Dynamic Conductance and the Scattering Matrix of Small Conductors

M. Büttiker,[a] A. Prêtre, and H. Thomas
Institut für Physik, Universität Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland
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The current response to oscillating electric or magnetic fields acting on the carriers in the probes of a multichannel, multilead conductor is investigated. For a noninteracting system we find a frequency-dependent admittance matrix which is expressed in terms of scattering matrices. A self-consistent potential method is used to include Coulomb interactions. The low-frequency departure of the admittance away from the dc conductance is discussed in terms of phase-delay times and RC times.

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Expressions which relate the dc conductance of a conductor to the scattering matrix have become useful tools for the investigation of phase-coherent electron transport [1, 2]. Departures from the steady state occur spontaneously and lead to the need to investigate the noise properties of the conductor [3, 4]. Alternatively the conductor can be driven away from its steady state by time-dependent external perturbations [5]. Here we are interested in the admittance of a mesoscopic conductor which is part of an external network. The conductor is driven away from the steady state through oscillating fluxes $\delta\Phi_\alpha(\omega)$ or oscillating voltages $\delta U_\alpha(\omega)$ applied at the contacts $\alpha = 1, 2, 3, \ldots$ of the sample. As in the dc case there exists an admittance matrix $g_{\alpha\beta}(\omega) \equiv \langle \delta I_\alpha(\omega)\rangle / \delta U_\beta(\omega)$ which relates the currents at the contacts of the sample to the voltages at the contacts. In contrast to the dc case for which the internal potential distribution is irrelevant, the ac response depends in a sensitive way on the distribution of the potential in the sample. This internal potential is a consequence of the charge distribution generated by the voltages (or currents) applied at the contacts and must be calculated self-consistently. The calculation of an admittance may thus be separated into three steps. First, the response to external potentials is determined for noninteracting carriers, then the internal potential distribution is found from the unscreened charges introduced externally, and finally the response to this internal potential is evaluated. Below, we present a calculation in which the first step is carried out exactly, and the charging effect is taken into account to leading order by taking the induced potential as spatially constant in the sample.

In a first step we generate chemical potential differences with the help of voltages U_α or fluxes Φ_α applied to each reservoir. The additional energy due to these external potentials is

$$H_1 = \sum_\alpha (Q_\alpha U_\alpha + I_\alpha \Phi_\alpha), \tag{1}$$

where Q_α is the total charge in reservoir α and I_α is the current in probe α (see Fig. 1). For a conductor characterized by M_α quantum channels in probe α and by a set of scattering matrices $\mathbf{s}_{\alpha\beta}$ of dimension $M_\alpha \times M_\beta$ we find an equilibrium admittance matrix with elements

$$\begin{aligned} g_{\alpha\beta}(\omega) &\equiv \langle \delta I_\alpha(\omega)\rangle / \delta U_\beta(\omega) \\ &= \frac{e^2}{h}\int dE\, \mathrm{Tr}[\mathbf{1}_\alpha \delta_{\alpha\beta} - \mathbf{s}^\dagger_{\alpha\beta}(E)\mathbf{s}_{\alpha\beta}(E+\hbar\omega)] \\ &\quad \times \frac{f(E) - f(E+\hbar\omega)}{\hbar\omega}. \end{aligned} \tag{2}$$

Equation (2) gives the currents at the sample contacts in response to the external potentials. It characterizes the boundary conditions needed for the solution of the full problem. Below we give a derivation of this result [6]. We discuss the lack of particle current conservation and show that with the help of self-consistent potentials total current conservation is restored.

Our starting point is in contrast to much of the literature which derives a formal linear response to a given potential distribution in the sample [7–9]. The difficulty with such an approach lies in the fact that the potential distribution is not known *a priori*. It seems unrealistic to use the potential distribution that would exist in vacuum. Instead, similarly to Pastawski [10], we investigate the ac response to an external perturbation which prescribes the potentials in the reservoirs only. The external potentials effectively determine the chemical potentials μ_α of the reservoirs and the potential distribution in the conductor must be considered a part of the response which is to be determined self-consistently. An additional justi-

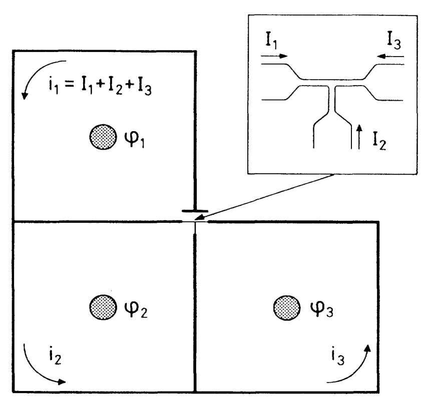

FIG. 1. Mesoscopic conductor (see inset) in an external network driven by fluxes ϕ_n, $n = 1, 2, 3, \ldots$.

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fication of our approach is given by the relation of Eq. (2) to the equilibrium current-noise spectra [4] via the fluctuation-dissipation theorem.

We begin our analysis with a more detailed discussion of Eq. (1). To define the total number of carriers Q_α in a precise way, it would be necessary to consider a closed system, where Q_α is the total number of carriers in reservoir α. Strictly speaking, a closed system in which carriers are subject only to elastic scattering does not dissipate energy. To make our system irreversible we assume that the reservoirs are so large that we can restrict our microscopic description to the currents entering the leads. Entering and leaving the reservoir is then described in a scattering formalism. The phase and energy of outgoing and incoming carriers are uncorrelated and the system is irreversible [11]. In the calculation presented below this step occurs when we relate the time derivative of Q_α to the current, $dQ_\alpha/dt = -I_\alpha$, and use the scattering expression for the current.

Similarly, it is necessary to discuss the electromagnetic term in Eq. (1). In a network (see Fig. 1) the fluxes ϕ_n are conjugate to *circulating* currents i_n which can be associated with each loop of the network. In contrast Eq. (1) is expressed in terms of particle currents incident at each lead of the mesoscopic conductors and fluxes Φ_α associated with each lead. Every analysis of frequency-dependent phenomena must deal with the fact that the conductor may temporarily deviate from a state of charge neutrality. The sum of the particle currents entering the conductor is not conserved but is related to the total charge Q_0 accumulated in the conductor, $dQ_0/dt = \sum I_\alpha$. In Fig. 1 total current conservation is achieved by assuming a separate, capacitively coupled path for the displacement current $i_1 \equiv dQ_0/dt = \sum I_\alpha$. For a conductor with N probes the particle currents are related to the network currents via $I_n = i_n - i_{n+1}$ for $n < N$ and $I_N = i_N$ for $n = N$. Consequently the fluxes in Eq. (1) are related to the network fluxes via $\Phi_n = \sum_{m=1}^{m=n} \phi_m$. Clearly, Fig. 1 is only an illustrative example of a transformation of the relationship between network currents and particle currents of the mesoscopic conductor. But its central feature, the differing paths followed by displacement currents and particle currents, can be expected to be part of any model. After all in a mesoscopic conductor that sits on a substrate and is often formed with the help of charged gates, displacement currents and particle currents do follow very different paths. Alternatively we could generate the electromagnetic perturbation, Eq. (1), by invoking local vector potentials which generate electric fields that act only on a particular lead [12].

Next we demonstrate that the electric and magnetic perturbations of Eq. (1) lead to the same response if they generate the same electrostatic potentials $d\delta\Phi_\alpha/dt = \delta V_\alpha = \delta U_\alpha$. The response function $\kappa^{\Phi}_{\alpha\beta}$ defined by $\langle \delta I_\alpha(\omega)\rangle = \sum_\beta \kappa^{\Phi}_{\alpha\beta}\delta\Phi_\beta(\omega)$ and the response function $\kappa^{U}_{\alpha\beta}$ defined by $\langle \delta I_\alpha(\omega)\rangle = \sum_\beta \kappa^{U}_{\alpha\beta}(\omega)\delta U_\beta(\omega)$ can be expressed in terms of the current and charge operators as follows [13]:

$$\kappa^{\Phi}_{\alpha\beta}(\tau) = -\frac{i}{\hbar}\langle [I_\alpha(\tau), I_\beta(0)]\rangle \Theta(\tau), \tag{3}$$

$$\kappa^{U}_{\alpha\beta}(\tau) = -\frac{i}{\hbar}\langle [I_\alpha(\tau), Q_\beta(0)]\rangle \Theta(\tau), \tag{4}$$

where $[\,,]$ denotes the commutator. I and Q are Heisenberg operators. Since for any operators A and B, $\langle [A(\tau), B(0)]\rangle = \langle [A(0), B(-\tau)]\rangle$, and since $dQ_\alpha/d\tau = -I_\alpha$, it follows that the electromagnteic response given by the time derivative of the electric response function $d\kappa^U/d\tau = \kappa^\Phi$. Both perturbations thus give rise to the same ac conductance. In the following we calculate the magnetic response function. With the help of Eq. (3) the ac conductance is determined by

$$g_{\alpha\beta} = \frac{1}{\hbar\omega}\int_0^\infty d\tau \exp[i(\omega + i0^+)\tau]\, \langle [I_\alpha(\tau), I_\beta(0)]\rangle . \tag{5}$$

To evaluate Eq. (5) we follow recent work on current fluctuations in mesoscopic conductors. In second quantization the operator of the total current in probe α is given by [4]

$$I_\alpha(t) = \frac{e}{h}\int dE\, dE' \left[\mathbf{a}^\dagger_\alpha(E)\mathbf{a}_\alpha(E') - \mathbf{b}^\dagger_\alpha(E)\mathbf{b}_\alpha(E')\right] \times \exp[i(E-E')t/\hbar], \tag{6}$$

where $\mathbf{a}^\dagger$, $\mathbf{a}$, $\mathbf{b}^\dagger$, $\mathbf{b}$ are vectors with M_α components which create (annihilate) incoming carriers and outgoing carriers. The a and b operators satisfy the same commutation relations. They are connected by a unitary transformation which is just the scattering matrix, $\mathbf{b}_\alpha = \sum_\beta \mathbf{s}_{\alpha\beta}\mathbf{a}_\beta$. Using Eq. (6) we find that the current operator in terms of the a operators only is determined by a matrix [4]

$$\mathbf{A}_{\beta\gamma}(\alpha, E, E') = \mathbf{1}_\alpha \delta_{\alpha\beta}\delta_{\alpha\gamma} - \mathbf{s}^\dagger_{\alpha\beta}(E)\mathbf{s}_{\alpha\gamma}(E'). \tag{7}$$

Equation (7) consists of normalized current matrix elements evaluated in probe α. The matrix elements are evaluated with the help of scattering states describing incident carriers in probes β and γ. In the presence of a time-dependent perturbation, the particle current in the leads is, strictly speaking, not spatially constant. As discussed in more detail in Ref. [4] there are oscillating contributions to the current both on a short length scale (the Fermi wavelength) as well as on a long length scale with a wavelength v_F/ω. The short-wavelength variations are a consequence of interference effects which can be neglected deep in the leads. The period of the long-wavelength oscillations, for a considerable range of frequencies, is much larger than the dimensions of a typical mesoscopic conductor [4]. In Eq. (6) these spatial variations are neglected and the particle current is taken to be spatially uniform along each lead. Using Eqs. (6) and (7) to evaluate Eq. (5) we find

$$g_{\alpha\beta}(\omega) = -\frac{e^2}{(2\pi)^2\hbar}\int dE\, dE'\, \mathrm{Tr}\,[\mathbf{A}_{\alpha\alpha}(\beta,E',E) + \mathbf{A}_{\beta\beta}(\alpha,E,E')]\,\frac{f(E)-f(E')}{\hbar\omega}\,\frac{1}{i(\hbar\omega+E-E'+i0^+)}. \quad (8)$$

Here we have used that at equilibrium the Fermi distribution f is the same in each contact. We have furthermore used the standard statistical assumption that only expectation values of pairs of creation and annihilation operators which create and annihilate carriers in the same quantum channel specified by the same quantum numbers have a nonvanishing statistical expectation value. Equation (8) is still a formal expression. A key problem in all linear response calculations is the appearance of the double energy integral in Eq. (8). For noninteracting carriers the final result [see Eq. (2)] contains a single energy integral. Baranger and Stone [7] perform this integral on the level of Green's functions in a veritable tour de force. Shepard [8] points to a more direct path by appealing to the analytic properties of the current matrix elements. We proceed here in an especially simple and direct way: The scattering matrix is itself a response function. It must obey the causality requirement expressed by the Kramers-Kronig relations [6]

$$\int_{-\infty}^{+\infty} dE'\,\frac{s(E')}{E_1-E'\pm i0^+} = \begin{pmatrix} -2\pi i s(E_1) \\ 0 \end{pmatrix}. \quad (9)$$

A similar relation holds for the adjoint scattering matrices. The scattering matrices in Eq. (8) occur in the form of bilinear products at energy E and E' multiplied by either $f(E)$ or $f(E')$. If $f(E)$ occurs we apply Eq. (9) to the integral over E'; if $f(E')$ occurs we apply it to the integral over E. The result of this calculation is Eq (2), i.e., a conductance determined by the trace of $\mathbf{A}_{\beta\beta}(\alpha,E,E+\hbar\omega)$. Equation (2) exhibits the microreversibility symmetry $g_{\alpha\beta}(\omega,-B) = g_{\beta\alpha}(\omega,B)$ and obeys the reality condition $g_{\alpha\beta}(\omega) = g^*_{\alpha\beta}(-\omega)$. The real (dissipative) part of the frequency-dependent conductance is $g'_{\alpha\beta}(\omega) = \frac{1}{2}[g_{\alpha\beta}(\omega) + g^*_{\beta\alpha}(\omega)]$ and thus is determined by $\frac{1}{2}\mathrm{Tr}[\mathbf{A}_{\beta\beta}(\alpha,E,E+\hbar\omega)+\mathbf{A}_{\alpha\alpha}(\beta,E+\hbar\omega,E)]$. It is related to the equilibrium current fluctuations

$$S_{\alpha\beta}(\omega) = \frac{1}{2}\int_{-\infty}^{\infty} d\tau\,\exp(i\omega\tau)\,\langle[I_\alpha(\tau),I_\beta(0)]_+\rangle$$
$$= 2\,\epsilon(\omega,kT)\,g'_{\alpha\beta}(\omega) \quad (10)$$

via the fluctuation-dissipation theorem. In Eq. (10) the energy of a harmonic quantum oscillator is denoted by $\epsilon(\omega,kT)$. The nondissipative (out of phase) part of the conductance is $g''_{\alpha\beta}(\omega) = \frac{1}{2}[g_{\alpha\beta}(\omega) - g^*_{\beta\alpha}(\omega)]$ and is determined by $\frac{1}{2}i\,\mathrm{Tr}[\mathbf{A}_{\beta\beta}(\alpha,E,E+\hbar\omega) - \mathbf{A}_{\alpha\alpha}(\beta,E+\hbar\omega,E)]$. Below we briefly investigate the low-frequency behavior of the conductance and link it to the density of states of the conductor and to phase delay times for carrier traversal and reflection [14, 15]. To first order in ω we find, from Eq. (2),

$$g_{\alpha\beta}(\omega) = g_{\alpha\beta}(0) - i\omega e^2\int dE\,(dN_{\alpha\beta}/dE)(-df/dE), \quad (11)$$

where

$$\frac{dN_{\alpha\beta}}{dE} = \frac{1}{4\pi i}\,\mathrm{Tr}\left[\mathbf{s}^\dagger_{\alpha\beta}(E)\frac{\partial\mathbf{s}_{\alpha\beta}(E)}{\partial E} - \frac{\partial\mathbf{s}^\dagger_{\alpha\beta}(E)}{\partial E}\mathbf{s}_{\alpha\beta}(E)\right] \quad (12)$$

is the density of states of the conductor accessed by carriers incident in probe β and leaving through probe α. The total density of states accessed by carriers incident from all the leads and exiting through all the probes is $\sum_{\alpha\beta} dN_{\alpha\beta}/dE$. Alternatively, the term proportional to ω in Eq. (11) defines a time scale $\tau_{\alpha\beta} = h(dN_{\alpha\beta}/dE)/\mathrm{Tr}[\mathbf{s}^\dagger_{\alpha\beta}\mathbf{s}_{\alpha\beta}]$ where h is Planck's constant. The time $\tau_{\alpha\beta}$ is a multichannel average of characteristic time scales related to derivatives of scattering matrix elements. The scattering channel with carriers incident in channel n in lead β and with carriers exiting in channel m in lead α contributes to the average time with a probability $|s_{\alpha\beta mn}|^2$ a time $\tau_{\alpha\beta mn} = \hbar\,\mathrm{Im}[d(\ln s_{\alpha\beta mn})/dE]$. Summing over all channels and dividing the result by the total probability $\sum_{mn}|s_{\alpha\beta mn}|^2$ gives $\tau_{\alpha\beta}$.

The expressions for the characteristic times are valid at zero temperature. At elevated temperature we can introduce effective time scales by weighting the nominator and denominator with $-df/dE$ and integrating over energy. The denominator in $\tau_{\alpha\beta}$ is proportional to the zero-frequency conductance $g_{\alpha\beta}$ for $\alpha \neq \beta$. For $\alpha = \beta$ the denominator is proportional to $-g_{\alpha\alpha} + g_{c,\alpha}$ where $g_{c,\alpha} = (e^2/h)M_\alpha$ is a contact conductance. Hence Eq. (11) can be expressed in the form

$$g_{\alpha\beta}(\omega) = g_{\alpha\beta}(0) + i[g_{\alpha\beta}(0) - g_{c,\alpha}\delta_{\alpha\beta}]\omega\tau_{\alpha\beta}. \quad (13)$$

This intuitive result could also have been obtained simply by assuming that the appearance of carriers in probe α is retarded with a time $\tau_{\alpha\beta}$ relative to their time of injection in probe β. We emphasize that the appearance of a phase delay time [14] as opposed to a time which depends both on the amplitude and on the phase [15] of the scattering matrix elements is due to the fact that the perturbation we treat is not spatially localized.

In contrast to the zero-frequency case, where $\sum_\beta g_{\alpha\beta} = \sum_\alpha g_{\alpha\beta} = 0$ due to current conservation, the sum of the frequency-dependent conductances Eq. (2) is in general not zero. To linear order in ω we find

$$\sum_\beta g_{\alpha\beta}(\omega) = -ig_{c,\alpha}\omega\bar{\tau}_\alpha, \quad (14)$$

$$\sum_\alpha g_{\alpha\beta}(\omega) = -ig_{c,\beta}\omega\tau_\beta. \quad (15)$$

Here $\bar{\tau}_\alpha = (1/M_\alpha)\sum_\beta \mathrm{Tr}[\mathbf{s}^\dagger_{\alpha\beta}\mathbf{s}_{\alpha\beta}]\tau_{\alpha\beta}$ is the channel averaged time that carriers exiting probe α have spent in the conductor irrespective of which probe they entered, and $\tau_\beta = (1/M_\alpha)\sum_\alpha \mathrm{Tr}[\mathbf{s}^\dagger_{\alpha\beta}\mathbf{s}_{\alpha\beta}]\tau_{\alpha\beta}$ is the time carriers entering the conductor through probe β have spent in the conductor irrespective of the probe through which they leave.

We conclude with a brief description of the effects of self-consistent potentials on the total response of the conductor. The main effect which we can take into account is the reduction of the charging of the sample due to a counteracting self-consistent potential whereas self-polarization effects would require a more detailed theory. The pileup of a net charge $dQ_0/dt = \sum_\alpha I_\alpha$ on the conductor gives rise to an induced potential $U_0^{\mathrm{ind}} = d_{00}Q_0 = (i/\omega)d_{00}I$ where $d_{00} = (\mathbf{C}^{-1})_{00}$ is an element of the inverse capacitance matrix $\mathbf{C}$. The potential distribution $(U_0^{\mathrm{ind}}, U_\alpha^{\mathrm{ext}})$ is equivalent to the potential distribution $(0, U_\alpha^{\mathrm{ext}} - U_0^{\mathrm{ind}})$. Thus the response of the interacting system $g^I_{\alpha\beta} = \delta I_\alpha/\delta U_\beta^{\mathrm{ext}}$ in a self-consistent potential approach [16] is determined by $\delta I_\alpha = g_{\alpha\beta}\delta U_\beta^{\mathrm{ext}} - \sum_\beta g_{\alpha\beta}\delta U_0^{\mathrm{ind}}$, where $g_{\alpha\beta}$ is the conductance of the noninteracting system. The solution of these equations gives for the admittance of the interacting system

$$g^I_{\alpha\beta}(\omega) = g_{\alpha\beta}(\omega) - \left(\frac{(i/\omega C)\sum_\gamma g_{\alpha\gamma}(\omega)\sum_\delta g_{\delta\beta}(\omega)}{1+(i/\omega C)\sum_{\gamma\delta} g_{\gamma\delta}(\omega)}\right), \tag{16}$$

and gives for the current induced into the substrate (the capacitance in Fig. 1) an admittance $g_{0\beta} = -(\sum_\alpha \delta I_\alpha)/\delta U_\beta^{\mathrm{ext}}$,

$$g^I_{0\beta}(\omega) = -\frac{\sum_\delta g_{\delta\beta}(\omega)}{1+(i/\omega C)\sum_{\gamma\delta} g_{\gamma\delta}(\omega)}, \tag{17}$$

where we have used the abbreviation $1/C = d_{00}$. The combined admittance matrix of Eqs. (16) and (17) is current conserving. The second term in Eq. (16) represents a self-consistent potential correction of the conductance of the noninteracting system. For small frequencies Eqs. (14) and (15) show that this term is proportional to ω. For a conductor with one lead only, Eq. (16) gives $g^I = g/[1+(i/\omega C)g]$. For small frequencies $g = -i\omega\tau g_c$ and hence $g^I = -i\omega C/[1+(\tau_{RC}/\tau)]$. Thus the interactions may be neglected if the RC time, $\tau_{RC} = C/g_c$, is large compared to the dwell time τ. If the RC time is short compared to the dwell time, $g^I = -i\omega C$. Interactions dominate the low-frequency behavior. The admittance matrix of the interacting system, Eqs. (16) and (17), has the property that each element is a function of all the noninteracting conductances. This has especially interesting consequences if, as is the case at a quantized Hall plateau, only certain conductances of the noninteracting system are nonvanishing. Further, an interacting system permits ac currents for purely capacitively coupled conductors for which all off-diagonal admittances of the noninteracting system vanish. Thus Eq. (2) and Eqs. (16) and (17) should be useful to characterize the low-frequency response of a large class of mesoscopic conductors.

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(a) Permanent address: IBM T. J. Watson Research Center, P.O. Box 218, Yorktown Heights, NY 10598.

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