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Capacitance, admittance, and rectification properties of small conductors

M Büttiker

IBM T J Watson Research Center, P O Box 218, Yorktown Heights, NY 10598, USA

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Abstract. We formulate microscopic expressions for capacitances, admittances and the rectification properties for small phase-coherent samples consisting of a number of metallic layers separated by insulators. The electric potential in such a structure is discussed with the help of characteristic functions which determine the variation of the microscopic potential inside the sample in response to an increase of the electro-chemical potential at a contact. An electro-chemical capacitance matrix is derived which allows for field penetration into the conductor. We discuss the admittance matrix for conductors with nearby capacitors (gates) and analyse its magnetic field symmetry. We use the characteristic potentials to discuss the rectification properties of a conduction channel in the presence of nearby capacitors.

1. Introduction

Modern conductors which are of scientific interest and of technological importance are often multilayered structures with several metallic regions and doping layers separated by insulators. Some of the metallic layers, called gates, are used to define the 'conductor' and can be used to change its conductance properties. Examples of such conductors are various types of transistors [1], quantum point contacts [2, 3] formed with the help of split gates [4], and configurations used to measure the 'electrostatic Aharonov-Bohm effect' [5]. The charges of these metallic layers interact via long-range Coulomb forces. Here we are interested in the properties of such a conductor which depend on the mutual coupling of the metallic layers used to create it. First we discuss a structure consisting only of capacitors (see figure 1) and evaluate the differential capacitance matrix. There is no DC transport in this arrangement of conductors but in the presence of time-dependent oscillating voltages AC currents are induced. The capacitance matrix gives directly the leading-order terms of the frequency-dependent admittance. Subsequently we consider metallic layers attached to several contacts such that DC transport is permitted. While the DC conductances depend only on the equilibrium potential, the transport coefficients which describe the conductor and capacitors in the presence of slowly oscillating potentials depend on the quasi-stationary non-equilibrium potential distribution. In the presence of AC transport we find that the generalization of a capacitance matrix is an emittance matrix which determines the number of carriers per unit time emitted by the conductor into a contact. Finally we also discuss the role of long-range Coulomb potentials in non-linear DC transport. The leading-order non-linear terms of the current-voltage characteristic are expressed in terms of the potential which builds up in the conductor and nearby capacitors if a current is driven through the sample.



Figure 1. Capacitors connected via leads to electron reservoirs at electro-chemical potentials μ_k , k = 1, 2, 3. Capacitors 1 and 2 are in the same plane, capacitor 3 lies in another plane. No electric field lines penetrate the surface S.

The discussion of an assembly of capacitors shown in figure 1 is interesting. The textbook notion which holds that capacitance is determined by the Coulomb law and the geometry of the metallic layers assumes that electric fields are completely screened at the surface of the conductor. In reality, electric fields penetrate into the conductor. The degree of field penetration depends on the screening properties of the conductors. Field penetration occurs over a distance of the order of a Thomas-Fermi screening length. This is a short distance if the conductor is a good (three-dimensional) metal, but can be quite large compared to the dimensions of a mesoscopic conductor. Indeed a sufficiently small conductor might not be able to screen an external field at all. The key point is that any degree of field penetration changes the capacitance from a geometrical quantity to an electrochemical and statistical entity which, like the conductance, depends on the properties of the conductor. We derive a microscopic expression of the capacitance matrix which takes the field penetration into account.

The electro-chemical nature of capacitance is at the heart of capacitance spectroscopy. In these experiments a small AC current is driven through the sample and the capacitance is measured with the help of a capacitance bridge. This method has been used to investigate single-electron charging effects of metallic grains embedded in an insulating layer by Lambe and Jaklevic [6]. Büttiker [7] considered a single grain and discussed an effective small-signal capacitance. Recently, Lafarge *et al* [8] have carried out an experiment where a single 'electron box' is coupled capacitively to an external circuit. The spectra of quantum dots have also been investigated by Ashoori *et al* [9] with the help of this method. In single-electron tunneling effects, the distinction between electro-chemical capacitance and electrostatic capacitance has been discussed by van Houten *et al* [10].

The capacitive measurement of the density of states of a two-dimensional electron gas by Smith *et al* [11] and discussed by Stern [11] provides another illustration of this technique. In all these experiments and discussions it is the corrections to the geometrical capacitance

which provide the interesting information. Novel applications based on the fact that a two-dimensional electron gas cannot screen a transverse field have been suggested [12].

A brief discussion of a mesoscopic capacitor and its admittance was recently given by Büttiker, Thomas and Prêtre [13]. In this discussion the potential was characterized by a single parameter on each capacitor plate. The work presented here extends this earlier discussion to permit the treatment of an arbitrarily complicated electric potential distribution. Despite the fact that the electro-chemical nature of capacitances has been appreciated in the perceptive works mentioned already we are not aware of any attempts to provide a general theoretical formulation. To be definite we consider an arbitrary number of metallic layers each of which is connected to one electron reservoir as shown in figure 1. Each conductor is considered to be mesoscopic: electron motion near the capacitor plate and in the lead connecting the capacitor to the electron reservoir is subject to elastic scattering and Coulomb interaction. To find the differential capacitance we assume that the equilibrium potential for a reference state is known. We then investigate the change in the electrostatic potential which occurs if the electro-chemical potential of an electron reservoir is changed by a small amount. We determine this potential in a (one-loop) random phase approximation generalizing a discussion by Levinson [14]. Since we deal with an interacting manyelectron problem the results depend on the method used to find a solution. Our discussion attempts to extract a maximum of information from a few basic principles which apply to this problem. First, we consider a volume with a surface S which intersects the reservoirs at such a large distance that there are no electrical field lines penetrating the surface. As a consequence the total charge Q within the volume enclosed by the surface S is conserved. Second, the electrostatic potential and the electro-chemical potentials at the reservoirs are only defined up to an arbitrary energy. Thus the potential solution must be invariant if all electro-chemical potentials are raised or lowered by the same amount. Third, we use the fact that microscopic dynamics obey microreversibility: in the presence of a magnetic field the Hamiltonian for this system is invariant under simultaneous reversal of all momenta and of the magnetic field. These three principles provide useful constraints which any solution of this problem, independent of the particular method used, must obey. The deviations of the electro-static potential away from an equilibrium reference state are discussed with the help of characteristic functions, which give the microscopic potential in the interior of the conductor in response to a variation of the electro-chemical potential at a reservoir. These characteristic potential functions have themselves a number of simple properties that can be derived from the principles mentioned above.

From the capacitance matrix we immediately obtain the AC currents which are induced in such a system if the electro-chemical potentials (voltages applied to the contacts) are subject to slow time-dependent oscillations. For slowly changing voltages, the system is driven adiabatically through a sequence of equilibrium states.

We next consider a more general structure in which one or several metallic layers are connected to several contacts. Now current can appear not only as a consequence of electric induction but also as a consequence of direct carrier transmission from one contact to another. The zero-frequency terms of the admittances are the DC conductances determined by the equilibrium reference potential. But the actual potential distribution in the conductor and in the nearby capacitors is a time-dependent non-equilibrium potential. For DC transport the potential distribution in the presence of transport in the vicinity of impurities has been discussed by Landauer [15]. As a guide to additional work, see Sorbello [16]. Our discussion emphasizes the global behaviour of the potential in the entire structure. In conductors with poor screening properties the potential is determined not only by the conduction electrons but also by charges induced on nearby capacitors. For conductors with several contacts the leading-order terms of the admittance are not determined by capacitances alone but also by kinetic contributions which stem from direct carrier transmission from one contact to another. A generalization of the concept of capacitance is thus required: long-range Coulomb forces lead to a modification of the number of carriers emitted by the conductor into a contact. We call the quantity which takes the role of the capacitance an *emittance*. If direct transmission dominates over induced currents the emittance behaves like an inductance, but if induced currents dominate over directly transmitted carriers the emittance is similar to a capacitance.

Finally we illustrate the role of potentials in such a structure by calculating the leading non-linear terms in the I-V characteristic of the conductor for the case of a DC current. While, as mentioned already, the linear conductances depend only on the equilibrium potential, the non-linear terms in the I-V characteristic contain contributions which depend on the transport potential. Again we emphasize that the transport potential, similar to the equilibrium potential, is characteristic of the entire structure.

2. Characteristic potentials

Figure 1 shows a collection of mesoscopic capacitors labelled k, l = 1, 2, 3, which are connected via wires to electron reservoirs with electro-chemical potentials μ_k . The capacitors might lie in the same plane or might lie in different planes as in a layered system. We will treat all capacitors equally treating them as phase coherent mesoscopic structures. In realistic situations one or more capacitors might in fact be macroscopic conductors. First, we deal with the situations where all conductors are capacitors, i.e. there is no DC transport. A generalization to conductors with several contacts which permit DC transport will be given below. If the electro-chemical potentials are held constant as function of time we have an equilibrium system of electrons interacting via long-range Coulomb forces. The equilibrium electrostatic potential U of this system is a complicated function of position r and is a function of the electro-chemical potentials μ_k ,

$$U([\mu_k], \boldsymbol{r}). \tag{1}$$

A small variation $d\mu_k$ of the electro-chemical potentials will bring us from the equilibrium state with potential given by equation (1) to a new equilibrium state with potential

$$U([\mu_k + \mathrm{d}\mu_k], \mathbf{r}). \tag{2}$$

We are interested in the differential capacitance and hence investigate the difference in the potentials $U([\mu_k + d\mu_k], r) - U([\mu_k], r)$. We expand this potential difference with respect to the variations of the electro-chemical potentials

$$e \,\mathrm{d}U([\mu_k], \boldsymbol{r}) = \sum_k u_k(\boldsymbol{r}) \,\mathrm{d}\mu_k. \tag{3}$$

Here we have introduced the characteristic potential functions

$$u_k(\boldsymbol{r}) = e \, \mathrm{d} U([\mu_k], \boldsymbol{r}) / \mathrm{d} \mu_k|_{\mathrm{d} \mu_k = 0}.$$

Figure 2 depicts the conduction band bottom and electro-chemical potentials for two capacitors. Figure 2 illustrates the variation of the conduction band bottom given by $u_1(r) d\mu_1$ in response to an increase in the electro-chemical potential of reservoir 1. The characteristic potential functions have the following interesting properties.

(1) For r deep in reservoir k the local potential must follow the electro-chemical potential of that reservoir and hence $u_k(r) = 1$.



Figure 2. Conduction band bottom eU(r) and electro-chemical potentials of two capacitors connected via leads to reservoirs. An increment $d\mu_1$ of the electro-chemical potential at contact 1 changes the potential landscape across the capacitor by $u_1(r) d\mu_1$. The characteristic potential function $u_1(r)$ is 1 deep inside reservoir 1 and vanishes in reservoir 2.

(2) A change in the electro-chemical potential of reservoir k cannot affect the potential deep inside any other reservoir. Thus for r deep inside reservoir $l \neq k$, the characteristic function must vanish, $u_k(r) = 0$.

(3) If we change all electro-chemical potentials simultaneously and by an equal amount $d\mu_k = d\mu$ then we have only changed our (global) energy scale. Hence at every space point r the potential U must also change by $d\mu$. This implies that the sum of all characteristic functions at every space point is equal to 1,

$$\sum_{k} u_k(\mathbf{r}) = 1. \tag{4}$$

The three properties of the characteristic functions u_k are important and will frequently be used below. To specify the characteristic functions in detail and in order to be able to calculate a capacitance we must now consider the changes in the electron density distribution which accompany a change in the electro-chemical potentials.

The changes in the electron density $dn_k(r)$ of conductor k consist of two contributions. A variation of the electro-chemical potential $d\mu_k$ can be achieved either by a variation of the chemical potential or by a variation of the electrostatic potential. An increment $d\mu_k$ at fixed electrostatic potential injects an additional carrier density $(dn(r, k)/dE) d\mu_k$ into the conductor k. The coefficient dn(r, k)/dE is the effective (temperature dependent) density of states of conductor k. It is calculated for non-interacting carriers which are subject to the effective one-electron potential of the reference state specified by equation (1). The carriers which contribute to this density are injected from contact k. Thus dn(r, k)/dEcharacterizes the injection properties of this contact and we will also refer to this quantity as the *injectivity* of contact k. The excess carriers injected into the various conductors give rise to a long-range Coulomb potential. This electro-static potential induces a density $dn_{ind,k}(r)$ into conductor k. Thus the total density in conductor k is The induced density $dn_{ind,k}(r)$ generated by a potential variation dU(r) can be specified by the Lindhard [17] function $\Pi_k(r, r')$,

$$dn_{ind,k}(r) = -\int d^3r' \Pi_k(r,r') e \, dU(r') = -\sum_l \int d^3r' \Pi_k(r,r') u_l(r') \, d\mu_l.$$
(6)

The second equation is obtained by expressing the potential variation in terms of the characteristic potential functions introduced above. In equation (6) the volume integrals can be taken over all space enclosed by the surface S. (This convention applies also to subsequent volume integrals in this work.) We will not give a detailed description of a classical or quantum mechanical calculation of the Lindhard function. It is a density-density correlation function which is long ranged if we deal with a conductor described by extended states [14] and is short ranged if we deal with a conductor which near the Fermi energy consists mostly of localized states. Fortunately, to make progress we only need a few properties of this response function which are a consequence of the charge neutrality of our system and are a consequence of microreversibilty. With the help of equation (6) we can express the total density variation (equation (5)) in conductor k as a function of the electro-chemical potential changes

$$\mathrm{d}n_k(\mathbf{r}) = (\mathrm{d}n(\mathbf{r},k)/\mathrm{d}E)\,\mathrm{d}\mu_k - \sum_l \int \mathrm{d}^3 r' \,\Pi_k(\mathbf{r},\mathbf{r}') u_l(\mathbf{r}')\,\mathrm{d}\mu_l. \tag{7}$$

From equations (7) and (4) we conclude that the invariance of the charge distribution under simultaneous changes in all electro-chemical potentials implies that the integral over the second spatial argument of the Lindhard function is equal to the injectivity of reservoir k,

$$dn(\mathbf{r},k)/dE = \int d^3r' \Pi_k(\mathbf{r},\mathbf{r}').$$
(8)

Equation (8) can be viewed [18] as an Einstein relation which connects the density response to a chemical potential variation (left-hand side of equation (8)) to the density response to an electro-static potential variation (right-hand side of equation (8)). Next we introduce the density obtained by integrating the Lindhard function over the first argument

$$dn(k,r)/dE = \int d^3r' \Pi_k(r',r).$$
(9)

Equation (9) gives the density of states at point r of carriers which will exit the conductor through contact k. We call this density of states the emissivity of contact k. The Coulomb energy of two charge densities dn(r) and dn(r') is equal to e dn(r) dU(r) or e dn(r') dU(r'), where dU(r) is the potential generated by dn(r') and dU(r') is the potential generated by dn(r). As a consequence, the Lindhard function is symmetric in its arguments, $\Pi_k(r', r) = \Pi_k(r, r')$. Hence the injectivity and emissivity are identical, dn(r, k) = dn(k, r). The density response described by the Lindhard function is a consequence of a change in the equilibrium potential. Since an equilibrium density is an even function of magnetic field, the Lindhard function is also an even function of the magnetic field, $\Pi_k(B, r', r) = \Pi_k(-B, r', r)$. For the conductor of figure 1 this has the consequence that all elements of the capacitance matrix (which we derive below) are even functions of the magnetic field. We emphasize that these symmetry properties are characteristic for conductors connected to a single reservoir.

So far we have discussed the induced densities in the conductor. In the insulator (index k = 0) separating the capacitors, a potential variation can polarize the insulator and induce a charge density

$$\mathrm{d}n_{\mathrm{ind},0}(\boldsymbol{r}) = -\int \mathrm{d}^3 r' \Pi_0(\boldsymbol{r},\boldsymbol{r}') e \,\mathrm{d}U(\boldsymbol{r}').$$

No external charges reach the insulating region and thus instead of equation (7) we find that the volume integral of the Lindhard function over either the first or the second argument vanishes

$$\int \mathrm{d}^3 r' \Pi_0(\boldsymbol{r},\,\boldsymbol{r}') = \int \mathrm{d}^3 r' \Pi_0(\boldsymbol{r}',\,\boldsymbol{r}) = 0.$$

Now we write down Poisson's equation for the potential U. If we differentiate U with respect to $d\mu_k$ we find that the characteristic function u_k is determined by

$$-\Delta u_k(r) + 4\pi e^2 \int d^3r' \sum_{l=0}^{l=N} \Pi_l(r,r') u_k(r') = 4\pi e^2 (dn(r,k)/dE).$$
(10)

Note that equation (10) contains the sum of all Lindhard functions of all the conductors k = 1, 2, ..., N and of the insulating region k = 0. The density of states of conductor k plays the role of a source term for the characteristic function u_k . Let us for a moment replace the source term by a test charge $e\delta(r - r_0)$ which is concentrated at one point r_0 . Then the solution to equation (10) is Green's function $g(r, r_0)$. With the help of Green's function we find for the characteristic function

$$u_{k}(\mathbf{r}) = \int d^{3}r'g(\mathbf{r},\mathbf{r}')(dn(\mathbf{r}',k)/dE) = \int d^{3}r' \int d^{3}r''g(\mathbf{r},\mathbf{r}')\Pi_{k}(\mathbf{r}',\mathbf{r}'').$$
(11)

Equation (4) implies for Green's function the property

$$\int d^{3}r'g(r,r') \sum_{k} (dn(r',k)/dE) = 1.$$
(12)

The total charge in conductor k is

$$\mathrm{d}Q_k = e \int \mathrm{d}^3 r[(\mathrm{d}n(r,k)) \,\mathrm{d}\mu_k + \mathrm{d}n_{\mathrm{ind},k}(r)]. \tag{13}$$

Overall charge neutrality of our assembly of conductors implies that the sum of all induced charges plus the test charge is zero, $\sum_k dQ_{ind,k} + e = 0$. This implies

$$\sum_{k} \int d^{3}r' (dn(k, r')/dE)g(r', r) = 1.$$
(14)

Equations (12) and (14) will be used to demonstrate charge and current conservation of the results derived below.

3. The capacitance matrix

We are now ready to calculate the capacitance coefficients. Using equations (7) and (11), the total charge (equation (13)) in conductor k can be expressed in terms of the density of states and Green's function. Differentiating the total charge dQ_k with respect to the voltage $dV_l = d\mu_l/e$ gives a capacitance $C_{kl} = e dQ_k/d\mu_l$ given by

$$C_{kl} = e^2 \int d^3r \int d^3r' (dn(k, r)/dE) \left[\delta_{kl} \delta(r - r') - g(r, r') (dn(r', l)/dE) \right].$$
(15)

Equation (15) is a key result of this paper. To arrive at this result we have in the diagonal term C_{kk} replaced $\int d^3r(dn(r,k)/dE)$ by $\int d^3r(dn(k,r)/dE)$. These integrated densities are equal independent of whether a magnetic field is applied or not. Equation (15) expresses the capacitances in terms of the density of states of non-interacting electrons and the Green's function which mediates interactions. The diagonal capacitances C_{kk} are positive. The off-diagonal capacitances (also called coefficients of inductance) are negative. On account of

equation (12) the sum over all capacitance matrix elements in a row is zero, $\sum_{l} C_{kl} = 0$, and due to equation (14) the sum over all elements in the column of the capacitance matrix is zero.

To gain some insight into the magnitude of the effect discussed here we consider a few simple but (exactly) solvable examples. Two metallic conductors of large cross section A fill the half spaces x > a/2 and x < -a/2. Neglecting fringe fields we can treat this as a one-dimensional problem. The density of states of the conductors are taken to be uniform right up to the surfaces. Screening is treated in the Thomas-Fermi approximation: the density is locally related to the potential, $dn_{ind,k}(r) = -(dn(k, r)/dE)eU(r)$ which is equivalent to taking $\Pi_k(r, r') = \delta(r - r')dn(k, r')/dE$. We have a Thomas-Fermi screening length $\lambda_1^{-2} = 4\pi e^2 dn_1/dE$ for the conductor to the left and a screening length $\lambda_2^{-2} = 4\pi e^2 dn_2/dE$ for the conductor to the right. For this simple case, Green's function and the characteristic functions can be calculated exactly. The characteristic potential functions are shown in figure 3. The capacitance $C \equiv C_{11} = C_{22} = -C_{21} = -C_{12}$ is

$$A/C = 4\pi(a + \lambda_1 + \lambda_2) \tag{16}$$

the geometrical capacitance in series with two quantum capacitors determined by the Thomas–Fermi screening lengths. Clearly the corrections to the geometrical capacitance are a consequence of the fact that the induced potential penetrates the conductors over a distance of order of a Thomas–Fermi screening length. The corrections have a simple interpretation. They are the product of the density of states multiplied by the surface volume penetrated by the electric field. The relevant surface volume for this example is the Thomas–Fermi screening length times the surface area A. Indeed equation (16) can be written in the form

$$\frac{1}{C} = \frac{4\pi a}{A} + \frac{1}{e^2 (dn_1/dE)\lambda_1 A} + \frac{1}{e^2 (dn_2/dE)\lambda_2 A}.$$
(17)

We emphasize that equation (17) only gives a lower estimate of the corrections of the geometrical capacitance. In reality the density of the conductor tends to zero continuously as the surface of the conductor is approached and hence cannot immediately screen out the induced field with the bulk screening length.

Another simple example consists of two-dimensional conductors lying in the y-zplane at x = -a/2 and x = +a/2. Their density of states is a two-dimensional sheet density $d\sigma_{1,2}/dE$. The three-dimensional effective densities are given by $dn_{1,2}(r) = \delta(x \pm a/2)(d\sigma_{1,2}/dE)(\mu_{1,2} - eU_{1,2}(\pm a/2))$ where $\mu_{1,2}$ are the electro-chemical potentials and $U(\pm a/2)$ is the potential U at x = -a/2 and x = +a/2. A two-dimensional gas (much smaller in thickness than the Thomas-Fermi screening length) cannot screen the potential. U(x) is a continuous function. The characteristic functions $u_{1,2}$ will not take on the value 1 and zero in these two conductors. With the lengths $\lambda_{1,2} = (4\pi e^2(d\sigma_{1,2}/dE))^{-1}$ we find $u_1 = (a + \lambda_2)/(a + \lambda_1 + \lambda_2)$ for x < -a/2 and find $u_1 = \lambda_2/(a + \lambda_1 + \lambda_2)$ for x > a/2. The capacitance is

$$\frac{1}{C} = \frac{4\pi a}{F} + \frac{1}{e^2(d\sigma_1/dE)F} + \frac{1}{e^2(d\sigma_2/dE)F}$$
(18)

where F is the area of the two-dimensional conductors. Again the geometrical capacitance is in series with two capacitances determined by the density of states of the electron gases. Note that in the discussion of this example we have not explicitly described the contacts (reservoirs) connected to the two-dimensional conductors. It is only in the bulk of the contacts where we can expect the characteristic potential functions to approach 1.



Figure 3. Characteristic functions u_1 and u_2 for two bulk conductors with density of states dn_1/dE and dn_2/dE .

As a third example we consider a two-dimensional electron gas between two bulk conductors. This geometry was also considered in [12]. The bulk conductors labelled k = 1 and k = 2 fill the space x < -a/2 and x > a/2 and the two dimensional conductor k = 3 is at x = 0. Unlike the previous examples which could be characterized by a single capacitance, this structure needs to be described by a capacitance matrix. For simplicity we neglect the penetration of the field into the bulk conductors. The most important effect is the lack of screening of the two-dimensional electron gas. As in the previous example we describe the two-dimensional electron gas with a density of states $dn(r)/dE = \delta(x)(d\sigma/dE)(\mu_3 - eU(0))$ and a length $\lambda = (4\pi e^2(d\sigma/dE))^{-1}$. The three characteristic functions u_k which need to be calculated are depicted in figure 4. Note that the three characteristic functions add up to one. The resulting capacitance matrix is

$$(4\pi/F)\mathbf{C} = \begin{pmatrix} \left(\frac{1}{a+a^2/4\lambda} + \frac{1}{a/2+2\lambda}\right) & -\frac{1}{a+a^2/4\lambda} & -\frac{1}{a/2+2\lambda} \\ -\frac{1}{a+a^2/4\lambda} & \left(\frac{1}{a+a^2/4\lambda} + \frac{1}{a/2+2\lambda}\right) & -\frac{1}{a/2+2\lambda} \\ -\frac{1}{a/2+2\lambda} & -\frac{1}{a/2+2\lambda} & \frac{2}{a/2+2\lambda} \end{pmatrix}.$$
 (19)

In the limit of a small density of states of the two-dimensional electron gas, $\lambda \to \infty$, the capacitance matrix is $\mathbf{C} = C_{11} = C_{22} = -C_{12} = -C_{21} = 4\pi F/a$. All other capacitance elements of the matrix vanish. In the limit of a very large density of states of the two-dimensional electron gas, $\lambda \ll a$, the mutual capacitance of the bulk conductors vanishes $C_{12} = C_{21} \to 0$ and the non-vanishing elements of the capacitance matrix have magnitude $8\pi F/a$.

The simple examples we have presented illustrate that capacitances are electro-chemical entities which depend on the properties of the conductor. If the conductors are placed in a magnetic field the capacitances through the density of states become symmetric functions of the applied field. In our discussion of the examples we have analysed field penetration M Büttiker



Figure 4. Characteristic functions u_k , k = 1, 2, 3 for a two-dimensional electron gas with sheet density of states $d\sigma/dE$ between two conductors with density of states dn_1/dE and dn_2/dE . Field penetration into the bulk conductors is neglected.

into the conductors only with the help of a Thomas-Fermi approximation. Our central result (equation (15)) is more general and can be used to investigate more subtle effects. The Lindhard function incorporates exchange effects and at large distances decays only algebraically [14]. There will, therefore, be long-range effects which stem from the algebraic decay of the Lindhard function. The possibility that the thermodynamic density of states $dn/d\mu$ is negative has been reported and linked to interaction properties of the electron gas [19].

A number of additional effects are possibly worth investigating. A small mesoscopic capacitor with a more complicated topology, for instance with a hole penetrated by an Aharonov–Bohm flux, will exhibit a flux-dependent capacitance. Capacitance spectroscopy of small islands leads to an effective capacitance which depends on the Coulomb blockade of the small island. We will not discuss these possibilities further here, but will now investigate the case where one or more of the electro-chemical potentials exhibits time-dependent oscillations away from an equilibrium value.

4. Admittance

In the presence of slowly oscillating potentials $d\mu_k(\omega) \exp(-i\omega t)$ the assembly of conductors is driven through the sequence of equilibrium states $U([\mu_k(t)], r)$. For slowly varying electro-chemical potentials, the time dependence of U is determined by replacing the equilibrium electro-chemical potentials μ_k by the time-dependent electro-chemical potentials $\mu_k(t) = \mu_k + d\mu_k(t)$. The quasi-stationary voltage distribution away from the reference state is

$$e \,\mathrm{d}U(\boldsymbol{r},t) = \sum_{k} u_{k}(\boldsymbol{r}) \,\mathrm{d}\mu_{k}(t). \tag{20}$$

From the relation between charges and electro-chemical potentials $dQ_k = \sum_l C_{kl} (d\mu_l/e)$ we directly obtain the leading-order terms of the admittance

$$I_k(\omega) = -\mathrm{i}\omega \,\mathrm{d}Q_k = -\mathrm{i}\omega \sum_l C_{kl} (\mathrm{d}\mu_l(\omega)/e)$$

or

$$g_{kl}(\omega) = eI_k(\omega)/d\mu_l(\omega) = -i\omega C_{kl}.$$
(21)

Below we discuss within the framework of a scattering theory of electrical conductance an approach which gives this result. But first we generalize the discussion given above to the case where there are conductors with several contacts.

The typical experimental arrangement consists of a number of conductors some of which are connected to several reservoirs. Different conductors are labelled by arabic numeral indices k, l = 1, 2, 3, ... The contacts of conductor k are labelled by Greek indices $\alpha, \beta = 1, 2, 3, 4$. First consider the capacitance matrix for the case that all electro-chemical potentials of conductor k are varied in synchronism, $d\mu_{k\alpha} = d\mu_k$. Then the discussion given above is readily generalized. To each contact $k\alpha$ there belongs a characteristic function $u_{k\alpha}$. Since the electro-chemical potentials at each conductor are the same we again have an equilibrium problem. The contributions of the characteristic functions are additive and the capacitance coefficients are

$$C_{kl} = e^2 \int \mathrm{d}^3 r \mathrm{d}^3 r' \sum_{\alpha} \frac{\mathrm{d}n(k\alpha, r)}{\mathrm{d}E} \left(\delta_{kl\alpha\beta} \delta(r - r') - g(r, r') \sum_{\beta} \frac{\mathrm{d}n(r', l\beta)}{\mathrm{d}E} \right).$$
(22)

A novel situation arises if we now permit the electro-chemical potentials at different contacts of conductor k to oscillate independently. In the presence of slowly oscillating electrochemical potentials, $d\mu_{k\alpha}(t)$, a quasi-stationary non-equilibrium potential distribution is established. For slowly oscillating electro-chemical potentials, the potential distribution inside the sample is governed by the time dependence of the external potentials and is given by

$$e \,\mathrm{d}U(\mathbf{r},t) = \sum_{k\alpha} u_{k\alpha}(\mathbf{r}) \,\mathrm{d}\mu_{k\alpha}(t). \tag{23}$$

Now there are two main differences in the admittance compared to equation (21). First, the admittance matrix also contains zero-frequency terms which are just the DC conductances,

$$dI_{k\alpha}(\omega) = \sum_{\beta} g_{k\alpha\beta}(0) (d\mu_{k\beta}(\omega)/e).$$
(24)

The DC conductances [7] $g_{k\alpha\beta}(0)$ can be expressed in terms of transmission probabilities $T_{k\alpha\beta}$ for carriers incident in contact $k\beta$ to reach contact $k\alpha$. As in DC transport the transmission probabilities (and reflection probabilities) are a function of the equilibrium (reference) potential $T_{k\alpha\beta}(U([\mu_k], r))$. The potential distribution (equation (23)) which forms as a consequence of transport plays no role in the evaluation of the transmission probabilities. But the transport potential distribution is essential if we want to find the leading-order term proportional to ω of the frequency-dependent admittance.

If transmission is permitted from one contact to another a change in electro-chemical potential at one of the contacts will not only cause capacitive effects but also purely kinetic effects. To discuss the response to a slowly oscillating potential we first give a different interpretation of the capacitance coefficients. The density of states $(dn(r, l\beta)/dE)$ which appears in equation (22) gives the density per unit energy of carriers at point r in response to a potential change at contact β in conductor l. This density is characteristic of the injection properties of contact β as viewed from a point r inside conductor l. We will henceforth

call this density of states the *injectivity* of contact β and will call the integrated density $\int d^3r(dn(r, l\beta)/dE)$ the *injectance* of contact β . The density of states $(dn(k\alpha, r)/dE)$ gives the number of carriers per unit energy which after being emitted from point r reach contact α in conductor k. Thus this density of states can be viewed as the *emissivity* into contact α of a source at point r. The integrated emissivity of charge

$$\mathrm{d}Q_{k\alpha}/\mathrm{d}E = e\int\mathrm{d}^3r\mathrm{d}n(k\alpha,r)/\mathrm{d}E$$

is the *emittance* into contact α of the conductor k. We now see that the capacitance coefficients $C_{kl\alpha\beta}$ are a measure of the change in emittance of contact $k\alpha$ in response to an electro-chemical potential variation at contact $l\beta$. It is the concept of emittance which is easily generalized to the situation, where we permit a number of contacts on each conductor.

A small oscillation of the electro-chemical potential $\mu_{l\beta}(t)$ injects a charge density $e(dn(r, l\beta)/dE)d\mu_{l\beta}(t)$ into conductor *l*. A fraction of the carriers which reach point r will eventually reach (through transmission or reflection) contact $k\alpha$. These carriers have a density of states $\delta_{kl}(dn(k\alpha, r, l\beta)/dE)$. The Kronecker delta function takes into account that direct transmission can only occur within the same conductor. Furthermore, the unscreeened density of external charges can change the emittance of contact $k\alpha$ via long-range Coulomb forces. Of course this effect occurs even if there is no transmission from contact $l\beta$ to contact $k\alpha$. The charge emissivity of contact $k\alpha$ due to Coulomb forces is $e(dn(k\alpha, r)/dE)u_{l\beta}(r) d\mu_{l\beta}(t)$, or, if we use the characteristic function expressed with the help of Green's function, equation (11),

$$e(\mathrm{d}n(k\alpha,\mathbf{r})/\mathrm{d}E)\int\mathrm{d}^{3}r'g(\mathbf{r},\mathbf{r}')e(\mathrm{d}n(\mathbf{r}',l\beta)/\mathrm{d}E)\,\mathrm{d}\mu_{l\beta}(t).$$

Integrating these two contributions over the volume enclosed by S gives a charge emittance $E_{kl\alpha\beta} \equiv e \, dQ_{k\alpha}(t)/d\mu_{l\beta}(t)$ with

$$E_{kl\alpha\beta} = e^2 \delta_{kl} \int d^3 r (dn(k\alpha, \mathbf{r}, l\beta)/dE) -e^2 \int d^3 r \int d^3 r' (dn(k\alpha, \mathbf{r})/dE) g(\mathbf{r}, \mathbf{r}') (dn(\mathbf{r}', l\beta)/dE).$$
(25)

If we oscillate the potentials slowly, equation (25) predicts that a current $-i\omega Q_{k\alpha}$ leaves the conductor k at contact α . For small frequencies the admittance $g_{kl\alpha\beta}(\omega) = e dI_{k\alpha}(\omega)/d\mu_{l\beta}(\omega)$ is given by the DC conductance and the emittance

$$g_{kl\alpha\beta}(\omega) = \delta_{kl}g_{k\alpha\beta}(0) - i\omega E_{kl\alpha\beta} + O((\omega)^2).$$
⁽²⁶⁾

The first term in equation (25), since it is integrated over the volume, can also be written as $e^{2}\delta_{kl}(dN_{kl\alpha\beta}/dE)$, i.e. a density of states of carriers injected in contact $k\beta$ reaching contact $k\alpha$. It is a purely kinetic term and, if it dominates the Coulomb term (second term in equation (25)), gives a current response which lags behind the voltage. If $e^{2}\delta_{kl}(dN_{kl\alpha\beta}/dE)$ is small compared to the second term of equation (25), the emittance is similar to a capacitance. It should be noted that the admittance given by equation (26) is current conserving, i.e. $\sum_{l\beta} g_{kl\alpha\beta}(\omega) = 0$ and $\sum_{k\alpha} g_{kl\alpha\beta}(\omega) = 0$.

As a simple example consider the quantum point contact [2, 3] shown in figure 5 with contacts labelled 1 and 2 formed with the help of split gates labelled 3 and 4. (For simplicity we label all reservoirs in sequence and use only arabic numeral indices.) Suppose we oscillate the gate voltage μ_3 . There is of course no transmission from this gate to the conductor. The current at contact 1 of the conductor is determined by E_{13} . But the first term in equation (25) is zero and $E_{13} = C_{13}$ describes purely capacitive coupling between the





Figure 5. Quantum point contact formed with the help of a split gate. The emittance matrix for this structure is given by equation (27).

two conductors. Similarly the current induced into contact 2 is purely capacitive $E_{23} = C_{23}$. By reciprocity if we oscillate the electro-chemical potentials at either contact 1 or 2, the current induced into contact 3 is purely capacitive $E_{31} = C_{31}$, $E_{32} = C_{32}$. In contrast, the current at contact 1 and 2 in response to an oscillating potential at contact 1 contains a kinetic contribution and is determined by the full emittance given by equation (25). Thus the matrix of transport coefficients multiplying $-i\omega$ in equation (26) is given by

$$\mathbf{E} = \begin{pmatrix} E_{11} & E_{12} & C_{13} & C_{14} \\ E_{21} & E_{22} & C_{23} & C_{24} \\ C_{31} & C_{32} & C_{33} & C_{34} \\ C_{41} & C_{42} & C_{43} & C_{44} \end{pmatrix}.$$
(27)

Current conservation requires that the coefficients in each row and in each column of this matrix add up to zero. Thus the sum of the two emittances in each row or column of equation (27) is always a capacitance.

Next we connect the results given above with the discussion of admittances of small conductors given by Büttiker, Thomas and Prêtre [21, 13]. According to these authors the admittance is determined by the sum of the response to an external potential and the internal electrical potential. We assume that deep in the reservoirs the Hamiltonian is separable into longitudinal motion and quantized transverse motion. This separable region permits the definition of incident and out-going quantum scattering channels. The scattering properties of conductor k are assumed to be given in terms of scattering matrices $s_{k\alpha\beta}$ which give the current amplitudes at contact α in response to the incident current amplitudes in contact β . The response to an (external) electro-chemical potential to leading order in ω is [21, 13, 22]

$$g^{\mathbf{e}}_{kl\alpha\beta}(\omega) = -\mathrm{i}e^2\omega\delta_{kl}(\mathrm{d}N_{k\alpha\beta}/\mathrm{d}E). \tag{28}$$

Here the density of states in terms of the scattering matrix of conductor k is given by $dN_{k\alpha\beta}/dE \equiv \int d^3r (dn(k\alpha, r, k\beta)/dE)$ is

$$\frac{\mathrm{d}N_{k\alpha\beta}}{\mathrm{d}E} = \frac{1}{4\pi\mathrm{i}} \int \mathrm{d}E \left(-\frac{\mathrm{d}f}{\mathrm{d}E}\right) \,\mathrm{Tr}\left[s_{k\alpha\beta}^{\dagger}(E)\frac{\mathrm{d}s_{k\alpha\beta}(E)}{\mathrm{d}E} - \frac{\mathrm{d}s_{k\alpha\beta}^{\dagger}(E)}{\mathrm{d}E}s_{k\alpha\beta}(E)\right].$$
(29)

To find the response to an induced oscillating electric potential we consider the scattering matrix as a *functional* of the electric potential $s_{k\alpha\beta}(E, U([\mu_{k\alpha}(t)], r))$. For small frequencies, carriers see the instantaneous potential. We can expand U away from its equilibrium value

$$U([\mu_{k\alpha}(t)], \mathbf{r}) = U([\mu_{k\alpha}], \mathbf{r}) + \sum_{l\beta} u_{l\beta}(\mathbf{r}) \,\mathrm{d}\mu_{l\beta}(t)$$

where the $u_{l\beta}$ are the static characteristic potential functions. The current response to the internal potential is then found by expanding the scattering matrix away from the time-independent equilibrium reference state. A calculation gives [22]

$$g^{i}_{kl\alpha\beta}(\omega) = ie^{2}\omega \int d^{3}r (dn(k\alpha, r)/dE)u_{l\beta}(r)$$
(30)

with a density of states

$$\frac{\mathrm{d}n(k\alpha,\mathbf{r})}{\mathrm{d}E} = -\frac{1}{4\pi\mathrm{i}}\int\mathrm{d}E\left(\frac{-\mathrm{d}f}{\mathrm{d}E}\right)\sum_{\beta}\mathrm{Tr}\left[s_{k\alpha\beta}^{\dagger}(E)\frac{\delta s_{k\alpha\beta}(E)}{\delta eU(\mathbf{r})} - \frac{\delta s_{k\alpha\beta}^{\dagger}(E)}{\delta eU(\mathbf{r})}s_{k\alpha\beta}(E)\right].$$
(31)

Note that the response to the internal potential (equation (30)) is proportional to the frequency ω . A static change in the internal potential leads from an equilibrium potential to another equilibrium potential. However, a static equilibrium potential cannot give rise to a current. Since the internal response is already proportional to the frequency the leading-order terms of the admittance are determined by the quasi-stationary potential distribution. Using equation (11) leads to the internal response

$$g_{kl\alpha\beta}^{i}(\omega) \equiv ie^{2}\omega \int d^{3}r \int d^{3}r' (dn(k\alpha, r)/dE)g(r, r') \frac{dn(r', l\beta)}{dE}.$$
 (32)

Taking into account that the total response of the system is the sum of the internal and external response, we find for the admittance to leading order in ω the result given by equation (26) with an emittance given by equation (25).

Equation (31) expresses the emissivity into contact $k\alpha$ in terms of the scattering matrix and its functional derivaties. The injectivity of contact $k\alpha$, $(dn(r, k\alpha)/dE)$ is given by an expression similar to equation (31) but with the indices α and β of the scattering matrix interchanged. Microreversibility [20] implies for the scattering matrix $s_{k\alpha\beta}(B, E) = s_{k\beta\alpha}(-B, E)$. Consequently, for a conductor with several contacts we have in general a reciprocal relationship between injectivites and emissivites $(dn(B, r, k\alpha)/dE) =$ $(dn(-B, k\alpha, r)/dE)$. Similarly the Lindhard functions $\prod_{k\alpha}(r, r')$, which give the induced density of mobile carriers which eventually reach contact $k\alpha$ are not even functions of the magnetic field. But Green's function is determined by the sum of all Lindhard functions which is again an even function of magnetic field. Consequently, the symmetry under magnetic field reversal of the chracteristic functions $u_{k\alpha}$ is determined by the source term of Poisson's equation, equation (10), i.e. by the injectivities. As a consequence the emittance is not an even function of magnetic field but obeys the reciprocity relation $E_{kl\alpha\beta}(B) = E_{lk\beta\alpha}(-B)$. For the conductor of figure 5 with the emittance matrix given by equation (27) this has the following interesting consequence: All diagonal coefficients of this matrix and in addition $C_{43} = C_{34}$ are even functions of the magnetic field. All other elements of this matrix contain, in addition to a term which is even, a term which is odd under magnetic field reversal. For instance, the capacitance coefficient C_{14} obeys $C_{14}(B) = C_{41}(-B)$ and in general contains terms which are odd under magnetic field reversal. Clearly the measurement of capacitance terms which are odd under magnetic field reversal would be an interesting experimental test of the ideas presented here.

5. Rectification properties

The non-linear current voltage characteristic of a small conductor [23] can also be represented in terms of an external response and a response to an internal potential like the capacitances and admittances discussed above. Non-linearites in metallic mesoscopic samples have been analysed by Al'tshuler and Khmelnitskii [24] using diagramatic techniques without a self-consistent potential. For transmission through a tunnel contact the effect of a potential which changes with increasing applied bias has been investigated by Frenkel [25]. Landauer has pointed to the necessity of a self-consistent treatment of the internal potential [26]. Below we derive the current-voltage characteristic taking into account non-linearities which are a consequence of the increase of the external electrochemical potential differences as well as the changing internal (self-consistent) potential We focus on the leading non-linear correction of the low-voltage ohmic distribution. behaviour of the sample. The I-V characteristic of a mesoscopic sample is rectifying, $I(V) \neq -I(-V)$. Furthermore, since rectification also depends on the internal potential, and since the internal potential in conductor k depends on the charge distribution of other nearby conductors, the rectification properties of a small sample are dependent on its entire electric environment.

To proceed we start again by viewing the scattering matrices as a functional of the potential distribution $s_{k\alpha\beta}(E, U([\mu_{k\alpha}], r))$ and expand U away from the equilibrium potential distribution. The scattering matrix in the neighbourhood of the equilibrium reference state (index 0) is

$$s_{k\alpha\beta}(E, eU(r)) = s^0_{k\alpha\beta}(E) + \int \mathrm{d}^3 r' (\delta s^0_{k\alpha\beta}(E) / \delta eU(r')) e \,\mathrm{d}U(r').$$

Here e dU(r) can now again be expressed in terms of the characteristic potential functions and the electro-chemical potentials of the reservoirs. The total current at probe $k\alpha$ is

$$I_{k\alpha} = (e/h) \sum_{\beta} \int dE (f_{k\beta} - f_{k0}) \operatorname{Tr} \left[\mathbf{1}_{k\alpha}(E) \delta_{\alpha\beta} - s^{\dagger}_{k\alpha\beta}(E, U(r)) s_{k\alpha\beta}(E, U(r)) \right]$$
(33)

where f_{k0} is the Fermi function of the equilibrium reference state in conductor k. To insert the Fermi function of the reference state we have made use of the unitarity of the **s**-matrix. The coefficients in equation (33) summed over β or α add up to zero. To proceed we now expand equation (33) in powers of the electro-chemical potential deviations $d\mu_{\alpha}$ from the equilibrium reference state. We find for the current at contact α in conductor k

$$I_{k\alpha} = \sum_{\beta} g_{k\alpha\beta} (\mathrm{d}\mu_{k\beta}/e) + (1/2) \sum_{lm\beta\gamma} g_{klm\alpha\beta\gamma} (\mathrm{d}\mu_{l\beta}/e) (\mathrm{d}\mu_{m\gamma}/e). \tag{34}$$

The terms linear in the electro-chemical potentials are determined by the DC conductances

$$g_{k\alpha\beta} = (e^2/h) \int \left(-\frac{\mathrm{d}f}{\mathrm{d}E}\right) \operatorname{Tr}\left[\mathbf{1}_{\alpha\beta} - s^{\dagger}_{k\alpha\beta}(E)s_{k\alpha\beta}(E)\right]$$

which are a functional of the equilibrium reference potential only. The leading-order nonlinear terms are given by transport coefficients which are composed of an external response and an internal response $g_{klm\alpha\beta\gamma} = g^{e}_{klm\alpha\beta\gamma} + g^{i}_{klm\alpha\beta\gamma}$. The external response arises from the expansion of the Fermi functions in powers of the electro-chemical potentials and is given by

$$g_{klm\alpha\beta\gamma}^{e} = -\left(\frac{e^{3}}{h}\right)\delta_{kl}\delta_{km}\delta_{\beta\gamma}\int dE\left(-\frac{df_{k0}}{dE}\right)\operatorname{Tr}\left[s_{k\alpha\beta}^{\dagger}(E)\frac{ds_{k\alpha\beta}(E)}{dE} + \frac{ds_{k\alpha\beta}^{\dagger}(E)}{dE}s_{k\alpha\beta}(E)\right].$$
(35)

The internal response is a consequence of the change in the potential distribution and is given by

$$g_{klm\alpha\beta\gamma}^{i} = -\left(\frac{e^{3}}{h}\right)\delta_{kl}\int dE\left(-\frac{df_{k0}}{dE}\right)$$

$$\times \int d^{3}r \operatorname{Tr}\left[s_{k\alpha\beta}^{\dagger}(E)\frac{\delta s_{k\alpha\beta}(E)}{\delta eU(r)} + \frac{\delta s_{k\alpha\beta}^{\dagger}(E)}{\delta eU(r)}s_{k\alpha\beta}(E)\right]u_{m\gamma}(r)$$

$$-\left(\frac{e^{2}}{h}\right)\delta_{km}\int dE\left(-\frac{df_{k0}}{dE}\right)$$

$$\times \int d^{3}r \operatorname{Tr}\left[s_{k\alpha\gamma}^{\dagger}(E)\frac{\delta s_{k\alpha\gamma}(E)}{\delta eU(r)} + \frac{\delta s_{k\alpha\gamma}^{\dagger}(E)}{\delta eU(r)}s_{k\alpha\gamma}(E)\right]u_{l\beta}(r). \tag{36}$$

The linear terms are given by the DC conductances and depend only on the potential differences existing at conductor k. The non-linear terms in equation (34) depend on all deviations of electro-chemical potentials away from the reference state including the voltages applied to the capacitors (gates). We deal with a stationary state and there is no current at the contact leading away from a capacitor if the capacitor is connected to a single reservoir. For a conductor with a single contact the traces in equation (35) and equation (36) vanish. Nevertheless since an increase in voltage at a capacitor changes the entire potential landscape the non-linear properties of a conductor do depend on the potentials of nearby capacitors. The rectification properties of a conductor depend on other nearby conductors. By tuning the gate voltage of a nearby capacitor we can tune the I-V characteristic. The non-linear terms also conserve current since

$$\sum_{k\alpha} g_{klm\alpha\beta\gamma} = 0 \qquad \sum_{l\beta} g_{klm\alpha\beta\gamma} = 0 \qquad \sum_{m\gamma} g_{klm\alpha\beta\gamma} = 0 \qquad (37)$$

on account of the unitarity of the total scattering matrix and on account of equation (4). Moreover, since these coefficients are composed of both the non-linear response to external potentials and the non-linear response to internal potentials, a theory which would consider only one of these effects [27] cannot be current conserving. Equation (34) can, for instance, be used to investigate the departure of the Hall resistance away from quantized values in a high-mobility two-dimensional electron gas.

6. Discussion

Based on a derivation of the microscopic electric potential we have formulated microscopic expressions for the electro-chemical capacitance of highly structured conductors. The quasi-stationary potential determines the leading-order frequency-dependent terms of the admittance. The variation of the local potential also affects crucially the non-linear behaviour of a small mesoscopic conductor. To derive the local potential we have used a simple one-loop random-phase approximation. In this procedure all response functions are calculated exactly. However, the response is to a field which is treated classically. Clearly, many more sophisticated schemes are available to treat many electron problems. The scheme used here has the benefit that it leads to transparent results which appeal to our physical intuition. Even for this simple scheme definite answers for the transport coefficients, except in the most simple situations, can be obtained only by using computational tools. It is clearly desirable to extend the discussion presented here beyond the quasi-stationary limit. Reference [13] also discusses the charge relaxation resistances of a capacitor connected via leads to

reservoirs. Together with the electro-chemical capacitance these resistances determine the RC-time. But the charge relaxation requires knowledge of the time dependence of the voltage distribution beyond the quasi-stationary time dependence discussed here.

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