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CHRISTEN, Thomas, BUTTIKER, Markus. Low frequency admittance of a quantum point contact. *Physical review letters*, 1996, vol. 77, no. 1, p. 143-146

DOI : 10.1103/PhysRevLett.77.143

arxiv : cond-mat/9601074

PMID : 10061792

Available at:

<http://archive-ouverte.unige.ch/unige:4211>

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Low frequency admittance of a quantum point contact

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Abstract

We present a current and charge conserving theory for the low frequency admittance of a quantum point contact. We derive expressions for the electrochemical capacitance and the displacement current. The latter is determined by the *emittance* which equals the capacitance only in the limit of vanishing transmission. With the opening of channels the capacitance and the emittance decrease in a step-like manner in synchronism with the conductance steps. For vanishing reflection, the capacitance vanishes and the emittance is negative.

PACS numbers: 72.10.Bg, 73.40.Gk

arXiv:cond-mat/9601074v1 18 Jan 1996

Typeset using REVTeX

There is growing interest in transport properties of electric nanostructures such as quantum point contacts, quantum wires, and quantum dots, to mention but a few [1,2]. These mesoscopic conductors can be so small that transport at low temperatures is phase coherent or even mainly ballistic including only a few elastic scattering events. The scattering approach to electrical conduction [2–4] has successfully been used to describe many experiments. For a phase coherent conductor with two probes this theory relates the transmission probabilities $T^{(j)}$ of the occupied one-dimensional subbands to the dc-conductance $G^{(0)} = (2e^2/h) \sum T^{(j)}$. The validity of this conductance formula was experimentally confirmed first by van Wees et al. [5] and Wharam et al. [6] who found a stepwise increase of the conductance by successively opening conduction channels of a quantum point contact.

A more novel concept concerns the notion of the *mesoscopic capacitance*. Usually, the capacitance C_μ is defined by the static change of the charge on a conductor as a response to the electrochemical voltage drop between the contacts. However, there exists also a dynamic point of view which is important for practical use: the capacitance is then associated with the phase shift between a current and a voltage oscillation at small frequencies ω , i.e. with the imaginary part of the low frequency admittance $G(\omega)$ of a resistor and condenser in parallel. A dynamical derivation of a mesoscopic capacitance was given by Büttiker, Thomas, and Prêtre [7]. To make a clear distinction between the static and the dynamic conceptions, we call $E_\mu = i(dG/d\omega)_{\omega=0}$ the *emittance* of a conductor. For a purely capacitive structure such as a condenser the static and dynamical derivations lead to identical results, i.e. $E_\mu = C_\mu$. This case is characterized by a displacement current entering the sample through the leads which is equal to the change of the charge on a condenser plate. We mention that in a mesoscopic sample the relevant density of states (DOS), dN_1/dE and dN_2/dE , of the ‘mesoscopic condenser plates’ can be so small that C_μ is no longer equal to the geometric capacitance C_0 but depends on the DOS [7]: $C_\mu^{-1} = C_0^{-1} + D_1^{-1} + D_2^{-1}$ with $D_k = e^2 dN_k/dE$. This is due to the fact that the voltage drop between the reservoirs can differ significantly from the drop of the electrostatic potential at the plates. On the other hand, for conductors which permit transmission $E_\mu = C_\mu$ is *not* valid. In this Letter, we derive expressions for the capacitance

and the emittance of a quantum point contact (Fig. 1). The model which we develop also describes a ballistic quantum wire containing an elastic scatterer or a mesoscopic condenser with tunneling between the two condenser plates (leakage). Capacitance properties of small conductors with transmission are also of great importance in tunneling microscopy [8].

First, we present our results for a single-channel conductor. Subsequently, their derivation and the generalization to many channels is provided using the scattering approach to low-frequency transport developed in Refs. [9,10].

Consider a phase-coherent single-channel conductor containing a localized scattering obstacle. It turns out that C_μ and E_μ decrease for increasing transmission probability $T = 1 - R$. In particular, we show that the capacitance is proportional to the reflection probability R

$$C_\mu = \frac{R}{C_0^{-1} + D_1^{-1} + D_2^{-1}} . \quad (1)$$

In general, also the geometric capacitance C_0 depends on R . For example, C_0^{-1} decreases for two condenser plates approaching each other. However, since the D_k are nearly independent of T and remain finite for $R \rightarrow 0$ one concludes from Eq. (1) that C_μ vanishes for $R \rightarrow 0$ even if C_0^{-1} vanishes. This is reasonable since for ideal transmission (no barrier) a charge accumulation does not occur. For $R = 1$, on the other hand, we recover from Eq. (1) the above mentioned expression for the electrochemical capacitance of a mesoscopic condenser.

The emittance of a single-channel conductor is given by

$$E_\mu = C_\mu R - \frac{D}{4} T^2 , \quad (2)$$

where $D = D_1 + D_2$ is associated with the total (relevant) DOS of the sample. As expected, $R = 1$ implies $E_\mu = C_\mu$. On the other hand, for total transmission ($R = 0$) the emittance is negative, $E_\mu = -D/4$. For the particular case where the geometric capacitance is sufficiently large and where the sample is spatially symmetric, i.e. $C_0 \gg D_1 = D_2$, we find $E_\mu = (D/4)(R - T)$. This illustrates a cross-over between positive and negative emittance. Negative emittances are characteristic for conductors with nearly perfect transmission. For

resonant tunnel junctions an inductive-like kinetic response is discussed in Refs. [11–13]. In Ref. [9] it is shown that the emittance remains negative even when the charge in the well is totally screened. It is interesting that the emittance for the symmetric tunnel resonance barrier in this limit can also be written as $E_\mu = (D/4)(R - T)$. A similar relation has been found by Mikhailov and Volkov [14] who calculated with a Boltzmann approach the low frequency plasma-wave spectrum for a tunnel junction. Introducing a time τ_T , they found a tunnel contribution C_T to the capacitance which is proportional to $\tau_T(R - T)$. Although their result is not in full accordance with Eq. (2), it holds $E_\mu = C_T$ if the barrier is symmetric, if capacitances in series and in parallel are neglected, and if one replaces τ_T by the expression $hD/(2e^2)$. Furthermore, we showed in Ref. [15] that positive and negative emittances exist in quantized Hall samples, depending on whether edge states provide perfect transmission or perfect reflection channels.

Consider now a quantum point contact (Fig. 1) connected on either side to reservoirs α ($= 1, 2$). A variation of the voltage $\delta V_\alpha = \delta\mu_\alpha/e$ in reservoir α changes the electrochemical potential $\delta\mu_\alpha$ of the incoming particles which are partly scattered back and partly transmitted. The admittance matrix $G_{\alpha\beta}(\omega) = \delta I_\alpha/\delta V_\beta$ represents the linear response of the current δI_α through contact α for a small voltage oscillation $\delta V_\beta \propto \exp(-i\omega t)$ in reservoir β . For low frequencies one can write

$$G_{\alpha\beta}(\omega) = G_{\alpha\beta}^{(0)} - i\omega E_{\alpha\beta} \quad , \quad (3)$$

where $E_{\alpha\beta}$ is the emittance matrix. A microscopic calculation of the emittance is a complicated task since the electrostatic potential is a complicated function of space. The aim of this work is to develop a simple model that captures the essential physical features.

First, we mention that an applied voltage can polarize the conductor but leaves the total charge unaffected. Hence, for a conductor in electrical isolation (no other nearby conductors or gates) charge and current are conserved, meaning $G_{11} = G_{22} = -G_{12} = -G_{21} \equiv G \equiv G^{(0)} - i\omega E_\mu$. The non-equilibrium charge distribution with the form of a dipole has a charge δq_1 to the left and a charge $\delta q_2 = -\delta q_1$ to the right of the barrier. Instead of

treating the entire potential landscape realistically we introduce only two potentials $\delta U_{1,2}$ for the regions $\Omega_{1,2}$ (dark regions in Fig. 1). These regions are characterized by an incomplete screening of the excess charge. Consider for a moment a voltage shift $\delta V_1 = \delta\mu_1/e$ only in the left reservoir. On the far left side of the point contact one has complete screening, thus the local electric potential shift follows the electrochemical potential, $\delta\mu_1/e$, while on the far right side it vanishes. As we move along the conductor from the left reservoir to the right reservoir the potential shift drops from $\delta\mu_1/e$ to δU_1 to δU_2 to zero. The potential drop will be strongly localized near the maximum of the barrier in the center of the quantum point contact. In fact, the potential drop will be localized within a screening length. We discretize this potential [16]. We emphasize that within the framework of the general approach provided by Ref. [10] the complicated full quantum mechanical and space dependent problem can be treated analogously.

In the basis of eigen-channels the transmission problem through a quantum point contact can be represented as a sum of single-channel transmission-problems [17,18]. The potential of a quantum point contact has the shape of a saddle [18] with a value eU_0 at the saddle point. Near the saddle the potential can also be separated into a longitudinal part $eU(x)$ and a transverse part $eU(y)$. Thus, in a first step we consider a single-channel transmission problem in a potential $eU(x)$. The variation of this potential is slow compared to the Fermi wavelength which allows us to use the semiclassical WKB approximation for the local density of states $dn(x)/dE$ and for the transmission probability T [19,20]. The regions Ω_k to the left and to the right of the barrier in which the potentials are not screened are $\Omega_1 = [-l_1, -x_1]$ and $\Omega_2 = [x_2, l_2]$, respectively, where the $l_{1,2}$ are of the order of the screening length. The x_k are determined by the WKB turning points if $E_F < eU_0$, and they are given by $x_k = 0$ (the location of the barrier peak) for $E_F \geq eU_0$. We express the DOS in the region Ω_k in the form of a quantum capacitance

$$D_k = e^2 \int_{\Omega_k} dx \frac{dn(x)}{dE} . \quad (4)$$

For the following we need the nonequilibrium state, i.e. the charge δq_k which resides in

Ω_k as a consequence of a voltage variation $\delta V_\alpha = \delta\mu_\alpha/e$ at contact α . This charge can be found with the help of the *partial densities of states* (PDOS) associated with carriers in Ω_k scattered from contact β to contact α [10]. In the semiclassical (WKB) case this PDOS is given by

$$D_{\alpha k\beta} = D_k (T/2 + \delta_{\alpha\beta}(R \delta_{\alpha k} - T/2)) \quad , \quad (5)$$

where δ_{kl} is the Kronecker delta. Note that $D_k = \sum_{\alpha\beta} D_{\alpha k\beta}$. Greek and roman indices label reservoirs and incompletely screened regions near the point contact, respectively. The injected charges lead to induced electrostatic potentials δU_k which counteract the built up of charge in the regions Ω_k , i.e. the shifts δU_k of the band bottoms induce a charge response. For a spatially slowly varying potential this response is local and is determined by the DOS, $\delta q_k^{ind} = -D_k \delta U_k$. The charge in region k is then given by

$$\delta q_k = \sum_{\alpha\beta} D_{\alpha k\beta} (\delta V_\beta - \delta U_k) \equiv \sum_{\beta} \bar{D}_{k\beta} (\delta V_\beta - \delta U_k) \quad , \quad (6)$$

where we introduced the *injectivity* [10] $\bar{D}_{k\beta} = \sum_{\alpha} D_{\alpha k\beta}$ which is the PDOS of region Ω_k associated with carriers injected at contact β .

We next determine the electrochemical capacitance. We introduce a geometrical capacitance matrix $C_{0,kl} = (-1)^{k+l} C_0$ associated with the regions Ω_k , which we assume to be known. In general, it is found by solving the Poisson equation. The electrostatic and electrochemical capacitance matrices $C_{0,kl}$ and $C_{\mu,k\beta}$, respectively, relate the charge to the potentials via

$$\delta q_k = \sum_l C_{0,kl} \delta U_l = \sum_{\beta} C_{\mu,k\beta} \delta V_\beta \quad . \quad (7)$$

Charge conservation implies $C_{\mu,k\beta} = (-1)^{k+\beta} C_\mu$. Using Eqs. (5)-(7) yields then the electrochemical capacitance (1).

To calculate the emittance matrix we remark that $E_{\alpha\beta} \delta V_\beta$ corresponds to the displacement charge δQ_α which passes contact α for a variation δV_β of the voltage in reservoir β . Note that $\delta q_k = \delta Q_{\alpha=k}$ is only valid if $R = 1$ but does not hold if $R < 1$. Since we restrict ourselves to the first-order frequency term, it is sufficient to calculate the quasi-static

displacement charge. We take the Coulomb interaction into account self-consistently by considering two contributions to δQ_α . A first part which neglects screening is given by the kinetic contribution $D_{\alpha\beta}\delta V_\beta$, where $D_{\alpha\beta} = \sum_k D_{\alpha k\beta}$ is the PDOS of carriers scattered from contact β to contact α at fixed electrostatic potentials. A second part corresponds to a screening charge which is due to the shifts δU_k of the band bottoms. The part of the screening charge which is eventually scattered to contact α is then given by $-\sum_{k\gamma} D_{\alpha k\gamma}\delta U_k \equiv -\sum_k \underline{D}_{\alpha k} u_{k\beta} \delta V_\beta$, where we defined the *emissivity* [10] $\underline{D}_{\alpha k} = \sum_\gamma D_{\alpha k\gamma}$ associated with the states scattered from the region Ω_k to contact α . Furthermore, we introduced the *characteristic potentials* [10] $u_{k\beta} = \partial U_k / \partial V_\beta$ which give the change of the electrostatic potential in region k due to a variation of the voltage in reservoir β . The negative sign of the screening charge is due to the fact, that a positive shift of the band bottom at fixed electrochemical potential diminishes the number of charge carriers. One finds from Eqs. (6) and (7) $u_{k\beta} = (\overline{D}_{k\beta} - c_{\mu,k\beta})/D_k$. The emittance matrix is the sum of kinetic and screening charges scattered to contact α [10]

$$E_{\alpha\beta} = D_{\alpha\beta} - \sum_k \underline{D}_{\alpha k} u_{k\beta} . \quad (8)$$

Using the total density of states $D = D_1 + D_2 = \sum_{\alpha k} \underline{D}_{\alpha k} = \sum_{\alpha\beta} D_{\alpha\beta}$ of both regions Ω_1 and Ω_2 , the expression (5) for the PDOS, and the characteristic potentials given above, we find Eq. (2) for the emittance of a single-channel mesoscopic conductor.

In order to generalize the results (1) and (2) to M channels $j = 1, \dots, M$ with channel thresholds $E_b^{(j)}$ we use the fact that the total PDOS is the sum of the PDOS of the single channels, i.e. $D_{\alpha k\beta} = \sum_j D_{\alpha k\beta}^{(j)}$. If $E_F < E_b^{(j)}$, the PDOS for the channel j vanish, $D_{\alpha k\beta}^{(j)}(E_F) \equiv 0$. If $E_F \geq E_b^{(j)}$, the PDOS $D_{\alpha k\beta}^{(j)}(E_F)$ are given by the single-channel PDOS (5) taken at an energy $E_F - E_b^{(j)}$. Proceeding the same way as above, we find an electrochemical capacitance (1) with a reflection probability $R = 1 - T_1/2 - T_2/2$, where $T_k = D_k^{-1} \sum_j T^{(j)} D_k^{(j)}$ is an average transmission probability weighted by the density of states of Ω_k . For the emittance we find

$$E_\mu = C_\mu R - \frac{1}{4}(D_1 T_1^2 + D_2 T_2^2) . \quad (9)$$

Equation (9) applies to a scattering obstacle in an N-channel wire. Let us now apply this result to the quantum point contact of Fig. 1. One expects a step-like behavior of the capacitance and the emittance as the number of open channels increases. In the following we consider a symmetric barrier with the quadratic potential $U(x) = U_0(b^2 - x^2)/b^2$ if $|x| \leq b$, and $U(x) = 0$ if $b < |x| \leq l$. For this special case, the PDOS and the transmission probability can be calculated analytically from the WKB expressions [19,20]. For simplicity, we assume a constant electrostatic capacitance $C_0 = 1 \text{ fF}$ between Ω_1 and Ω_2 and a fixed number of occupied channels in these regions. The only parameter to be varied is the potential height U_0 . We assume that no additional channels enter into the regions Ω_k during the variation of U_0 . In Fig. 2 we show the result for a constriction with $b = 500 \text{ nm}$, $l = 550 \text{ nm}$, and with three equidistant channels separated by $E_F/3 = 7/3 \text{ meV}$. The dotted, dashed, and solid curves correspond to the dc-conductance, the electrochemical capacitance, and the emittance, respectively. For small U_0 where all channels are open, the capacitance vanishes and the emittance is negative. At each conductance step, the capacitance and the emittance increase and eventually merge when all channels are closed. Due to a weak logarithmic divergence of the WKB density of states at particle energies $E = eU_0$ (where WKB is not appropriate), the WKB emittance diverges weakly (steep edges of the emittance below and above the steps). A more accurate quantum mechanical calculation of the PDOS from the scattering matrix [9,10] yields a suppression of these divergencies, i.e. the regions between the steps become more flat.

To summarize, we present a theory for the capacitance and the low frequency admittance of one-dimensional mesoscopic two-terminal conductors. The electrochemical capacitance defined as the charge variation on a conductor for a voltage drop in the reservoirs turns out to be proportional to the reflection probability. The quantity which is usually measured in an experiment is not the charge (or the dipole moment) but rather the displacement current which is determined by the emittance. The emittance equals the capacitance for vanishing transmission but becomes negative if transmission predominates. Quantum point contacts which provide the possibility to vary the number of open one-dimensional channels should

thus show not only conductance steps but also steps in the capacitance and the emittance. The generalization to conductors which are not in electrical isolation will be published elsewhere. We only mention that metallic gates used to form the point contact couple with a purely capacitive emittance which exhibits peaks as new channels are opened. Furthermore, the presence of gates causes the zero in the emittance of the point contact to be shifted to larger values of T (< 1). We believe that the presented theory is also a starting point in order to treat the finite-frequency noise of quantum point contacts including Coulomb interactions [21].

Acknowledgement This work has been supported by the Swiss National Science Foundation.

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FIGURES

FIG. 1. Quantum point contact connected to reservoirs with electrochemical potentials $\mu_\alpha = \mu_0 + \delta\mu_\alpha$, and for the particular case of one transmitted and two backscattered channels inside Ω_k (dark regions) with electric potentials δU_k .

FIG. 2. Dependence of the conductance (in units $2e^2/h$; dotted curve), capacitance and emittance (in units of fF ; dashed and full curves, respectively) on the barrier height eU_0 for a quantum point contact with three relevant channels (see Fig. 1).



