is assumed to be large ($k_F l \gg 1$). The probability that an electron gets scattered in segment δL is small, of order $\delta L/l$ (the ballistic regime). The corresponding reflection and transmission coefficients are

$$|(\delta r)_{\alpha\beta}|^2 \equiv (\delta R)_{\alpha\beta} = c\delta L/lN ,$$
$$(\delta T)_{\alpha\beta} = \begin{cases} c\delta L/lN, & \text{for } \alpha \neq \beta , \\ 1 - c(\delta L/lN)(2N-1), & \text{for } \alpha = \beta , \end{cases} \tag{4}$$

where coefficient c is of order 1 and, for simplicity, short-range scatterers have been assumed. The scattering probability is then independent of the angle (i.e., of the channel), so that all $\delta R_{\alpha\beta}$ are the same and are equal to $\delta T_{\alpha\beta}$, for $\alpha \neq \beta$. The element $\delta T_{\alpha\alpha}$ is then determined by current conservation. The matrices for reflection and transmission amplitudes, $\delta\underline{r}$ and $\delta\underline{t}$, are obtained from Eq. (4) by taking a square root and introducing corresponding phase factors:

$$\delta r_{\alpha\beta} = (c\delta L/lN)^{1/2} \exp(i\phi_{\alpha\beta}) ,$$
$$\delta t_{\alpha\beta} = \begin{cases} (c\delta L/lN)^{1/2} \exp(i\theta_{\alpha\beta}), & \alpha \neq \beta , \\ 1 - (c\delta L/2lN)(2N-1)\exp(i\theta_{\alpha\alpha}), & (\alpha = \beta) , \end{cases} \tag{5}$$

where smallness of the ratio $\delta L/l$ has been used in the last equation. Unitarity and time-reversal symmetry (if not broken, e.g., by an external magnetic field) impose certain relations among phases. Otherwise, the phases are arbitrary and, in a disordered system, should be treated as random variables. Note that in the most general case the coefficient c also should be allowed to fluctuate from one member of the ensemble to another. Besides, as was already mentioned, c can also depend on channel number i.e., generally one has a random matrix $c_{\alpha\beta}$ instead of just a number c. This randomness (in contrast to randomness in phases) is of no particular interest, and it is neglected here: It can only contribute to the standard (small) resistance fluctuations, of the kind one encounters in classical resistor networks.

In order to calculate the change Δg in the conductance under increase δL of the wire length, one has to calculate the corresponding change $\Delta\underline{T}$ in the transmission matrix ($\Delta\underline{T} \equiv \underline{T}_{L+\delta L} - \underline{T}_L$, and it should not be confused with the transmission matrix $\delta\underline{T}$ of the segment δL). Alternatively, and a bit more simply, one can calculate the change $\underline{\Delta R} \equiv \underline{R}_{L+\delta L} - \underline{R}_L$ in the reflection matrix. Using Eq. (3) and the smallness of the ratio $\delta L/l$, one can write the reflection matrix $\underline{r}_{L+\delta L}$ for the combined segment $L+\delta L$ in terms of the matrices describing segments L and δL:

$$\underline{r}_{L+\delta L} = \underline{r} + \underline{t}'(\delta\underline{r})\underline{t} , \tag{6}$$

where $\underline{t}$, $\underline{t}'$, and $\underline{r}$ refer to the segment L. For the purpose of this paper it is sufficient to keep only linear terms in $\delta\underline{r}$.

Writing Eq. (6) in algebraic notations and multiplying it by its complex conjugate, one obtains

$$|(r_{L+\delta L})_{\alpha\beta}|^2 \equiv (R_{L+\delta L})_{\alpha\beta} = |r_{\alpha\beta}|^2 + t'_{\alpha i}(\delta r)_{ij} t_{j\beta} (t')^*_{\alpha i'} (\delta r)^*_{i'j'} t^*_{j'\beta} + [r^*_{\alpha\beta} t'_{\alpha i} (\delta r)_{ij} t_{j\beta} + \text{c.c.}] , \tag{7}$$

where summation over repeated latin indices is implied. One thus has a sum of random complex numbers or, alternatively, a sum of real numbers with random signs (since each complex number occurs with its complex conjugate). There is, however, a special class of terms which do not contain any phase factors and thus always give a positive contribution to $R_{L+\delta L}$. These are terms with $i = i'$, $j = j'$. Retaining for the moment only these terms (the others will be discussed later), one has

$$(R_{L+\delta L})_{\alpha\beta} = R_{\alpha\beta} + T'_{\alpha i} (\delta R)_{ij} T_{j\beta} , \tag{8}$$

where $R_{\alpha\beta} \equiv |r_{\alpha\beta}|^2$, etc. and again summation over i and j is implied. In matrix notation,

$$\underline{R}_{L+\delta L} = \underline{R} + \underline{T}'(\delta\underline{R})\underline{T} . \tag{9}$$

This is the same as Eq. (6) but with reflection and transmission *probabilities* instead of amplitudes. This immediately suggests that Eq. (9) is a classical analog of Eq. (6), with quantum interference effects (i.e., phases) neglected. This is an entirely reasonable result which, for a strictly one-dimensional (i.e., single-channel) case, was recognized already in the early work of Landauer.[3] He noticed that the classical Ohm's law for two obstacles in series is obtained by combining directly the corresponding reflection coefficients (i.e., probabilities) rather than amplitudes, as prescribed by quantum mechanics. Note, however, that Eq. (9) is not yet the complete equivalent of the Boltzman transport equation, since in general the matrices in Eq. (9) are random matrices (depending on a particular realization of the random impurity potential), whereas the Boltzmann equation operates with averaged quantities. However, as has been mentioned above, this randomness in probabilities (as opposed to randomness in phases) is of little interest. It has, in fact, already been neglected in Eq. (4) for $\delta\underline{R}$ and $\delta\underline{T}$, since these equations refer to averaged quantities. Thus, with the fluctuations neglected, Eq. (9) should be equivalent to the classical Boltzmann equation. This equivalence is demonstrated below.

Substituting $\delta\underline{R}$ from Eq. (4) into Eq. (8) and denoting $c\delta L/l \equiv \Delta x$ (a dimensionless element of length), one obtains the following differential equation for $R_{\alpha\beta}$:

$$dR_{\alpha\beta}/dx = N^{-1} \left[\sum_i T'_{\alpha i} \right] \left[\sum_j T_{j\beta} \right] . \tag{10}$$

Summing this equation over α and β and using Eq. (1) for the conductance, one obtains

$$dg/dx = -g^2/N , \tag{11}$$

where the equality $\sum_{ij} T'_{ij} = \sum_{ij} T_{ij}$, following from unitarity (even in the absence of time-reversal symmetry), has

been used. Equation (11) implies that the inverse conductance scales as x, i.e., it is proportional to the length of the wire. It is also clear that g is proportional to the number of channels, i.e., to the wire cross section. Thus, the standard classical scaling (Ohm's law) is obtained, provided that only the $i=i'$, $j=j'$ terms in Eq. (7) are kept. This is quite natural since it is just such terms that appear in any Boltzman-type theory. Indeed, in such a theory one always assumes, implicitly or explicitly, random uncorrelated phases for different scattering processes and then averages over these phases at some early stage of the calculation. It is clear that the $i=i'$, $j=j'$ terms do survive such averaging.

I now briefly discuss the other terms in Eq. (7), which so far have been neglected. First, note that if time-reversal symmetry is obeyed (i.e., reflection and transmission matrices satisfy the symmetry relations $\underline{r}=\underline{\tilde{r}}$, $\underline{r}'=\underline{\tilde{r}}'$, $\underline{t}=\underline{\tilde{t}}'$), then there is an additional class of terms which survive the above mentioned averaging. Indeed, consider a scattering process $\beta\rightarrow j\rightarrow i\rightarrow\alpha$, i.e., the electron is impinging (on the left) in channel β, transmitted through the first segment into channel j, then reflected from the second segment into channel i and, finally, transmitted back through the first segment into channel α. The amplitude for this process is $t'_{\alpha i}(\delta r)_{ij}t_{j\beta}$. This process has its time-reversed counterpart $\alpha\rightarrow i\rightarrow j\rightarrow\beta$, with an amplitude $t'_{\beta j}(\delta r)_{ji}t_{i\alpha}$ which, due to time reversal symmetry, is exactly equal to the "direct" process amplitude $t'_{\alpha i}(\delta r)_{ij}t_{j\beta}$. Therefore two processes, $\alpha\rightarrow i\rightarrow j\rightarrow\alpha$ and $\alpha\rightarrow j\rightarrow i\rightarrow\alpha$, describing reflection in the backward direction, are completely correlated (coherent), rather than completely uncorrelated as a Boltzmann-type theory assumes for different processes. This correlation leads to the doubling of reflection probability in the backward direction.[13] Correspondingly, terms with $i=j'$, $j=i'$, and $\alpha=\beta$ in Eq. (7) (the second sum on the right-hand side) survive the aforementioned averaging[20] (in addition to the $i=i'$, $j=j'$ terms).

Finally, the great majority of terms in Eq. (7), in particular the sum in square brackets (cross terms), do not survive averaging over random phases. It does not mean, however, that therefore these terms can be safely neglected. The point is that the conductance fluctuations generated by these terms are not necessarily small. Moreover, even when these fluctuations are small, they are quite different from the standard fluctuations in classical resistor networks. In particular, it is these terms that produce the recently discovered anomalously large (as compared to the classical case) conductance fluctuations[14-16,21] in the metallic regime.

It is perhaps worthwhile to discuss in this context the strictly one-dimensional (i.e., single channel) case. Equation (7), in this case reduces to

$$R_{L+\delta L}=R+T^2\delta R+2T(R\delta R)^{1/2}\cos\theta\ , \tag{12}$$

where R and T are the reflection and transmission coefficients for a chain of length L, δR refers to the segment δL, and θ is the phase difference between r and δr. Note that it is only the $\cos\theta$ term that leads to localization and large resistance fluctuations: Without this term a chain of any length would exhibit classical behavior. From Eq. (12), or from a corresponding equation for resistances [the dimensionless resistance ρ is related to R by $\rho=R/(1-R)$], one can derive an equation for the resistance distribution $P_L(\rho)$. This equation describes the evolution of the distribution under increase of L and it is given by[22-24]

$$\frac{\partial P}{\partial L}=\alpha\frac{\partial}{\partial\rho}\left[(\rho^2+\rho)\frac{\partial P}{\partial p}\right]\ , \tag{13}$$

where $\alpha\equiv\delta\bar{\rho}/\delta L$ is the small-scale (average) resistivity. For short chains, $L\ll l$ (the mean free path l, in one dimension, coincides with the localization length ξ), one can neglect the ρ^2 term and obtain the solution[24,25]

$$P_L(\rho)=(1/\bar{\rho}_L)\exp(-\rho/\bar{\rho}_L)\ ,$$

where $\bar{\rho}_L\sim L$ is the average resistance. Thus, even for $L\ll\xi$, there are large (of order 1) resistance fluctuations. In other words, classical Ohm's law is obeyed only on the average, whereas a particular member of the ensemble (i.e., a given chain) will typically exhibit a nonmonotonic, strongly fluctuating dependence of ρ on L. When L increases beyond ξ, the typical resistance becomes large and the ρ^2 term in Eq. (13) dominates. The distribution $P_L(\rho)$ then approaches the well known log-normal distribution,[22,23] with $\overline{\ln\rho}\sim L$.

In conclusion, the composition rule for adding two multichannel scatterers in series has been applied to derive classical transport within the scattering approach. Three distinct types of scattering processes in the composition rule have been identified: (i) processes leading to classical scaling, i.e., Ohm's law (ii) processes responsible for weak-localization effects, in the presence of time-reversal symmetry, and (iii) processes related to fluctuations, i.e., to (sometimes broad) statistical distributions. The work seems to provide a natural starting point for a systematic expansion, in weak disorder, within the scattering approach.

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[18]Although this approximate expression can be used for the overwhelming majority of the random potential configurations, there are few configurations (i.e., few members in the ensemble) for which this expression fails. This point can be illustrated with the simple, strictly one-dimensional case. In this case Eq. (1) gives $g=|t|^2\equiv T$, whereas the exact expression is $g=T/(1-T)$. For a long chain ($L\gg l$), T is, typically, exponentially small and thus can be neglected in the denominator. Certain configurations, however, can have almost perfect transmission, $T\approx 1$ (transmission resonances). Clearly, for those configurations one should use the full expression for g.

[19]In more precise terms one should speak not about a single conductance but rather about a distribution of conductances, for a given ensemble of disordered systems.

[20]If time-reversal symmetry is broken, then the enhanced backscattering appears only in second order with respect to $\delta\underline{R}$.

[21]See in particular Ref. 16 for a similar discussion of various scattering sequences, in a path-integral formulation.

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