Low Frequency Admittance of a Quantum Point Contact

T. Christen and M. Büttiker

Département de Physique Théorique, Université de Genève, 24 Quai Ernest-Ansermet, CH-1211 Genève, Switzerland

(Received 17 January 1996)

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 steplike manner in synchronism with the conductance steps. For vanishing reflection, the capacitance vanishes and the emittance is negative. [S0031-9007(96)00603-5]

PACS numbers: 73.23.Ps, 72.10.Bg, 73.40.Gk

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 [1–4] 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*. Besides the definition of the capacitance C by the static charge response to an electrochemical voltage drop, 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 capacitor 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 concepts, we call $E = i(dG/d\omega)_{\omega=0}$ the *emittance* of a conductor. For a purely capacitive structure the static and dynamical derivations lead to identical results, i.e., $E = C$. 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 capacitor plate. We mention that in a mesoscopic sample the relevant density of states (DOS), dN_1/dE and dN_2/dE, of the "mesoscopic capacitor plates" can be so small that C is no longer equal to the geometric capacitance C_0 but depends on the DOS [7]: $C^{-1} = C_0^{-1} + D_1^{-1} + D_2^{-1}$ 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 $E = C$ is *not* valid. In this Letter, we derive expressions for E and C of a quantum point contact (Fig. 1). We emphasize the dipolar structure of the charge distribution. The model which we develop also describes a mesoscopic capacitor with tunneling between the two capacitor plates (leakage), which is of great interest in, e.g., tunneling microscopy [8].

First, we present our results for a single-channel conductor. Subsequently, we present the derivation of the results using the scattering approach to low-frequency transport developed in Refs. [9,10]. Finally, the results are generalized to the many channel case of a quantum point contact.

C and E for a single channel.—The single-channel case is described by a one-dimensional scattering problem with a localized potential region describing a constriction or a tunneling barrier. It turns out that C and E decrease for increasing transmission probability $T = 1 - R$ of this

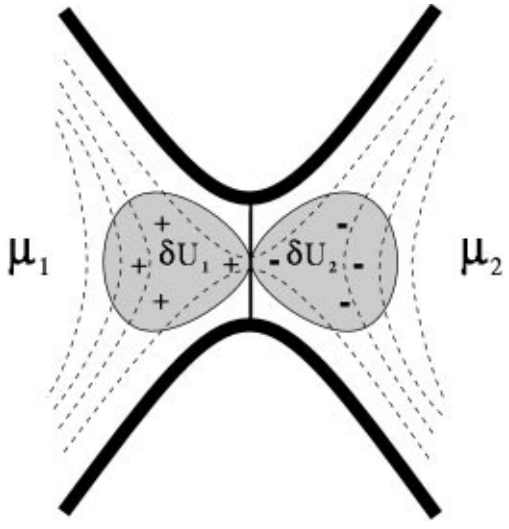

FIG. 1. Quantum point contact connected to reservoirs with electrochemical potentials $\mu_\alpha = \mu_0 + \delta\mu_\alpha$, and for the particular case of one transmitted and two backscattered channels inside Ω_k (dark regions) with electric potentials δU_k.

region. In particular, we find that the capacitance is proportional to the reflection probability R

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

In general, also the geometric capacitance C_0 depends on R. For example, C_0^{-1} decreases for two capacitor plates approaching each other. However, since the D_k are nearly independent of T and remain finite for $R \longrightarrow 0$ one concludes from Eq. (1) that C vanishes for $R \longrightarrow 0$ even when C_0^{-1} vanishes. This is reasonable since for ideal transmission (no barrier) a charge accumulation (dipole moment) 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 capacitor.

Below we will also show that in the single channel case the emittance is given by

$$E = CR - \frac{D}{4} T^2, \quad (2)$$

where $D = D_1 + D_2$ is the total (relevant) DOS. As expected, $R = 1$ implies $E = C$. On the other hand, for total transmission ($R = 0$) the emittance is negative, $E = -D/4$. 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 $E = (D/4)(R - T)$. This illustrates a crossover 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 $E = (D/4)(R - T)$. 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 tunneling contribution C_T to the capacitance proportional to $\tau_T(R - T)$. Although their result is not in full accordance with Eq. (2), it holds $E = C_T$ if the barrier is symmetric and if one replaces τ_T by a dwell time $hD/2e^2$. Furthermore, we show 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.

Derivation of C and E.—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 $\{\beta\}$. For low frequencies one can write

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

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 (with no other nearby conductors or gates) charge and current are conserved, meaning $G_{11} = G_{22} = -G_{12} = -G_{21} \equiv G \equiv G^{(0)} - i\omega E$. The nonequilibrium 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. 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, so the shift of the local electric potential follows the electrochemical potential $\delta\mu_1/e$. For the same reason, the electrostatic potential shift vanishes on the far right side. The drop of the voltage shift from $\delta\mu_1/e$ to zero is strongly localized within a screening length near the center of the quantum point contact. Instead of treating the entire potential landscape realistically, we discretize it [16]. We introduce two potentials $\delta U_{1,2}$ for the regions $\Omega_{1,2}$ (dark regions in Fig. 1) which are characterized by an incomplete screening of the excess charge. 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 eigenchannels 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 size of the Ω_k is 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 $D_k = e^2 \int_{\Omega_k} dx\, dn(x)/dE$.

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) $D_{\alpha k\beta}$ which are defined as the DOS associated with carriers in Ω_k scattered from contact β to contact α [15]. For example, D_{211} is given by the transmission probability times the DOS of Ω_1 associated with carriers with positive velocity, hence $D_{211} = TD_1/2$. Since there are no states in Ω_1 associated with scattering from contact 2 back to contact 2 one concludes $D_{212} = 0$. With similar arguments one finds in the semiclassical case for the PDOS

$$D_{\alpha k\beta} = D_k[T/2 + \delta_{\alpha\beta}(R\delta_{\alpha k} - T/2)], \qquad (4)$$

where δ_{ij} is the Kronecker delta. Note that $D_k = \sum_{\alpha\beta} D_{\alpha k\beta}$. The injected charges lead to induced electrostatic potentials δU_k which counteract the buildup 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, $\delta q_k^{\text{ind}} = -D_k\delta U_k$. The charge in Ω_k is then given by

$$\delta q_k = \sum_{\alpha\beta} D_{\alpha k\beta}(\delta V_\beta - \delta U_k) \equiv \sum_\beta \overline{D}_{k\beta}(\delta V_\beta - \delta U_k), \qquad (5)$$

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

To determine the electrochemical capacitance, we introduce first the geometrical capacitance matrix $C_{0,kl} = (-1)^{k+l}C_0$ associated with the regions Ω_k and which can be obtained from the Poisson equation. The electrostatic and electrochemical capacitances, $C_{0,kl}$ and $C_{k\beta}$, respectively, relate the charge to the potentials via

$$\delta q_k = \sum_l C_{0,kl}\delta U_l = \sum_\beta C_{k\beta}\delta V_\beta. \qquad (6)$$

Charge conservation implies $C_{k\beta} = (-1)^{k+\beta}C$. The result (1) follows now immediately from Eqs. (4)–(6).

To calculate the emittance we remark that $E_{\alpha\beta}\delta V_\beta$ corresponds to the displacement charge δQ_α, which passes contact α due to 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 quasistatic 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 global 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 response 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. (5) and (6) $u_{k\beta} = (\overline{D}_{k\beta} - C_{k\beta})/D_k$. The emittance matrix is obtained from the sum of kinetic and screening charges scattered to contact α [10]: $E_{\alpha\beta} = D_{\alpha\beta} - \sum_k \underline{D}_{\alpha k}u_{k\beta}$. 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 (4) for the PDOS, and the characteristic potentials given above, we find Eq. (2) for the emittance of a single-channel mesoscopic conductor.

The quantum point contact.—In order to generalize the results (1) and (2) to M channels $j = 1, \ldots, M$ 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 (4) taken at an energy $E_F - E_b^{(j)}$. Proceeding the same way as above, we find an electrochemical capacitance of the form of (1) with $R = 1 - T_1/2 - T_2/2$, 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

$$E = CR - \frac{1}{4}(D_1T_1^2 + D_2T_2^2). \qquad (7)$$

Let us now apply this result to the quantum point contact of Fig. 1. One expects a steplike behavior of the capacitance and the emittance as the number of open channels increases. As a specific example 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 $b < |x| \leq l$. In this case, $T_1 = T_2$ and the PDOS and the transmission probability can be calculated analytically from the WKB expressions [19,20]. For simplicity, we assume a constant electrostatic capacitance $C_0 = 1$ 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 $b = 500$ nm, $l = 550$ nm, and with three equidistant channels separated by $E_F/3 = 7/3$ 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. Because of a weak logarithmic divergence of the WKB density of states at particle energies $E = eU_0$ (where WKB is not appropriate), the WKB emittance shows steep edges between the steps. A more accurate quantum mechanical calculation of the PDOS from the scattering matrix [9,10] should yield a suppression of these divergencies.

In conclusion, a theory has been presented for the capacitance and the low frequency admittance of quasi-one-dimensional mesoscopic two-terminal conductors in electrical isolation. 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). The theory presented here is also a starting point for a treatment of the finite-frequency noise of quantum point contacts including Coulomb interactions [21].

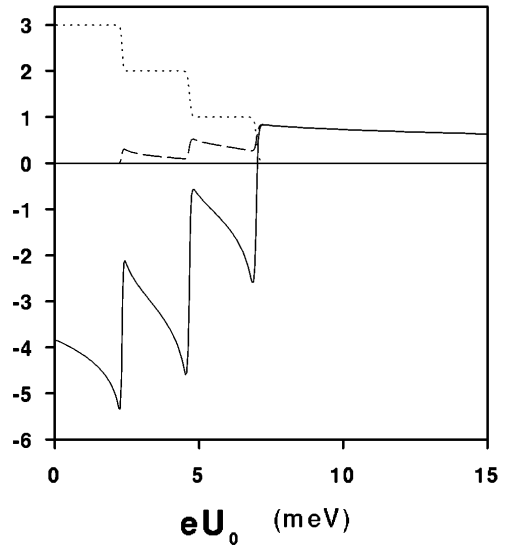

FIG. 2. Dependence of the conductance (in units $2e^2/h$; dotted curve), capacitance, and emittance (in units of fF; dashed and full curves, respectively) on the barrier height eU_0 for a quantum point contact with three relevant channels (see Fig. 1).

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

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