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Relation between conductivity and transmission matrix

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The dc conductance Γ of a finite system with static disorder is related to its transmission matrix t by the simple relation $\Gamma = (e^2/2\pi\hbar)\,\mathrm{Tr}(t^\dagger t)$. This relation is derived from the Kubo formula and is valid for any number of scattering channels with or without time-reversal symmetry. Differences between various definitions of the conductance of a finite system are discussed.

Some time ago Landauer[1] proposed that the dc conductance Γ of noninteracting (spinless) electrons in a disordered medium in strictly one dimension is given by $\Gamma = (e^2/2\pi\hbar)|t|^2/|r|^2$ where t and r are the transmission and reflection amplitudes. A relation of this kind, especially if it can be generalized to higher dimensions, is of great interest for at least two reasons. First, the cost of numerical computation may be greatly reduced compared with the conventional use of the Kubo formula.[2–6] Second, such a relation emphasizes the fundamental role of the conductance which is assumed to be the only relevant variable in a recent scaling theory treatment of the localization problem.[7,8] This point of view was discussed in a recent analysis of the conductivity of a one-dimensional (1D) chain[9] in which Landauer's expression was used. The argument given by Landauer is a heuristic one and not easily generalized to higher dimensions.

Recently Economou and Soukoulis[2] derived from the Kubo formula an expression for the conductance of a one-dimensional chain, $\Gamma = (e^2/2\pi\hbar)|t|^2$. This result is in agreement with Landauer for long chains for which $|r|^2 \sim 1$, but in disagreement with his result for short chains. Their derivation is, however, also restricted to 1D. In this paper a completely general relation between the conductance and the transmission matrix is derived, and some implications for numerical calculations are discussed.

In the derivation of Landauer[1] and Anderson *et al.*[9] the conductance is obtained by dividing the current I by the chemical potential difference, $\Delta\mu$, between the left and the right of the sample. (To avoid additional complications of long-range Coulomb interaction, we consider the transport of neutral particles.) Thus some inelastic scattering mechanism must be introduced outside the sample to allow the regions to the left and right to reach local thermal equilibrium. The interface between the nonequilibrium region in the sample and the outside regions is difficult to treat, particularly in the multichannel case. However, even in the absence of a precise treatment, it is clear that in the limit of a perfect sample ($|t| = 1$), $\Delta\mu$ must vanish and the conductance will be infinite, a feature satisfied by the Landauer formula. Traditionally the nonequilibrium problem is bypassed using the Kubo formula, which relates via linear response the conductance to the equilibrium properties of the system. However, in applying the Kubo formula to a finite sample, we are faced with some ambiguity. If the sample is isolated, its energy levels are discrete and $\sigma(\omega)$ is a sum of closely spaced δ functions. Some procedure for averaging over these δ functions is then necessary in order to obtain a useful result.[5,6] Alternatively, we can embed the disordered region of interest in an infinite system with no disorder, and probe the system with an electric field (or potential gradient) of frequency ω which exists only in the vicinity of the disordered region. The energy spectrum for the whole system will be continuous and $\sigma(\omega)$ will be smooth with a well-defined limit as $\omega \to 0$. This latter procedure was used by Economou and Soukoulis, and we shall adopt it here. The result, however, has the feature that the conductance is finite in the limit of a perfect conductor. This is because in the presence of a finite electric field, there is no mechanism for establishing thermal equilibrium outside the sample, a situation that can be realized if the frequency is high compared with the inelastic scattering rate. While a fully satisfactory expression for the conductance based on the chemical potential difference is not yet available, the expectation[9] is that in the limit of a large number of channels, $\Gamma = (e^2/2\pi\hbar)\,\mathrm{Tr}(t^\dagger t)$, a result that we shall derive here from the Kubo formula. In most cases of interest (2D, 3D, and $t \ll 1$ in 1D) the difference between the different definitions of conductance will be small.

To be specific we consider a disordered sample of length L in the z direction ($0 < z < L$) and cross-sectional area A. Perfect regions of cross section A are attached to the $\pm z$ directions so that the total length of the system is Λ (to be taken to infinity), and we assume periodic boundary conditions in the transverse directions [$\vec{\rho} = (x,y)$] for the entire system. We apply an electric field in the z direction with

frequency ω to the disordered region. The energy absorption rate P is related to the conductance $\Gamma(\omega)$ of the system by $P=\Gamma E_{\rm rms}^2 L^2$, where $E_{\rm rms}$ is the root-mean-square electric field. Standard linear-response theory then gives, at zero temperature,[10]

$$\Gamma(\omega)=\frac{\pi}{\omega L^2}\int dE\sum_{\alpha\beta}\left|\int_0^L dz\, J_{\alpha\beta}(z)\right|^2\delta(E+\omega-E_\beta)\delta(E-E_\alpha)\ , \tag{1}$$

where the sum is over eigenstates $\psi_\alpha(\vec{r})$ of the entire system [$\vec{r}=(\vec{\rho},z)$] with the restriction that $E_\alpha<E_F<E_\beta$, where E_F is the Fermi energy. The matrix element of the current in the z direction between states α and β is

$$J_{\alpha\beta}(z)=\int d\vec{\rho}\,\frac{e}{2im}\left[\frac{\partial\psi_\alpha^*(\vec{r})}{\partial z}\psi_\beta(\vec{r})-\psi_\alpha^*(\vec{r})\frac{\partial\psi_\beta(\vec{r})}{\partial z}\right]\ . \tag{2}$$

(For ease of presentation we work in a continuum representation; in a tight-binding picture derivatives become finite differences.) Conservation of current implies that

$$J_{\alpha\beta}(z_1)-J_{\alpha\beta}(z_2)=i\omega\int_{z_1}^{z_2}dz\int d\vec{\rho}\,\psi_\alpha^*(\vec{r})\psi_\beta(\vec{r})\ . \tag{3}$$

Following Economou and Soukoulis,[2] we note from Eq. (3) that in the limit $\omega\to 0$, $J_{\alpha\beta}(z)$ is independent of z and hence the integral over z in Eq. (1) can be done trivially. In particular, $J_{\alpha\beta}$ can be evaluated *outside* of the disordered region, where the eigenstates sufficiently far from the disordered region will be simple combinations of plane waves. Each plane wave corresponds to a scattering channel b characterized by spin σ_b, transverse momenta $\vec{q}_b$, and z momenta k_b, with energy $E=(1/2m)(k_b^2+|\vec{q}_b|^2)$. We note that only a certain fraction of the possible transverse momenta $\vec{q}$ will be allowed for each energy E; the others will correspond to exponential growth or decay in the z direction and hence will be negligible except near the disordered region. All sums over "channels" b will include only the allowed wave vectors.

It is convenient to define the Green's functions $G^{(\pm)}(E)=(E\pm i\eta-H)^{-1}$ with matrix elements between scattering channels b and a.

$$G_{ba}^{(\pm)}(z,z')=A^{-1}\int d\vec{\rho}\int d\vec{\rho}\,'\exp(-i\vec{q}_b\cdot\vec{\rho})\exp(i\vec{q}_a\cdot\vec{\rho}\,')\langle\vec{r},\sigma_b|G^{(\pm)}|\vec{r}\,',\sigma_a\rangle\ . \tag{4}$$

The energy E of the Green's functions will henceforth be taken to be E_F and will be suppressed. The zero-frequency limit of the conductance given by Eq. (1) then becomes

$$\Gamma=\Gamma(\omega=0)=\frac{-e^2}{4m^2}\frac{\pi}{(2\pi)^2}\,{\rm Tr}\left[\frac{\partial}{\partial z'}\frac{\partial}{\partial z}(G^{(+)}-G^{(-)})(\tilde{G}^{(+)}-\tilde{G}^{(-)})+(G^{(+)}-G^{(-)})\frac{\partial}{\partial z}\frac{\partial}{\partial z'}(\tilde{G}^{(+)}-\tilde{G}^{(-)})\right.$$
$$\left.-\frac{\partial}{\partial z}(G^{(+)}-G^{(-)})\frac{\partial}{\partial z'}(\tilde{G}^{(+)}-\tilde{G}^{(-)})-\frac{\partial}{\partial z'}(G^{(+)}-G^{(-)})\frac{\partial}{\partial z}(\tilde{G}^{(+)}-\tilde{G}^{(-)})\right]\ , \tag{5}$$

where the trace is over the channel index and $G^{(\pm)}$ is the matrix $G_{ba}^{(\pm)}(z,z')$ (over the channel indices a,b) and $\tilde{G}^{(\pm)}=G_{ba}^{(\pm)}(z',z)$.

We can now proceed in analogy with the well-known scattering problem,[11] except that the scattering geometry here is such that there are plane waves instead of spherical waves outside the scattering region. We may take $z'\ll 0$ and $z\gg L$ so that the wave functions assume their asymptotic form. Then $G_{ba}^{(+)}$ consists of outgoing waves only (the exponentially decaying parts can be ignored) so that $G_{ba}^{+}(z,z')$ is proportional to $\exp(-ik_a z')$ and $\exp(ik_b z)$. Similarly $G^{(-)}$ consists only of incoming waves. The z derivatives in Eq. (5) can hence be done trivially and have the effect of converting the $G^{(+)}-G^{(-)}$ in the last two terms to $G^{(+)}+G^{(-)}$. Equation (4) then simplifies to

$$\Gamma=\frac{e^2}{4\pi}\sum_{ab}[|G_{ab}^{(+)}(z,z')|^2+|G_{ab}^{(+)}(z',z)|^2]v_a v_b\ , \tag{6}$$

where $v_b=k_b/m$ (or more generally dE/dk_b) is the velocity in channel b.

It remains to relate the Green's function to the transmission matrix. Again in analogy with the scattering problem, we find the stationary scattering state

$$\hat{\psi}_{La}^{(+)}=\hat{\phi}_a+G^{(+)}V\hat{\phi}_a\ , \tag{7}$$

where $\hat{\phi}_a$ is the plane wave $(AL)^{-1/2}\exp(ik_a z+i\vec{q}_a\cdot\vec{\rho})$. The function $\hat{\psi}_{La}^{(+)}$ consists of incoming and outgoing (reflected) plane waves to the left of the disordered region and purely outgoing (transmitted) waves to the right. It is natural to define the matrix $\hat{t}_{ba}^{L}$ as the amplitude of the transmitted wave from the left; i.e., $\hat{\psi}_{La}^{(+)}(z)\to\sum_b\hat{t}_{ba}^{L}\hat{\phi}_b(z)$ for $z\gg L$. This can be calculated using the relation

$$\langle\hat{\phi}_b|V|\hat{\psi}_{La}^{(+)}\rangle=\Lambda^{-1}iv_b\hat{t}_{ba}^{L}\ , \tag{8}$$

where V is the scattering potential. Equation (8) is

derived along the same lines as an analogous relation for the spherical scattering geometry.[11] We next insert Eq. (7) into Eq. (8) and eliminate $V(\vec{r})$ and $V(\vec{r}')$ in favor of ∇^2 and ∇'^2 using the equations satisfied by the Green's function. After a number of partial integrations we obtain

$$i v_b \hat{t}^L_{ba} = \left[\frac{\exp[-i(k_b z - k_a z')]}{(2m)^2}\left(\frac{\partial}{\partial z} + ik_b\right)\right. \times \left.\left(\frac{\partial}{\partial z'} - ik_a\right) G^{(+)}_{ba}(z,z')\right]\Bigg|_{z=z_1}^{z=z_2}\Bigg|_{z'=z_1'}^{z'=z_2'} , \quad (9)$$

where $z_2, z_2' > L$ and $z_1, z_1' < 0$ are *anywhere* outside the disordered region. Now we again take z_2, z_2' to the asymptotic limit to the right and z_1, z_1' to the left so that the z derivatives again become simple. Only a single term survives ($z = \infty$, $z' = -\infty$) and we obtain

$$\hat{t}^L_{ba} = -i v_a G^{(+)}_{ba}(z,z') \exp[-i(k_b z - k_a z')] . \quad (10)$$

A similar relation exists between the transmission matrix from the right $\hat{t}^R$ and $G^{(+)}(-\infty, \infty)$.

At this point it is necessary to discuss normalization of the channels. In the present scattering geometry, the conserved quantity is the total flux in the z direction. It is therefore convenient to normalize the channels to carry unit flux in the z direction and define wave functions normalized in this manner, i.e., $\phi_a = v_a^{-1/2}\hat{\phi}_a$ and $\psi^{(+)}_{La} = v_a^{-1/2}\hat{\psi}^{(+)}_{La}$. The transmission matrix t^L corresponding to this normalization is then simply related to $\hat{t}^L$ defined above by

$$t^L_{ba} = (v_b/v_a)^{1/2}\hat{t}^L_{ba} . \quad (11)$$

The reflection matrices r^L and r^R normalized to unit flux may be analogously defined. In terms of these, the S matrix relating incident to scattered waves is simply

$$S = \begin{pmatrix} r^L & t^R \\ t^L & r^R \end{pmatrix} . \quad (12)$$

By combining Eqs. (6), (10), and (11) we obtain for the conductance

$$\Gamma = \frac{e^2}{4\pi\hbar} \sum_{ab} (|t^L_{ab}|^2 + |t^R_{ab}|^2) . \quad (13)$$

With the normalization to unit flux, conservation of probability is equivalent to the unitarity of the S matrix, $S^\dagger S = SS^\dagger = I$. This implies that the two terms in Eq. (13) are actually equal after the sum over a and b even if time-reversal symmetry is broken (i.e., $S \neq \tilde{S}$). We hence conclude that

$$\Gamma = \frac{e^2}{2\pi\hbar} \mathrm{Tr}(t^\dagger t) , \quad (14)$$

where t is the transmission matrix from *either* the left or the right.

The conductance as given by Eq. (14) can also be obtained directly from Eq. (5) without use of scattering theory by directly calculating $G^{(+)}(\vec{r}, \vec{r}') - G^{(-)}(\vec{r}, \vec{r}')$ and hence $G^{(+)}_{ba} - G^{(-)}_{ba}$. It is found that

$$G^{(+)}(\vec{r}, \vec{r}') - G^{(-)}(\vec{r}, \vec{r}') = -2\pi i \sum_\alpha \psi^*_\alpha(\vec{r})\psi_\alpha(\vec{r}')\delta(E - E_\alpha)$$
$$= -2\pi i \Lambda \sum_a \{[\psi^{(+)}_{La}(\vec{r})]^* \psi^{(+)}_{La}(\vec{r}') + [\psi^{(+)}_{Ra}(\vec{r})]^* \psi^{(+)}_{Ra}(\vec{r}')\} \quad (15)$$

for z and z' sufficiently far from the disordered region. The sum runs over the scattering states at energy E normalized to unit flux. Note that the $\psi^{(+)}_{La}$ are neither conventionally normalized nor orthogonal. The direct proof of Eq. (15) involves averaging over the actual eigenstates of a finite system, and is somewhat subtle; we will not discuss it here.

When the amount of disorder is reduced to zero, there is no reflection and $t = I$. The conductance from the power absorption as given by Eq. (14) thus remains finite and is equal to $N_c e^2/2\pi\hbar$, where N_c is the number of allowed channels. This is because an electric field imposed over a finite region of a perfect conductor can be absorbed. For a translationally invariant system, such as a perfect conductor, the $\Gamma(\omega)$ discussed here is related to $\sigma(\vec{q}, \omega)$ by

$$\Gamma(\omega) = \frac{A}{L^2}\int \frac{dq_z}{2\pi}\frac{4}{q_z^2}\sin^2\left(\frac{q_z L}{2}\right)\sigma(q_x = q_y = 0, q_z, \omega) , \quad (16)$$

which is perfectly finite as $\omega \to 0$ for a perfect conductor. It is only $\sigma(q = 0, \omega \to 0)$ which is infinite. The discrepancy with the Landauer formula is due to the fact that a finite electric field cannot be maintained across a perfect conductor if the outside wires are in local equilibrium.

For a large disordered system, with both $A \sim L^{d-1}$ and L large (where d is the dimensionality), it is natural to relate the conductance Γ which we have calculated to the zero-frequency conductivity σ. We will assume σ to be nonzero, i.e., that the system is a metal. (We note that if all states are localized in two dimensions, as obtained by Abrahams *et al.*,[7] then the following analysis will only be valid in more than two dimensions.) In the limit as $L \to \infty$

$$\Gamma = \frac{A}{L}\sigma . \quad (17)$$

For any finite L, however, there will be corrections to this which may arise from at least two sources. First,

there will be corrections due to the lack of equilibrium in the region of the perfect conductor outside the disordered region, as discussed in the opening paragraphs. Second, there may be an effective boundary resistance between the ordered and disordered regions. Both of these effects will lead to corrections to the conductivity of order $1/L$, and an underestimate of σ from Eqs. (14) and (17). We further note that if the energy E_F is outside the band edge of the ordered region, Eq. (14) fails. The derivation becomes invalid in this regime because the eigenvalues are discrete and the $\omega \rightarrow 0$ limit in Eq. (3) can no longer be taken. Just inside the band edge the number of allowed channels becomes small and the boundary resistance becomes very large.

Finally, we comment on the numerical computation of the conductivity. In principle the most efficient method to evaluate the transmission matrix is to calculate the transfer matrix in a real-space representation and then invert the transfer matrix.[12,13] The cost for an L^d sample is L^3 in 2D and L^6 in 3D. However, the transfer matrix blows up exponentially so that the matrix inversion necessary to obtain t rapidly becomes singular. This technique is thus limited to relatively small L and hence will involve relatively large errors, especially due to the boundaries. Alternatively one can calculate the Green's function via a generalization of the method of Ref. 5 to higher dimensions. In this case the transmission matrix can be calculated via Eq. (9). In fact it is more efficient to bypass the transmission matrix altogether and use Eq. (5) directly. The cost is L^4 in 2D and L^7 in 3D with storage requirements that go as L^2 and L^4, respectively. These computational schemes have been implemented, and the results will be presented elsewhere.

Note added in proof. After this work was completed, the authors received two reports of work prior to publication (one by D. Langreth and E. Abrahams, and the other by D. Thouless) on 1D conductance dealing with the effects of requiring charge neutrality in the wires attached to the disordered sample. For the one-channel case, both papers obtain Landauer's result,[1] while for the many-channel case, the results are rather complicated. We would like to thank the above authors for sending us copies of their papers and for stimulating discussions.

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