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Dynamic admittance of mesoscopic conductors: Discrete-potential model

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We present a discussion of the low-frequency admittance of mesoscopic conductors in close analogy with the scattering approach to dc conductance. The mesoscopic conductor is coupled via contacts and gates to a macroscopic circuit which contains ac-current sources or ac-voltage sources. We find the admittance matrix which relates the currents at the contacts of the mesoscopic sample and of nearby gates to the voltages at these contacts. The problem is solved in two steps: we first evaluate the currents at the sample contacts in response to the oscillating voltages at the contacts, keeping the internal electrostatic potential fixed. In a second stage an internal response due to the potential induced by the injected charges is evaluated. The self-consistent calculation is carried out for the simple limit in which each conductor is characterized by a single induced potential. Our discussion treats the conductor and the gates on equal footing. Since our approach includes all conductors on which induced fields can change the charge distribution, the admittance of the total response is current conserving, and the current response depends only on ac-voltage differences. We apply our approach to a mesoscopic capacitor for which each capacitor plate is coupled via a lead to an electron reservoir. We find an electrochemical capacitance with density-of-state contributions in series with the geometrical capacitance. The dissipative part of the admittance is governed by a charge-relaxation resistance which is a consequence of the dynamics of the charge pileup on the capacitor plates. We specialize on a geometry displaying an Aharonov-Bohm effect only at nonzero frequencies. For a double barrier with a well coupled capacitively to a gate the low-frequency admittance terms may have either sign, reflecting either a capacitive or a kinetic-inductive behavior. The validity of a second-quantization-current-operator expression which neglects spatial information is examined for perfect leads in both the frequency and the magnetic-field domain. [S0163-1829(96)06332-1]

I. INTRODUCTION

Investigation of the ac properties of electrical conductors provides important information on the internal charge and potential distribution of the sample. Pieper and Price[1] have measured the complex dynamic magnetoconductance of disordered mesoscopic rings, Chen *et al.*[2] have measured the magnetic-field symmetry of a capacitance tensor, and Kouwenhoven *et al.*[3] have observed the dependence of photon-assisted tunneling on the interaction with a microwave field. Theoretical studies of the frequency dependence of current-current correlation spectra[4–8] and of the current response to oscillating fields[9–26] have been carried out. In contrast to dc transport, which is fully characterized if the transmission probabilities are known, the ac-transport properties are sensitive to the *phases* of the scattering matrix elements. Derivatives of the scattering-matrix elements with respect to the energy are related to the charge injected into the conductor. In nonstationary conditions charge accumulation occurs and causes induced fields. Consequently a self-consistent treatment of the electron-electron interactions plays an important role. What is needed is an ac conductance which is charge and current conserving.[20,21] It is the purpose of this work to extend our earlier discussions,[19–21] and to provide some of the technical details omitted.

Our approach to the ac conductance of mesoscopic conductors is in a close conceptual analogy with the scattering approach to dc conduction, especially to the version which emphasizes coherent transmission from one electron reservoir to another.[27–29] To be definite we envisage a system of capacitively coupled mesoscopic conductors which may be defined with the help of gates (see Fig. 1). The conductors and gates are connected via electron reservoirs (contacts) to a

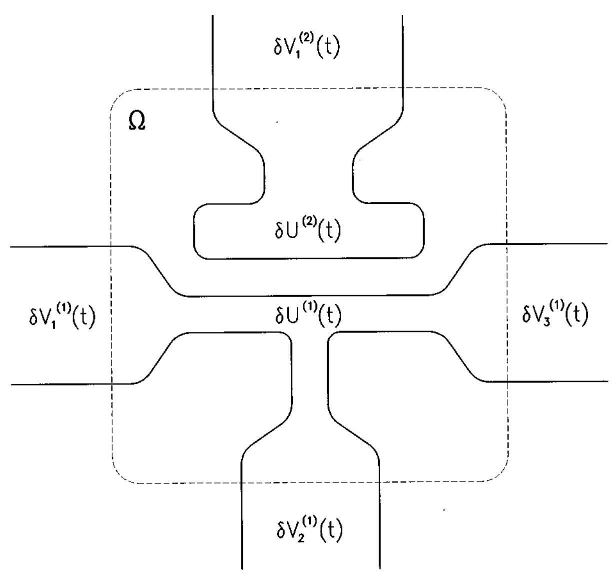

FIG. 1. A mesoscopic conductor with a nearby gate. The long-range Coulomb forces acting among different conductors ensure that the total charge in the volume Ω vanishes.

macroscopic circuit which contains ac-current and ac-voltage sources. Since in ac transport we can induce current from the conductor into the gates, and vice versa, it is necessary to treat all metallic constituents of the sample on equal footing. Consequently in the treatment given here, there is no distinction between conductors and gates. All constituents are considered as conductors. Each conductor may have an arbitrary number of contacts. We want to determine the current $\langle \delta I_{\alpha}^{(m)}(\omega)\rangle$ at contact α of conductor m in linear response to an oscillating voltage $\delta V_{\beta}^{(n)}(\omega)$ at contact β of conductor n,

$$\langle \delta I_{\alpha}^{(m)}(\omega)\rangle = \sum_{n\beta} g_{\alpha\beta}^{(mn)}(\omega)\,\delta V_{\beta}^{(n)}(\omega). \tag{1}$$

The theoretical task is to find an expression for the dynamical conductance coefficients (admittances) $g_{\alpha\beta}^{(mn)}(\omega)$. Everywhere in the system a stationary magnetic field is allowed: it is arbitrary inside the sample, and in each lead it is required to be constant and perpendicular to the lead.

In order to start from a conceptually clear situation we assume that all electric-field lines emanating from one of the conductors terminate at nearby conductors. Then a sufficiently large Gauss volume Ω (see Fig. 1) can be chosen[30] through which there is no electric flux. Consequently the total charge is conserved. Conservation of the overall charge on all conductors implies that the currents are conserved. Thus the columns of the admittance matrix must add up to zero. If the circuit is in an electrically insulating environment, then applying a uniform ac potential on the whole *external* circuit leads to an overall spatially uniform effective potential. This only affects the phases of the wave functions but has no observable effect. Hence the ac-current response can depend only on voltage differences. This implies that the rows of the conductance matrix must also add up to zero.

To achieve these sum rules of the columns and rows of the admittance matrix, the presence of interactions is crucial. Only because of the interactions does a simultaneous and equal potential shift at all contacts cause the same potential shift everywhere in the sample. Were the electrons uncharged particles, instead, then a simultaneous and equal potential shift at the contacts would lead to an oscillatory accumulation and depletion of particles inside the conductors. For ‘‘neutral electrons’’ this particle distribution would cost no electrostatic energy, or, in other words, it would bear no induced potential. According to the continuity equation the sum of all particle currents at the contacts of the samples is equal to the time derivative of the total particle number inside the samples. Consequently, for neutral (i.e., noninteracting) electrons the sum of all currents is not conserved. The current response of noninteracting electrons does not represent an acceptable approximation of the actual system: it is crucial to take the Coulomb interaction into account. Theoretically, ac transport is interesting, since it requires an explicit treatment of interactions. It is under the influence of the mutually interacting charges distributed over the various samples that current conservation is restored.

Our first step, however, is to consider the (non-current-conserving) response of the electrons to an externally applied potential. In this step the internal effective electrostatic potential is kept fixed. The electrons are treated as noninteracting. This external potential is *a priori* arbitrary except for the boundary conditions that must be satisfied in the reservoirs. In reality the electrons ‘‘see’’ a total potential and not only the external potential. The total current response must be independent of the initial choice of the external potential and is unique. Thus in this inital step we are permitted to choose an arbitrary ‘external-potential profile.’’ In many works an arbitrary potential profile (for instance one corresponding to a uniform external field) is taken with the implicit but incorrect understanding that the response to such a field already represents the complete answer. The choice of the external perturbation which we adopt is motivated by the geometry of our samples. In our structure with contacts (reservoirs) it is natural to choose an external perturbation which acts only on the carriers in the leads but not inside the sample. Thus within the noninteracting treatment the sample can be described by its global scattering law. In the dc limit this perturbation leads in a direct way to the dc conductances known from the transmission approach. But even in the ac case this choice of perturbation lets us find an answer which can be expressed in terms of the scattering matrix.

The amplitudes $b_{\alpha w}^{(m)}(E)$ of electron waves leaving the conductor m in channel w of lead α at energy E are related to the amplitudes $a_{\beta u}^{(m)}(E)$ of electron waves which are incident on the same conductor m in channel u of lead β by the relation[4]

$$\mathbf{b}_{\alpha}^{(m)}(E) = \sum_{\beta} \mathbf{s}_{\alpha\beta}^{(m)}(E)\mathbf{a}_{\beta}^{(m)}(E). \tag{2}$$

Here $\mathbf{s}_{\alpha\beta}^{(m)}(E)$ is a submatrix of the unitary scattering matrix $\mathbf{S}^{(m)}(E)$ of conductor m. For $\alpha\neq\beta$ it contains the transmission amplitudes of waves incident from reservoir β into reservoir α, and for $\alpha=\beta$ the reflection amplitudes of waves incident from reservoir α. For the external response (superscript ext), we obtain the admittance

$$g_{\alpha\beta}^{\mathrm{ext}(m)}(\omega) = \frac{e^2}{h}\int dE\,\mathrm{Tr}[\hat{1}_{\alpha}^{(m)}(E)\,\delta_{\alpha\beta} - \mathbf{s}_{\alpha\beta}^{(m)\dagger}(E) \times \mathbf{s}_{\alpha\beta}^{(m)}(E+\hbar\omega)]\frac{f_{\beta}^{(m)}(E)-f_{\beta}^{(m)}(E+\hbar\omega)}{\hbar\omega}. \tag{3}$$

Here the unit matrix $\hat{1}_{\alpha}^{(m)}(E)$ denotes the identity operator on the space spanned by all active channels in lead α of conductor m at energy E. In Eq. (3), $f_{\beta}^{(m)}(E) = f(E-\mu_{\beta}^{(m)})$ is the Fermi-Dirac distribution in reservoir β of conductor m. Equation (3) gives the particle current at contact α in response to an external perturbation which acts on the carriers in lead β. Note that the noninteracting response is zero between contacts belonging to different conductors.

Our second step contains the crucial point: the calculation of the effective potential seen by interacting particles and the determination of the internal response. For this purpose we consider all conducting units which interact via long-range Coulomb forces. Any charge pileup on one conductor induces counterbalancing charges on the other conductors. Up to here the approach is very general, and is actually the common starting point for a more detailed treatment which takes the electrostatic potential landscape into account.[30] Here we

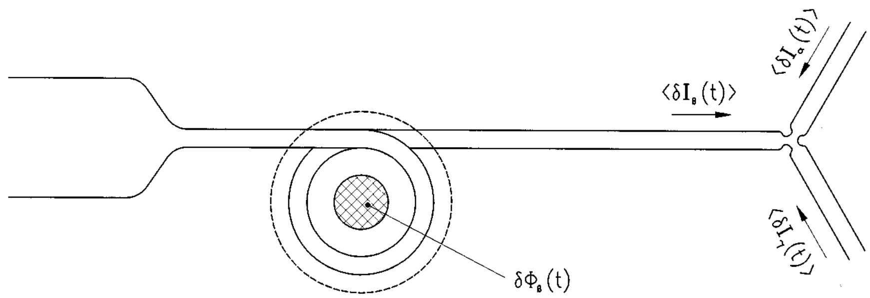

FIG. 2. Magnetic external perturbation: the lead is formed into a loop which is threaded by an Aharonov-Bohm flux. To screen the electric fields generated by the oscillating flux, a compensating flux is applied through a thin ring area outside the loop.

approximate the potential landscape by a single potential $U^{(n)}$ which is locally induced on each conductor n. We introduce the long-range Coulomb interactions via formal geometrical capacitances C_{mn} which relate the (instantaneous) total charges $Q^{(m)}$ accumulated on the conductors m to the local potential parameters. In matrix notation, $\mathbf{Q}=\mathbf{C}\mathbf{U}$. Such an assumption is commonly used to treat Coulomb-blockade effects.

The central result of this paper is the following expression for the true admittance of the system including interactions (superscript I):

$$g_{\alpha\beta}^{I(mn)}(\omega)=\delta_{mn}g_{\alpha\beta}^{\mathrm{ext}(m)}(\omega)-\left[\sum_{\gamma} g_{\alpha\gamma}^{\mathrm{ext}(m)}(\omega)\right](M^{-1})_{mn}(\omega)\times\left[\sum_{\delta} g_{\delta\beta}^{\mathrm{ext}(n)}(\omega)\right]. \tag{4}$$

The matrix

$$M_{mn}(\omega)=\delta_{mn}\sum_{\alpha\beta} g_{\alpha\beta}^{\mathrm{ext}(m)}(\omega)-i\omega C_{mn} \tag{5}$$

mediates the interaction and insures charge conservation. The interacting admittance Eq. (4) fulfills current conservation

$$\sum_{m\alpha} g_{\alpha\beta}^{I(mn)}(\omega)=0, \tag{6}$$

and invariance under an overall potential shift,

$$\sum_{n\beta} g_{\alpha\beta}^{I(mn)}(\omega)=0, \tag{7}$$

as required, and the reality condition

$$g_{\alpha\beta}^{I(mn)}(\omega)=g_{\alpha\beta}^{I(mn)*}(-\omega). \tag{8}$$

The discreteness of this theory makes it suitable to structures where the effective potential can reasonably be approximated by a single parameter (for example, for a ballistic wire). A more sophisticated analysis[30,31] has refined this approach, and relates an effective potential landscape to a local density of states. However, this local theory has only been developed to leading order in frequency, in contrast to the closed result of the discrete-potential model. Our theory can even be applied to tunneling systems (single- or double-barrier problems) for which it is reasonable to include only the voltage in the well. It cannot be applied to a single junction, where the dipole across the junction matters. To treat this case, the theory presented here has been extended by Christen and Büttiker.[32] Finally we stress that our theory does not treat charge quantization,[33–35,23] and strictly speaking cannot be applied to a system where such effects are important.

We note here that the external ac-response $g_{\alpha\beta}^{\mathrm{ext}(m)}(\omega)$ of Eq. (3) is also valid in the presence of dc *transport*. From $g_{\alpha\beta}^{\mathrm{ext}(m)}(\omega)$ the mixed (dc,ac) coefficients of the second-order external response to simultaneous dc and ac-voltage perturbations in a transport state can be obtained. At zero frequency, these nonlinear coefficients coincide with the (dc,dc) coefficients of the external quadratic dc response derived in Ref. 30. On the other hand, the interacting ac response $g_{\alpha\beta}^{I(mn)}(\omega)$ of Eq. (4) is *only* valid for an *equilibrium* reference state. If the reference state carries a steady current, the effective dc potential inside the conductors is in general not the same as at equilibrium. This dc-potential difference influences the ac admittance. For small dc voltages this field effect can be treated with a self-consistent scheme which is analogous to that used here for the internal ac response.[30]

II. GENERAL ASPECTS OF THE ac RESPONSE

We consider a conductor[36] with time-oscillating voltages applied to the contacts. First we calculate the response to an *external perturbation* which treats the carriers as noninteracting particles. The internal potential is kept fixed. Only the total interacting response has physical significance and is unique: the external perturbation itself is arbitrary up to boundary conditions. Therefore, we choose a simple form of the external perturbation. We assume that the external perturbation acts on the carriers only in the leads and reservoirs.

We give two alternative but equivalent ways of experimental configurations which achieve this situation: we can accelerate the carriers either electrically or magnetically.

For an external circuit with zero impedance, we can accelerate the carriers with time-oscillating magnetic fluxes (see Fig. 2). Two requirements should be fulfilled: the external perturbation is restricted to the contacts, and it preserves the equilibrium state in each reservoir. Then only the leads are left for the acceleration. We imagine bending each lead to form a wire loop over a length $2\pi R_\beta$, as in Fig. 2. Each lead loop is threaded by a magnetic Aharonov-Bohm flux $\delta\phi_\beta(t)$ which does not penetrate into the multiprobe structure. The influence of this flux on the carriers in the corresponding loop is easily visualized. In order to avoid the perturbation to act anywhere else on the structure, just outside the loop the flux is counterbalanced by an opposite flux of equal magnitude. Thus the total flux beyond the loop is zero.

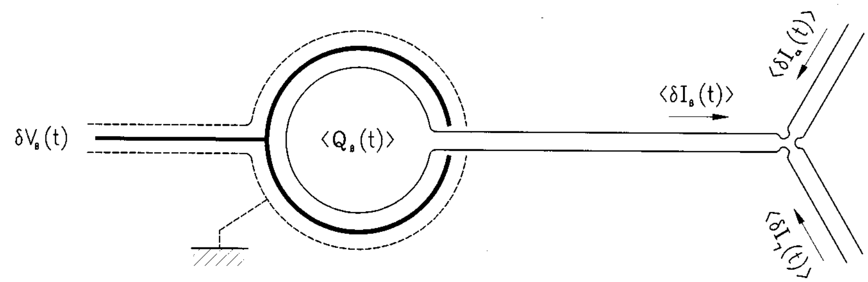

FIG. 3. Electric external perturbation: the reservoir is surrounded by a capacitor shifting its electric potential: the fields of the inner plate and the wire connecting it to an ac source are fully screened by the outer plate everywhere beyond the reservoir. Fringing fields accelerate the carriers in the portion of the lead passing through the opening of the capacitor.

If the typical cross-section diameter of the lead is much smaller than the loop radius, then a tangential vector potential of nearly constant magnitude acts on the carriers in the loop. For the microscopic Hamiltonian $\hat{H}=\Sigma_h(\mathbf{p}_h-e\mathbf{A})^2/2m+V(\mathbf{r})$, with $\mathbf{A}(\mathbf{r},t)=\mathbf{A}_0(\mathbf{r})+\delta\mathbf{A}(\mathbf{r},t)$, the perturbation

$$\hat{H}_1=\hat{H}-\hat{H}_0=-\int dr^3\mathbf{j}(\mathbf{r},t)\cdot\delta\mathbf{A}(\mathbf{r},t), \tag{9}$$

where $\hat{H}_0=\Sigma_h(\mathbf{p}_h-e\mathbf{A}_0)^2/2m+V(\mathbf{r})$, can be expressed in terms of macroscopic variables,

$$\hat{H}_1=\sum_\beta \hat{I}_\beta\delta\phi_\beta. \tag{10}$$

Here $\hat{I}_\beta$ denotes the current at contact β, and $\delta\phi_\beta$ denotes the magnetic flux threading the lead loop β.

Alternatively, we can imagine an external circuit with an infinite impedance. The electrochemical potential μ_β of reservoir β is the sum of its electric and its chemical potential. We can shift μ_β by $e\delta V_\beta(t)$ by embedding reservoir β in a capacitor whose outer plate is put to ground and whose inner plate is at a voltage $\delta V_\beta(t)$, as shown in Fig. 3. Then the accelerating fields due to the external perturbation act on the carriers only in the portion of the lead between one capacitor plate and the other. Under these assumptions the usual microscopic electric perturbation $\int dr^3\varrho(\mathbf{r},t)V(\mathbf{r},t)$ can be expressed again in terms of macroscopic variables,

$$\hat{H}_1=\sum_\beta \hat{Q}_\beta\delta V_\beta. \tag{11}$$

Here $\hat{Q}_\beta$ denotes the total charge in reservoir β, which is a well-defined quantity because the impedance of the external circuit is infinite. We are interested in the averaged variation of the current $\hat{I}_\alpha$, which is related to $\hat{Q}_\alpha$ by $\hat{I}_\alpha=-d\hat{Q}_\alpha/dt$.

When these two perturbations generate the same voltage, $\delta V_\beta(t)=d\delta\phi_\beta/dt$, then the linear response generated by an oscillating flux,

$$\langle\delta\hat{I}_\alpha(\omega)\rangle^\phi=\sum_\beta \kappa^\phi_{\alpha\beta}(\omega)\delta\phi_\beta(\omega), \tag{12}$$

and the linear response generated by an oscillating voltage,

$$\langle\delta\hat{I}_\alpha(\omega)\rangle^V=\sum_\beta \kappa^V_{\alpha\beta}(\omega)\delta V_\beta(\omega), \tag{13}$$

are the same. This is ensured by the equality $d\kappa^V_{\alpha\beta}(\tau)/d\tau=\kappa^\phi_{\alpha\beta}(\tau)$ demonstrated in Appendix A. Thus the electric and magnetic perturbations are equivalent.

Equations (12) and (13) are the starting point for a conventional linear-response calculation[19,20] as reviewed in Appendix A. In contrast to this standard method, in Sec. III we obtain the ac admittance with an elementary approach which is closer to physical intuition. Moreover, this approach also applies to a situation where a time-dependent perturbation is superimposed on a reference state carrying a steady current.

III. CURRENTS INDUCED BY EXTERNAL PERTURBATIONS

The response we are looking for is the time-dependent current variation $\langle\delta\hat{I}_\alpha\rangle$ away from the reference state. This response is defined as the difference of the expectation values of the current operator $\hat{I}_\alpha$ in the perturbed (p) and in the reference (0) ensemble, respectively,

$$\langle\delta\hat{I}_\alpha\rangle=\langle\hat{I}_\alpha\rangle_p-\langle\hat{I}_\alpha\rangle_0. \tag{14}$$

While standard linear-response theory would extract such an expectation value from correlations averaged over the reference ensemble, we calculate $\langle\delta\hat{I}_\alpha\rangle_p$ directly for the perturbed ensemble. For independent electrons it is sufficient to specify the population of a complete set of one-particle states in the presence of the perturbation.

When an oscillating magnetic flux threads loop β, the carriers ''feel'' the perturbing fields along the loop of length $2\pi R_\beta$. The magnetic perturbation takes the form of an electric dipolar energy on this loop, $-(e\hat{p}_\parallel/m)[\delta\phi_\beta\exp(-i\omega t)+\delta\phi^*_\beta\exp(i\omega t)]/(2\pi R_\beta)$. Here $\hat{p}_\parallel$ stands for the longitudinal component of the momentum operator. Carriers coming from the reservoir and traversing the loop either absorb or emit an energy $n\hbar\omega$, $n=1,2,\ldots$, or are transmitted at their incident energy. To first order in the perturbation, only one energy quantum $\hbar\omega$ is absorbed or emitted. On both sides of the loop the wave function can be expressed as a linear combination of incident $(+)$ and outgoing $(-)$ unperturbed eigenstates $|\varphi^{(+)}_{\beta u,E}\rangle\exp(-iEt/\hbar)$ and $|\varphi^{(-)}_{\beta u,E}\rangle\exp(-iEt/\hbar)$, where u is the channel index. These states form a complete orthonormal set. This is known as the completeness theorem in scattering theory.[37] Explicit expressions for these states are given in Appendix B. Independent of the perturbation, the reservoir injects carriers with a population according to $f_\beta(E)$ into incident eigenstates $|\varphi^{(+)}_{\beta u,E}\rangle \exp(-iEt/\hbar)$ in the portion between reservoir and loop. These Fermi-Dirac distributed states emerge from the loop into the portion between the loop and the sample in a time-dependent state

$$|\tilde{\Psi}'_{\beta u,E}(t)\rangle = |\varphi^{(+)}_{\beta u,E}\rangle e^{-iEt/\hbar} + c_\beta |\varphi^{(+)}_{\beta u,E_+}\rangle e^{-iE_+t/\hbar} - c_\beta |\varphi^{(+)}_{\beta u,E_-}\rangle e^{-iE_-t/\hbar} \tag{15}$$

with $c_\beta = e\delta V_\beta/\hbar\omega$ and $E_\pm = E \pm \hbar\omega$. Equation (15) is obtained by matching the wave functions at the two loop ends, and is valid up to corrections of the order of $(k_\pm - k)/|k|$, where k and $k_\pm$ are the longitudinal wave vectors in lead β and channel u associated with the energies E and $E_\pm$, respectively. Equation (15) is, therefore, valid for high-velocity states along the lead. Only these states couple effectively to the sample. As we discuss in Appendix B, the low-velocity states can be neglected.

Similar considerations can be carried out for an electric perturbation. We suppose the junction to be adiabatic between reservoir and lead β. In the absence of a perturbation, there is a reservoir state $|\varphi^{(\text{res})}_{\beta u,E}\rangle \exp(-iEt/\hbar)$ which is transmitted into the incident state $|\varphi^{(+)}_{\beta u,E}\rangle \exp(-iEt/\hbar)$ in the lead, and $|\Psi_{\beta u,E}(t)\rangle$ designates the corresponding unperturbed (reservoir plus lead) state. Let us adiabatically switch on the electric time-dependent perturbation $e[\delta V_\beta \exp(-i\omega t) + \delta V^*_\beta \exp(i\omega t)]$, which is uniform in the reservoir and vanishes in the lead. The state $|\Psi_{\beta u,E}(t)\rangle$ evolves into $|\Psi'_{\beta u,E}(t)\rangle$. This state gains additional time-dependence, $\exp(-iEt/\hbar) \rightsquigarrow \exp(-i[Et+\xi_\beta(t)]/\hbar)$, in the reservoir, and consists of a superposition of unperturbed eigenstates in the lead. The extra phase obeys $\xi_\beta(t) = \int dt [e\delta V_\beta \exp(-i\omega t) + e\delta V^*_\beta \exp(i\omega t)]$. For the wave function in the reservoir we find

$$|\Psi'_{\beta u,E}(t)\rangle = |\varphi^{(\text{res})}_{\beta u,E}\rangle e^{-iEt/\hbar} + c_\beta |\varphi^{(\text{res})}_{\beta u,E}\rangle e^{-iE_+t/\hbar} - c_\beta |\varphi^{(\text{res})}_{\beta u,E}\rangle e^{-iE_-t/\hbar}. \tag{16}$$

In the lead we find the same result [Eq. (15)] as for the magnetic perturbation. The range of validity is again restricted to high-velocity states. The states $|\Psi'_{\beta u,E}(t)\rangle$ which evolve adiabatically from $|\Psi_{\beta u,E}(t)\rangle$, have the same occupation probability $f_\beta(E)$ in the presence of the perturbation as the $|\Psi_{\beta u,E}(t)\rangle$ in the unperturbed case.

Let us introduce operators $\hat{a}_{\alpha u}$ which annihilate an incoming carrier in channel u in lead α and operators $\hat{b}_{\alpha u}$ which annihilate an outgoing carrier in channel u in lead α. Let us denote by $\hat{\mathbf{a}}_\alpha$ and $\hat{\mathbf{b}}_\alpha$ the vector of these operators. The number of components of these vectors is equal to the number of open channels in the lead α. At moderate frequencies the current operator is given by

$$\hat{I}_\alpha(t) = \frac{e}{h}\int dE\, dE' [\hat{\mathbf{a}}^\dagger_\alpha(E)\hat{\mathbf{a}}_\alpha(E') - \hat{\mathbf{b}}^\dagger_\alpha(E)\hat{\mathbf{b}}_\alpha(E')] e^{i(E-E')t/\hbar}. \tag{17}$$

Equation (17) has been derived in Refs. 4 and 38. In Appendix B this derivation is discussed for the case of a nonzero magnetic field. In the presence of the time-dependent electric or magnetic perturbation acting in the contacts, the incident wave in lead β has the form $\Sigma_u \int dE\, a'_{\beta u}(E) |\tilde{\Psi}'_{\beta u,E}(t)\rangle$. Here the amplitudes $a'_{\beta u}(E)$ obey Fermi-Dirac statistics, and $|\tilde{\Psi}'_{\beta u,E}(t)\rangle$ is expression (15). The most general incident wave is formed by a superposition of the incident waves at all leads $\Sigma_\beta \int dE\, \mathbf{a}'_\beta(E) |\tilde{\Psi}'_{\beta,E}(t)\rangle$.

In Fourier space the relation for the incident amplitudes (or for the corresponding annihilation operators) is

$$\hat{\mathbf{a}}_\alpha(E) = \{\hat{\mathbf{a}}'_\alpha(E) - c_\alpha \hat{\mathbf{a}}'_\alpha(E_+) + c_\alpha \hat{\mathbf{a}}'_\alpha(E_-)\}. \tag{18}$$

The outgoing amplitudes are found with the help of Eq. (2),

$$\hat{\mathbf{b}}_\alpha(E) = \sum_\beta \mathbf{s}_{\alpha\beta}(E)\{\hat{\mathbf{a}}'_\beta(E) - c_\beta \hat{\mathbf{a}}'_\beta(E_+) + c_\beta \hat{\mathbf{a}}'_\beta(E_-)\}. \tag{19}$$

In Eqs. (18) and (19) the amplitudes $\mathbf{a}_\alpha(E)$ and $\mathbf{b}_\alpha(E)$ of the unperturbed eigenstates in lead α consist of contributions of particles incident in lead β at energy E which are unaffected by the time-modulated perturbation, and at energies $E_\pm$ which have emitted or absorbed a modulation quantum.

We use Eqs. (18) and (19) in Eq. (17) to replace $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ with $\hat{\mathbf{a}}'$ and $\hat{\mathbf{b}}'$. Now $\langle \hat{I}_\alpha \rangle_p$ can be calculated as an expectation value of a single-particle operator obeying $\langle \hat{a}'^\dagger_{\beta u}(E)\hat{a}'_{\beta u}(E)\rangle_p = f_\beta(E)$. This yields the current response $\langle \delta\hat{I}_\alpha \rangle_p$ according to Eq. (14). The resulting admittance is given by Eq. (3).

The external admittance Eq. (3) fulfills the following basic properties. For a general reference state, the reality condition Eq. (8) is satisfied. Further, the ac admittance for a vanishing frequency reduces to the differential dc conductance. If the reference state is an equilibrium state, the reciprocity relation $g^{\text{ext}}_{\alpha\beta}(\omega,-B) = g^{\text{ext}}_{\beta\alpha}(\omega,B)$, and the fluctuation-dissipation theorem $S_{\alpha\beta}(\omega) = \epsilon(\omega,kT)[g_{\alpha\beta}(\omega) + g^*_{\beta\alpha}(\omega)]$ is obeyed, where the current-current correlations $S_{\alpha\beta}(\omega)$ are provided by Ref. 38. If, on the other hand, the reference state is a transport state, the real parts of the admittances do not show much similarity to the corresponding current-current correlations, which contain fourfold products of scattering-matrix elements. For a steady state, the admittance depends on the Fermi distributions of the various reservoirs, $f_\beta(E) = f(E-\mu_\beta)$.

An expansion of the admittance to the lowest orders in frequency is instructive. To second order we find, from Eq. (3),

$$g^{\rm ext}_{\alpha\beta}(\omega)=g_{\alpha\beta}(0)-i\omega e^2\frac{dN_{\alpha\beta}}{dE}+\omega^2e^4\left(\frac{dN_{\alpha\beta}}{dE}\right)^2D_{\alpha\beta}+\mathcal{O}(\omega^3). \tag{20}$$

Here

$$\frac{dN_{\alpha\beta}}{dE}=\frac{1}{4\pi i}\int dE\,{\rm Tr}\left[\mathbf{s}^\dagger_{\alpha\beta}(E)\frac{\partial\mathbf{s}_{\alpha\beta}(E)}{\partial E}-\frac{\partial\mathbf{s}^\dagger_{\alpha\beta}(E)}{\partial E}\mathbf{s}_{\alpha\beta}(E)\right]\times\left(\frac{-df_\beta(E)}{dE}\right) \tag{21}$$

is a partial density of states, and

$$D_{\alpha\beta}=\frac{h}{2e^2}\,\frac{\int dE\,{\rm Tr}\left[4\left(\frac{\partial\mathbf{s}^\dagger_{\alpha\beta}(E)}{\partial E}\frac{\partial\mathbf{s}_{\alpha\beta}(E)}{\partial E}\right)-\frac{\partial^2}{\partial E^2}(\mathbf{s}^\dagger_{\alpha\beta}(E)\mathbf{s}_{\alpha\beta}(E))\right]\left(\frac{-df_\beta(E)}{dE}\right)}{(4\pi)^2\left(\frac{dN_{\alpha\beta}}{dE}\right)^2} \tag{22}$$

has the dimension of a resistance.

Let us first concentrate on the first-order term. Under the action of the external oscillating potential δV_β, the total charge Q_Ω accumulated within a volume Ω which encloses the sample satisfies $\dot{Q}_\Omega(\omega)=-i\omega Q_\Omega(\omega)=\Sigma_\alpha\langle\delta I_\alpha(\omega)\rangle$. A simultaneous and equal variation of all chemical potentials gives an excess charge in the sample determined by the total density of states $\Sigma_{\alpha\beta}dN_{\alpha\beta}/dE$. Comparing with Eq. (20), we see that we can interpret $dN_{\alpha\beta}/dE$ as the *partial* density of states of Ω, associated with carriers coming from probe β and leaving through probe α. Note that, as a *partial* density of states, $dN_{\alpha\beta}/dE$ does not need to be positive.

Like the first-order admittance term, the second-order term does in general not have a definite sign either. Expression (22) is positive in the simplest case of a one-terminal structure. In that case $S^\dagger_{\alpha\alpha}S_{\alpha\alpha}\equiv$const, and the second term in the square bracket of $D_{\alpha\alpha}$ vanishes. Then $D_{\alpha\alpha}$ can be interpreted as a charge-relaxation resistance.[21] The expression for this particular case is given below [Eq. (32)] in terms of the eigenfunctions. We notice that in the general case only the first term in the numerator of $D_{\alpha\beta}$ is always positive.

IV. CURRENTS INDUCED BY INTERNAL PERTURBATIONS

The admittance of noninteracting electrons derived above is neither charge nor current conserving. The lack of charge and current conservation is typical for any time-dependent external response, and is not a feature of the particular approach discussed here. We now introduce a simple self-consistent scheme to achieve overall charge and current conservation. We consider an assembly of N conductors representing both the proper conductors and the gates used to form it, and restrict ourselves from now on to an *equilibrium* reference state: all reservoirs connected to the same conductor have the same electrochemical potential, $\mu^{(m)}_\beta=\mu^{(m)}$. Within a discrete-potential approach, we derive the interacting admittance matrix g^I, which relates the current variation $\langle\delta I^{(m)}_\alpha(\omega)\rangle$ to the voltage variation $\delta V^{(n)}_\beta(\omega)$ as in Eq. (1). Here each conductor l is connected to one or several reservoirs (l,γ), and is characterized by a noninteracting admittance matrix $\mathbf{g}^{\text{ext}(l)}_{\gamma\gamma'}$ as in Sec. III. It is assumed that no tunneling occurs between different conductors, and that the Coulomb interaction enters solely via the long-range part between conductor pairs. We introduce a discrete set of induced *internal potentials* $\delta U^{(n)}$ which are related to the piled-up charges $\delta Q^{(m)}$ with the help of electrostatic-capacitance elements C_{mn},

$$\delta Q^{(m)}(\omega)=\sum_n C_{mn}\delta U^{(n)}(\omega), \tag{23}$$

with $C_{mn}=C_{nm}$ and $\Sigma_nC_{mn}=0$. To proceed we must find the relationship between the internal potentials and the electrochemical potentials.

The current at contact α in conductor m is the sum of the responses of noninteracting carriers to the oscillating external potentials $\delta\mu^{(m)}_\beta(\omega)\equiv e\,\delta V^{(m)}_\beta(\omega)$, and to the oscillating internal potential $\delta U^{(m)}(\omega)$,

$$\langle\delta I^{(m)}_\alpha(\omega)\rangle=\sum_\beta g^{\text{ext}(m)}_{\alpha\beta}(\omega)\,\delta V^{(m)}_\beta(\omega)+g^{\text{int}(m)}_\alpha(\omega)\,\delta U^{(m)}(\omega), \tag{24}$$

where $g^{\text{int}(m)}_\alpha(\omega)$ describes the current response of noninteracting carriers at contact α in conductor m to the oscillating internal potential $\delta U^{(m)}(\omega)$. Below we determine $\delta U^{(m)}(\omega)$ self-consistently. Note that at this stage the current $\langle\delta I^{(m)}_\alpha\rangle$ depends only on the potentials applied to its own conductor m. The wave functions of carriers of one conductor vanish in all other conductors and, do not feel any effect of the potential beyond their conductor. Here the absence of tunneling is crucial. Now we make use of the fact that the current response of the interacting system is invariant under an overall potential shift. Fixing attention on conductor m and shifting the overall potential by $-\delta U^{(m)}$ yields

$$\langle\delta I^{(m)}_\alpha(\omega)\rangle=\sum_\beta g^{\text{ext}(m)}_{\alpha\beta}(\omega)[\delta V^{(m)}_\beta(\omega)-\delta U^{(m)}(\omega)]. \tag{25}$$

Comparision with Eq. (24) implies that the internal response is given by $g^{\text{int}(m)}_\alpha(\omega)=-\Sigma_\beta g^{\text{ext}(m)}_{\alpha\beta}(\omega)$. The internal potentials $\delta U^{(m)}$ depend via long-range Coulomb forces on the external potentials at the other conductors.[39] The charge on each conductor m is that permitted by the long-range Coulomb interaction Eq. (23). This yields a self-consistent condition for each conductor,

$$\sum_{\alpha} \langle \delta I_{\alpha}^{(m)}(\omega)\rangle = -i\omega \sum_{n} C_{mn}\delta U^{(n)}(\omega). \tag{26}$$

Combining (25) and (26) and solving the resulting inhomogeneous linear system, we obtain

$$\delta U^{(m)}(\omega) = \sum_{n} (M^{-1})_{mn}(\omega) \sum_{\alpha\beta} g_{\alpha\beta}^{\text{ext}(n)}(\omega)\delta V_{\beta}^{(n)}(\omega), \tag{27}$$

where the matrix M has been defined in Eq. (5). Thus we recover the individual currents from Eq. (25) and obtain Eq. (4) for the admittance matrix of the interacting system.

The interacting admittance (4) fulfills the key properties (6), (7) and (8) stated in Sec. I, and reduces to the noninteracting admittance at zero frequency where no charge accumulation occurs. In particular, property (7) follows from Eqs. (4) and (23) and the sum rules of the electrostatic-capacitance elements. It also fulfills the fluctuation-dissipation theorem[40] and the reciprocity relations.[28,2] For the admittance elements relating different $(m \neq n)$ conductors with a purely capacitive response, i.e., $g_{\alpha\beta}^{I(mn)}(\omega) = -i\omega c_{\mu,\alpha\beta}^{(mn)} + \mathcal{O}(\omega^2)$, microreversibility implies $c_{\mu,\alpha\beta}^{(mn)}(B) = c_{\mu,\beta\alpha}^{(nm)}(-B)$. On the other hand, $c_{\mu,\alpha\beta}^{(mn)}(B)$ is in general different from $c_{\mu,\alpha\beta}^{(mn)}(-B)$.[2] Only their sums $c_{\mu}^{\text{tot}(mn)} = \Sigma_{\alpha\beta} c_{\mu,\alpha\beta}^{(mn)}$ are even functions of the magnetic field, $c_{\mu}^{\text{tot}(mn)}(B) = c_{\mu}^{\text{tot}(nm)}(B)$, since they are the second derivatives of a thermodynamic potential.[2]

In the limit of a large capacitance element C_{jk} between the two conductors j and k, the two internal potentials U_j and U_k become locked: $U_j \cong U_k$. On the other hand, if one has a partition of the total assembly of conductors into subsets with vanishing mutual capacitance, then the charge vanishes separately in each subset.

The situation considered in Ref. 20 is a special limit of the model considered here. There, a mesoscopic conductor was capacitively coupled to a macroscopic environment characterized by an infinite density of states dN/dE. With $dN/dE >> |C|/e^2$, the interacting admittance provided by Ref. 20 follows directly from Eqs. (4) and (5).

V. DISCRETE-POTENTIAL MODEL: EXAMPLES

Coherent two-plate capacitor

In this section, we compare the standard macroscopic picture with the mesoscopic description of a capacitor consisting of two plates connected via leads to electron reservoirs, as sketched in Fig. 4(a). Here the dc part of $g^{\text{ext}(m)}$, $m=1$ and 2, vanishes. A conventional macroscopic capacitor, depicted in Fig. 4(b), is described by an electrostatic geometrical capacitance C in series with dc-resistances R_1 and R_2. The current response of this system has the form $\delta I = \{-iC\omega + RC^2\omega^2 + O(\omega^3)\}\delta V$, with $R = R_1 + R_2$. The parameters C, R_1, and R_2 express features which are specific to the separate constituents of the macroscopic system. In this respect, the situation is very different for a coherent capacitor. The mesoscopic capacitor consists of two conducting units whose capacitive coupling is determined by a single parameter C playing the role of an electrostatic geometry-dependent capacitance. Because of the current conservation, Eq. (6), and the invariance under an overall potential shift, Eq. (7), the four admittance elements are all identical up to the sign, $\langle \delta I^{(1)}\rangle = -\langle \delta I^{(2)}\rangle = g^I(\delta V^{(1)} - \delta V^{(2)})$. From Eqs. (4) and (5) we obtain

$$\frac{1}{g^I(\omega)} = \frac{1}{-iC\omega} + \frac{1}{g^{\text{ext}(1)}(\omega)} + \frac{1}{g^{\text{ext}(2)}(\omega)}. \tag{28}$$

Up to second order in ω, $g^{\text{ext}(m)}$ is given in terms of the corresponding scattering matrices $\mathbf{S}^{(m)}$ and Fermi functions $f^{(m)}(E) = f(E - \mu^{(m)})$ of the reservoirs on each side, according to Eqs. (20)–(22) specialized to one-lead conductors.[21] For each m, $g^{\text{ext}(m)}(\omega)$, and $dN^{(m)}/dE$, and $D^{(m)}$ are scalars. Expansion in powers of frequency in a form analogous to the macroscopic picture determines the electrochemical capacitance and the charge-relaxation resistance,

$$g^I(\omega) = -iC_\mu\omega + R_q C_\mu^2\omega^2 + O(\omega^3), \tag{29}$$

$$\frac{1}{C_\mu} = \frac{1}{C} + \frac{1}{e^2}\left(\frac{1}{dN^{(1)}/dE} + \frac{1}{dN^{(2)}/dE}\right), \tag{30}$$

$$R_q = R_q^{(1)} + R_q^{(2)} = D^{(1)} + D^{(2)}. \tag{31}$$

In contrast to the macroscopic case, the capacitance C_μ and resistance R_q governing the ac admittance of a coherent capacitor are thermodynamic quantities which reflect the behavior of the system as a whole. In fact, the charge-relaxation resistance $R_q^{(m)}$ on each side and the corrections to the standard classical capacitance are determined by the scattering properties of the whole reservoir-to-plate arm, statistically averaged at the corresponding reservoir.

To leading order in frequency, the purely capacitive response of the system is governed by the electrochemical capacitance $C_\mu = e\,\delta Q^{(m)}/\delta\mu^{(m)}$: the deviation of this mesoscopic capacitance C_μ from the conventional capacitance $C = \delta Q^{(m)}/\delta U^{(m)}$ relating charges and on-plate voltages can be appreciated from Eq. (30): C_μ formally looks like a series connection of C and of two quantum capacitances. In mesoscopic systems all three may be of the same order of magnitude. For a mesoscopic sample, it has to be taken into account that the two capacitor plates do not accomodate the capacitively induced charges directly at the surface. As discussed by Luryi[41] in the context of a spatially confined two-dimensional electron gas, the quantum capacitance is a consequence of the Pauli principle, which requires an extra energy for filling a limited space with electrons. As a result, such limited space does not completely screen an applied (transverse) electric field. In our case, the screening length over which the fields penetrate into the conductor may be comparable to the plate dimension. The injected charge $e\,dN^{(m)}/dE$ is stored inside plate m over this screening length. Thus $\delta U^{(m)}$ represents an average of the change in the effective potential landscape over the plate. The key point is that $e\,\delta U^{(m)}$ cannot be identified with the experimentally controlled electrochemical potential change at the contact, $\delta\mu^{(m)} = e\,\delta V^{(m)}$. The distinction of electrostatic capaci-

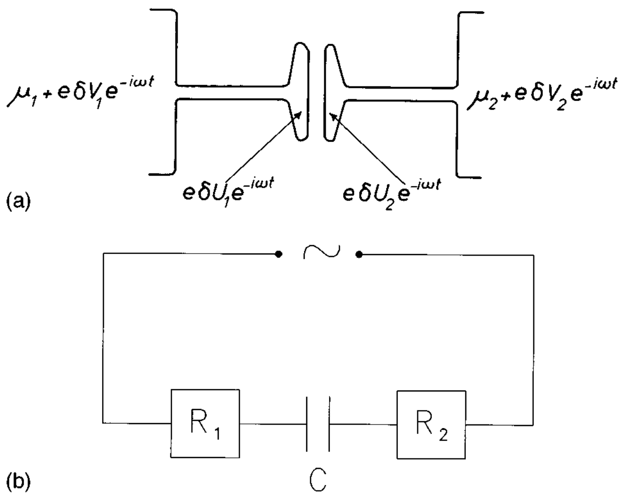

FIG. 4. (a) Mesoscopic coherent two-plate capacitor. (b) Macroscopic two-plate capacitor.

tance and electrochemical capacitance becomes irrelevant if both densities of states to the left and to the right are large compared to C.

Let us give an interpretation of the charge-relaxation resistance R_q. The first factor in $R_q^{(m)}$ is *half* the resistance quantum, the lead-reservoir interface resistance of a single quantum channel discussed by Sharvin and Imry.[42] This resistance is multiplied by the ratio[21] $\langle \tau_\phi^{(m)2}\rangle / \langle \tau_\phi^{(m)}\rangle^2$, where $\tau_\phi^{(m)}$ is the time carriers incident from the leads dwell [39] on the mth capacitor plate,[43]

$$R_q^{(m)} = \frac{h}{2e^2} \frac{\langle \tau_\phi^{(m)2}\rangle}{\langle \tau_\phi^{(m)}\rangle^2} = \frac{h}{2e^2} \frac{\langle \Sigma_n (d\phi_n^{(m)}/dE)^2\rangle_m}{\{\langle \Sigma_n (d\phi_n^{(m)}/dE)\rangle_m\}^2}. \quad (32)$$

The brackets $\langle\rangle$ denote both a quantum-mechanical and a statistical average. $R_q^{(m)}$ can be directly expressed in terms of energy derivatives of the eigenvalues $\mathbf{s}_{nn}^{(m)} = \exp(i\phi_n^{(m)})$. The presence of such a ratio in the current response suggests a non-self-averaging system. For a small number of channels M_m the resistance $R_q^{(m)}$ usually scales as $1/M_m$. For large M_m, on the other hand, Pendry and co-workers [44] have shown that in the diffusive regime the probability distribution of the conductance makes extreme excursions, or ‘‘maximal fluctuations.’’ We may expect this non-self-averaging system to react to an energy change with maximal changes of the phases ϕ for a minimum number of eigenchannels, whereas in the other eigenchannels no phase changes take place. Thus a non-self-averaging system is likely to exhibit a larger charge-relaxation resistance than a usual system. In addition, the charge distribution of localized states in the insulator between the capacitor plates is likely to be another important source of mesoscopic fluctuations.[45] To study this effect an approach is required which treats the microscopic potential landscape.

Next we consider a very asymmetric capacitor. One capacitor arm is macroscopic with an infinite density of states, the other capacitor arm is a one-contact quantum well: the ‘‘plate’’ contains a long-lived state which is separated from the wire by a tunneling barrier. We treat this example only to illustrate our theory. A more realistic discussion has to take charge quantization into account. We introduce the width Γ of the resonance and use the abbreviation $|\Delta|^2 = (E_F - E_r)^2 + \Gamma^2/4$. Here, E_F is the Fermi energy and E_r is the energy of the resonant state of the quantum well. For the external admittance of the quantum-well arm we find

$$g^{\text{ext}}(\omega) = -i\omega e^2 \frac{dN}{dE} + \omega^2 e^4 \left(\frac{h}{2e^2}\right)\left(\frac{dN}{dE}\right)^2, \quad (33)$$

$$\frac{dN}{dE} = \frac{\Gamma}{2\pi|\Delta|^2}, \quad (34)$$

and for the interacting admittance,

$$g^I(\omega) = -i\omega C_\mu + \omega^2 C_\mu^2 \left(\frac{h}{2e^2}\right), \quad (35)$$

$$\frac{1}{C_\mu} = \frac{1}{C} + \frac{1}{e^2(dN/dE)}. \quad (36)$$

The charge-relaxation resistance is just equal to $h/2e^2$ (half a resistance quantum). The lack of an energy dependence in the charge-relaxation resistance is implied by the fact that $\langle \tau_\phi^2\rangle = \langle \tau_\phi\rangle^2$, due to the effective *single-channel* nature of the scattering matrix.

If the quantum well is threaded by a magnetic flux ϕ as in Fig. 5, then the resonating energy E_r depends periodically on ϕ with period h/e, implying a ϕ dependence of the scattering amplitudes but not of the scattering probabilities. Consequently the electrochemical capacitance exhibits an Aharonov-Bohm effect.[46,35] This implies that an Aharonov-Bohm effect shows up in the admittance at nonzero frequencies only. This is a striking example for the observability of the scattering phases in the ac response.

Capacitively coupled quantum well with long-lived state

As a next example we consider a quantum well which contains a long-lived state connected to two ‘‘probes’’ via tunneling barriers and capacitively coupled to a nearby gate (see the inset of Fig. 6). The scattering matrix amplitudes are

$$S_{\alpha v,\beta u}(E) = [\delta_{\alpha\beta}\delta_{vu} - i(\Gamma_{\alpha v}\Gamma_{\beta u})^{1/2}/\Delta]\exp(i\delta_{\alpha v} + i\delta_{\beta u}),$$

where $\Delta = E - E_r + i\Gamma/2$, $\alpha,\beta = 1$ and 2, and u and v are channel indices. Here $\Gamma_{\alpha v}$ is the width of the resonance due to decay into channel v in lead α, $\Gamma_\alpha = \Sigma_v \Gamma_{\alpha v}$ is the total decay width into lead α, and $\Gamma = \Sigma_\alpha \Gamma_\alpha$ is the total width of the resonance. The phases $\delta_{\alpha v}$ and $\delta_{\beta u}$ are taken to be energy independent. For simplicity we assign to the gate an infinite density of states as in Ref. 20. At zero temperature for the admittance at the contacts of the two-barrier quantum well we find

$$g_{\alpha\beta}^I(\omega) = g_{\alpha\beta}(0) - i\omega E_{\alpha\beta} + \omega^2 D_{\alpha\beta}. \quad (37)$$

Here

$$g_{11}(0)=-g_{12}(0)=-g_{21}(0)=g_{22}(0)=\frac{e^2}{h}T$$
$$=\frac{e^2}{h}\frac{4\Gamma_1\Gamma_2}{\Gamma^2(x^2+1)} \tag{38}$$

are the dc conductances, $x=2(E_F-E_r)/\Gamma$, and E_F is the Fermi energy of the reference state. The terms multiplying ω are called emittances and are given by

$$E_{\alpha\beta}=e^2\frac{dN}{dE}\frac{\Gamma_\alpha}{\Gamma(x^2+1)}\left\{\delta_{\alpha\beta}(x^2-1)-\frac{\Gamma_\beta}{\Gamma}\left(\frac{x^2-1-4\gamma(x^2+1)}{1+2\gamma(x^2+1)}\right)\right\}. \tag{39}$$

The density of states $dN/dE=2/[\pi\Gamma(x^2+1)]$ is evaluated at E_F. Note that the total density of states $\Sigma_{\alpha\beta}dN_{\alpha\beta}/dE$ defined in Eq. (20) is identical with the one-contact density of states Eq. (34). The degree of screening present in the system is determined by the parameter γ, whose inverse is proportional to the ratio of the geometrical charging energy and the quantum charging energy $\gamma^{-1}=4(dN/dE)_{\text{res}}(e^2/2C)$. Here $(dN/dE)_{\text{res}}=2/(\pi\Gamma)$ is the total density of states at resonance. The term multiplying ω^2 is already a complicated expression given by

$$D_{\alpha\beta}=e^4\left(\frac{dN}{dE}\right)^2\left(\frac{h}{2e^2}\right)\frac{\Gamma_\alpha}{2\Gamma(x^2+1)}\left\{\delta_{\alpha\beta}(3x^2-1)-\frac{\Gamma_\beta}{\Gamma}\times\left((3x^2-1)-\frac{8\gamma^2(x^2+1)^3}{[1+2\gamma(x^2+1)]^2}\right)\right\}. \tag{40}$$

The dependence of the diagonal emittance element $E_{11}(E_F)$ on the Fermi energy is depicted in Fig. 6 for various values of γ^{-1} and a ratio $\Gamma_1/\Gamma=0.75$. Similarly, $D_{11}(E_F)$ is depicted in Fig. 7 as a function of the Fermi energy for various values of γ^{-1}. In the absence of screening $(\gamma^{-1}=0)$, the Coulomb effects vanish and the admittance g^I reduces to the external admittance. In this case $\Sigma_{\alpha\beta}E_{\alpha\beta}=e^2(dN/dE)$, where dN/dE is given by Eq. (34) with $\Gamma=\Gamma_1+\Gamma_2$. On the other hand, for perfect screening $(\gamma=0)$ the induced Coulomb effects are most effective and enforce charge neutrality in the quantum well.

The diagonal elements $E_{\alpha\alpha}$ and $D_{\alpha\alpha}$ are negative for Fermi energies E_α close to the resonance energy (kinetic-inductive behavior), except for sufficiently large γ and for Γ_α larger than $\Gamma^E_{\text{crit}}=\Gamma/2$ and $\Gamma^D_{\text{crit}}=\Gamma/3$. The diagonal elements are always positive far from resonance (resistive-capacitive behavior). For $\Gamma_\alpha<\Gamma^{E,D}_{\text{crit}}$, $E_{\alpha\alpha}$ and $D_{\alpha\alpha}$ are positive functions of E_F for any value of γ.

Positive off-diagonal elements $E_{\alpha\beta}$ and $D_{\alpha\beta}$ indicate kinetic-inductive behavior, whereas negative $E_{\alpha\beta}$ and $D_{\alpha\beta}$ indicate resistive-capacitive behavior. We always find kinetic-inductive behavior sufficiently near to the resonance, whereas far from resonance, usually resistive-capacitive behavior occurs. However, if $\gamma>1/4$ then $E_{\alpha\beta}$ is kinetic-inductive for any Fermi energy.

For a two-terminal sample, a macroscopic analog exhibiting a negative linear term and a negative second-order term in the admittance can be thought of as a self-inductance in series with a parallel connection of a capacitor and a resistor.

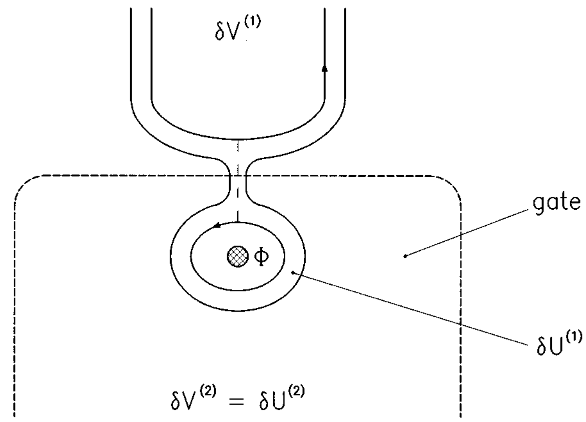

FIG. 5. One-contact quantum well with a long-lived state threaded by an Aharonov-Bohm flux Φ, with capacitive coupling to a macroscopic gate. Edge states (→) follow the contours of the conducting tip and the quantum well, and there is a transmission probability (--) for hopping between the edge state and the resonating state.

The admittance $G(\omega)=\delta I(\omega)/\delta V(\omega)$ of this electric circuit up to second order in the frequency is $G(\omega)=(1/R)-i\omega[C-L/R^2]+\omega^2(L/R)[2C-L/R^2]$. Neither the first nor second order have a definite sign. The first-order term switches from capacitive behavior to inductive behavior if $L=CR^2$. The second-order term becomes negative if $L>2CR^2$.

At low frequencies a correction $-i\omega E$ to the dc conductance may be difficult to measure. The emittance elements $E_{01}=C_{01}$ and $E_{02}=C_{02}$, which give the capacitively induced current into the gate in response to voltage oscillations at contacts 1 and 2, are easier to measure.[2] For our system it turns out that these capacitance coefficients are $C_{01}=-(\Gamma_1/\Gamma)C_\mu$ and $C_{02}=-(\Gamma_2/\Gamma)C_\mu$ with C_μ given by Eq. (30).

VI. DISCUSSION

In this work we have discussed the currents at the contacts of a system of conductors in response to small time-oscillating changes in the electrochemical potentials at these contacts. Our result for the admittances [Eqs. (4) and (5)] describes the transition from a regime where the samples can be charged at negligible electrostatic-energy expense to a regime where the electrostatic energy completely prevents charge from piling up in the samples. This transition is characterized by an increasing strength of the response of the system to the internal potentials. The internal response is peculiar to interacting carriers, and allows us to restore the invariance under an overall shift of the electrochemical potentials. This invariance is intimately related to total charge conservation. In this description, any gates are included in the system and are treated on equal footing with the conductors.

We have illustrated our results by treating a mesoscopic capacitor as well as a quantum well with capacitive coupling to a gate. If one capacitor plate has the form of a ring,[46] an Aharonov-Bohm effect results, which is peculiar to ac rather than to dc transport.

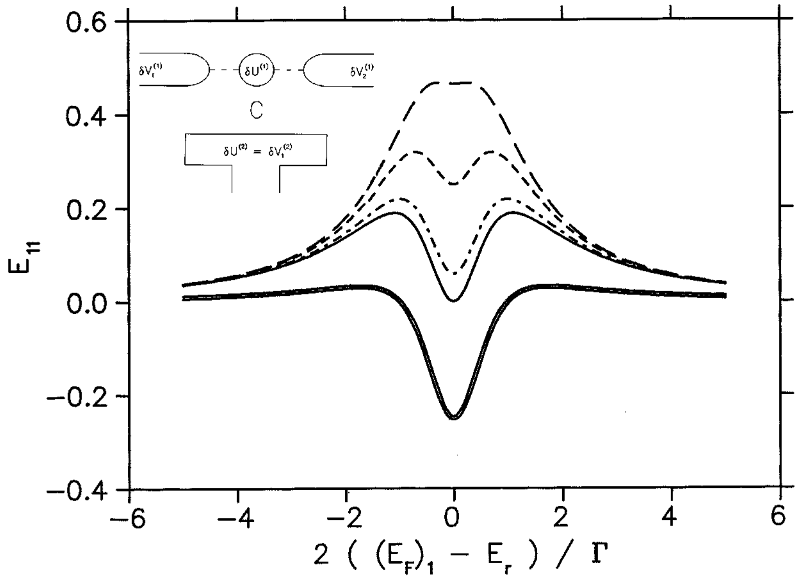

FIG. 6. Dependence of the diagonal admittance element E_{11} on the Fermi energy E_F, for an asymmetrically coupled quantum well (see the inset) with $\Gamma_1/\Gamma=0.75$. E_{11} is in units of $e^2(dN/dE)_{\rm res}(\Gamma_1/\Gamma)$ and is shown as a function of $2(E_F-E_r)/\Gamma$ for $\gamma=0$, 0.25, 0.35, 1, and 10 (from bottom to top). At $\gamma=0$ (double line) the quantum well is charge neutral. At $\gamma=0.25$ (full line) the crossover takes place between kinetic-inductive and capacitive behaviors of $E_{11}(E_F)$ near resonance.

ACKNOWLEDGMENTS

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APPENDIX A: LINEAR RESPONSE VIA RESPONSE KERNEL

In this appendix we find the external linear-current response, Eq. (3), using standard linear response theory.[19,20] The derivation is restricted to the case of a perturbation away from an equilibrium state; i.e. the reference state is an equilibrium state with zero average currents in the leads. A magnetic field is allowed which is constant in the leads and perpendicular to them.

The generalized susceptibilities given in Eqs. (12) and (13) in response to a magnetic perturbation [Eq. (10)] or to an electric perturbation [Eq. (11)], respectively, are given in terms of commutator expectations by the following expressions:[47,20]

$$\kappa^V_{\alpha\beta}(\tau)=-\frac{i}{\hbar}\langle[\hat{I}_\alpha(\tau),\hat{Q}_\beta(0)]\rangle_0\Theta(\tau), \qquad (A1)$$

$$\kappa^\phi_{\alpha\beta}(\tau)=-\frac{i}{\hbar}\langle[\hat{I}_\alpha(\tau),\hat{I}_\beta(0)]\rangle_0\Theta(\tau). \qquad (A2)$$

$d\kappa^V_{\alpha\beta}(\tau)/d\tau=\kappa^\phi_{\alpha\beta}(\tau)$ follows from Eqs. (41) and (42), and from $\langle\hat{I}_\alpha\rangle_0=-\langle d\hat{Q}_\alpha/dt\rangle_0$ by making use of the property $\langle[\hat{A}(\tau),\hat{B}(0)]\rangle_0=\langle[\hat{A}(0),\hat{B}(-\tau)]\rangle_0$. Both perturbations thus give rise to the same ac conductance if $\delta V_\beta=d\delta\phi_\beta/dt$.

In the following we calculate the magnetic response function. From Eqs. (1), (12), and (42), and from $\delta V_\beta(\omega)=-i\omega\delta\phi_\beta(\omega)$ the ac conductance in frequency space is determined by

$$g_{\alpha\beta}(\omega)=\frac{1}{\hbar\omega}\int_0^\infty d\tau e^{i(\omega+i0^+)\tau}\langle[\hat{I}_\alpha(\tau),\hat{I}_\beta(0)]\rangle_0. \qquad (A3)$$

We recall that at moderate frequencies the asymptotic current operator is expressed in terms of incoming and outgoing amplitudes according to Eq. (17). Since no perturbation acts on the sample, the outgoing-amplitude operators are related to the incoming ones according to relation (2). This gives rise to a lead-current operator expressed with the help of a new matrix **A** in the form[4,38]

$$\hat{I}_\alpha(t)=\frac{e}{h}\sum_{\gamma\delta}\int dE'dE''\hat{\mathbf{a}}^\dagger_\gamma(E')A_{\gamma\delta}(\alpha,E',E'')\times\hat{\mathbf{a}}_\delta(E'')e^{i(E'-E'')t/\hbar},$$

$$A_{\gamma\delta}(\alpha,E',E'')=\hat{1}_\alpha\delta_{\alpha\gamma}\delta_{\alpha\delta}-\mathbf{s}^\dagger_{\alpha\gamma}(E')\mathbf{s}_{\alpha\delta}(E''). \qquad (A4)$$

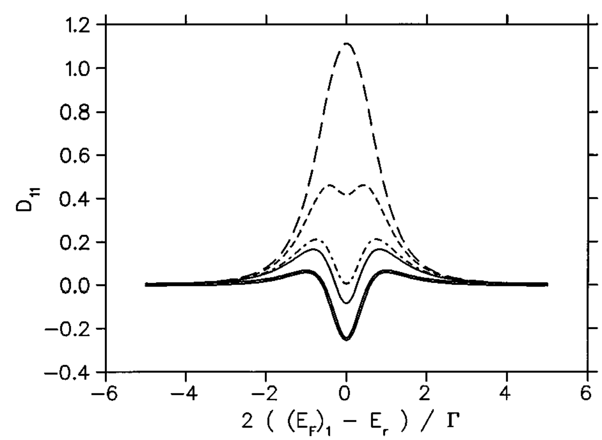

FIG. 7. Dependence of the diagonal admittance element D_{11} on the Fermi energy E_F, for an asymmetrically coupled quantum well with $\Gamma_1/\Gamma=0.75$. D_{11} is in units of $e^4(dN/dE)^2_{\rm res}(h/2e^2)(\Gamma_1/2\Gamma)$ and is shown as a function of $2(E_F-E_r)/\Gamma$ for $\gamma=0$, 0.25, 0.35, 1, and 10 (from bottom to top). At $\gamma=0$ (double line) the quantum well is charge neutral. Around $\gamma=0.35$ (dash-dotted line) the crossover takes place between kinetic-inductive and capacitive behaviors of $D_{11}(E_F)$ near resonance.

The averages $\langle\rangle_0$ are both quantum mechanical and statistical averages in the reference equilibrium state, $\langle\hat{O}\rangle_0=\mathrm{Tr}\{\hat{\rho}_0\hat{O}\}$. Within the independent-electron approximation, the density operator $\hat{\rho}_0$ is determined by the population at equilibrium of the incoming one-particle states, which is just the equilibrium distribution $f(E)$ common to all reservoirs. Defining $\hat{n}_{\beta m}(E)=\hat{a}^{\dagger}_{\beta m}(E)\hat{a}_{\beta m}(E)$ we have $\langle\hat{n}_{\beta m}(E)\rangle_0=f(E)$, and for $A\neq B$ we have $\langle\hat{n}_A\hat{n}_B\rangle_0=\langle\hat{n}_A\rangle_0\langle\hat{n}_B\rangle_0$. In (A4), $\hat{1}_\alpha$ is the identity operator on the space of all active channels in lead α. Strictly speaking it is an energy-dependent operator because the number of open channels increases with increasing energy. However, as discussed in Appendix B, the low-velocity channels with thresholds close to the Fermi energy are weakly coupled to the mesoscopic structure and their contribution may be neglected. Thus at sufficiently low temperatures, such that the region over which $f(E)$ changes is smaller than the typical interchannel energy, it is justified to consider $\hat{1}_\alpha$ as well as the scattering-matrix dimensions, as energy independent.

Since the lead currents vanish at equilibrium, instead of $\hat{I}_\alpha(\tau)$ and $\hat{I}_\beta(0)$ in Eqs. (A2) and (A3) one can equivalently use the current variations $\delta\hat{I}_\alpha(\tau)$ and $\delta\hat{I}_\beta(0)$ defined in Eq. (14). Consequently, the sums and integrals in the operators $\hat{I}_\alpha(\tau)$ and $\hat{I}_\beta(0)$ contain only nondiagonal terms. For example, in Eq. (44) the terms with $\alpha=\gamma$ and $E'=E''$ make no contribution to $\hat{I}_\alpha(t)$.

The quantum statistical average of the commutator in Eq. (43) is

$$\begin{aligned}&\langle[\hat{a}^{\dagger}_{\gamma m}(E)\hat{a}_{\theta n}(\widetilde{E}),\hat{a}^{\dagger}_{\theta' n'}(\widetilde{E}')\hat{a}_{\gamma' m'}(E')]\rangle_0\\&=\delta(E-E')\delta(\widetilde{E}-\widetilde{E}')\delta_{\gamma\gamma'}\delta_{\theta\theta'}\delta_{mm'}\delta_{nn'}\\&\quad\times[f(E)-f(E')]:,\end{aligned}\tag{A5}$$

where again the diagonal terms $(\gamma,n,E)=(\theta,n,\widetilde{E})$ and $(\gamma',n',E')=(\theta',n',\widetilde{E}')$ do not contribute. Furthemore, we use the identity[38]

$$\begin{aligned}&\mathrm{Tr}\left[\sum_{\gamma\theta}A_{\gamma\theta}(\alpha,E,\widetilde{E})A_{\theta\gamma}(\beta,\widetilde{E},E)\right]\\&=\mathrm{Tr}[2\delta_{\alpha\beta}\hat{1}_\alpha-\mathbf{s}^{\dagger}_{\alpha\beta}(E)\mathbf{s}_{\alpha\beta}(\widetilde{E})-\mathbf{s}^{\dagger}_{\beta\alpha}(\widetilde{E})\mathbf{s}_{\beta\alpha}(E)].\end{aligned}\tag{A6}$$

The sum of all terms of the type $\mathrm{Tr}[S^{\dagger}SS^{\dagger}S]$ has given rise to $\mathrm{Tr}[\delta_{\alpha\beta}\hat{1}_\alpha]$ due to the unitarity of the scattering matrix and the cyclic invariance of the trace. After performing the τ-integration, we find

$$\begin{aligned}g_{\alpha\beta}(\omega)=&-\frac{e^2}{2\pi h}\int dE\int d\widetilde{E}\,\mathrm{Tr}[2\delta_{\alpha\beta}\hat{1}_\alpha-\mathbf{s}^{\dagger}_{\alpha\beta}(E)\mathbf{s}_{\alpha\beta}(\widetilde{E})\\&-\mathbf{s}^{\dagger}_{\beta\alpha}(\widetilde{E})\mathbf{s}_{\beta\alpha}(E)]\frac{f(E)-f(\widetilde{E})}{\hbar\omega}\\&\times\frac{1}{i(\hbar\omega+E-\widetilde{E}+i0^+)}.\end{aligned}\tag{A7}$$

The double integral over the product of the scattering matrices can be removed in a direct and elegant way owing to causality requirements.[19,20,11,12] In fact, the scattering matrix is itself a response function. It is related to the retarded T matrix $\mathbf{T}(E)$.[48] Correspondingly the scattering matrix is analytic in the complex upper-half plane: for each scattering element

$$\int_{-\infty}^{+\infty}dE'\frac{\mathbf{s}(E')}{E_1-E'\pm i0^+}=\begin{pmatrix}-2\pi i\mathbf{s}(E_1)\\0\end{pmatrix}.\tag{A8}$$

Regarding the double integral over the first term (the term proportional to the identity), we argue in Appendix B that only the high-velocity states couple effectively to the sample. These states have thresholds much below the Fermi energy. Thus we can extend the lower integration limits, which for each channel are determined by their thresholds, to $-\infty$. The principal value of this double integral vanishes. The total integral proportional to the identity matrix is

$$\begin{aligned}&\int dE\int dE'\frac{f(E)-f(E')}{\hbar\omega+E-E'+i0^+}\\&=-i\pi\int dE[f(E)-f(E+\hbar\omega)].\end{aligned}\tag{A9}$$

With the help of Eq. (A9), and of Eq. (A8) and its complex conjugate, we find Eq. (3) for the admittance.

APPENDIX B: CURRENT OPERATOR IN THE LEADS

In this appendix we justify expression (17) for the asymptotic current operator in lead α, at moderate frequencies, in the presence of a stationary magnetic field $(0,0,B_{0,\alpha})$ constant in the lead and perpendicular to it. For simplicity, carrier motion in the lead is taken to be two dimensional, with x_α the longitudinal coordinate and y_α the transverse coordinate. In the following we drop the subscripts α and 0.

In the perfect lead which is considered to be infinite and invariant under longitudinal translations, the Hamiltonian can be written as

$$\hat{H}=\frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2+V(y),\tag{B1}$$

with $\mathbf{A}(\mathbf{x})=(-By,0,0)$. The motion is separable with a complete set of eigenvectors $\chi_{u,k}(x,y)=f_{u,k}(y)\exp(ikx)$ and energies $E_{u,k}$. We take $f_{u,k}(y)$ to be normalized to unity, $\int dy|f_{u,k}(u)|^2=1$. Writing $k=\sigma|k|$ $(\sigma=\pm1)$ and $E_{u,k}=E$, the two sets of quantum numbers (u,k) and (u,E,σ) are equivalent. The reduced Schrödinger equation in y space is k dependent,

$$\left\{\frac{\hbar^2}{2m}\left[-\frac{d^2}{dy^2}+\left(\frac{y}{l_B^2}+k\right)^2\right]+V(y)-E_{u,k}\right\}f_{u,k}(y)=0,\tag{B2}$$

where $l_B^{-2}=|eB|/\hbar$ defines the magnetic length. Hence, unless $B=0$, $f_{u,k}$ fulfill orthogonality relations only for a common k. The creation and annihilation operators $\hat{\mathbf{a}}(E)$ and $\hat{\mathbf{b}}(E)$ entering the current expression (17) refer to states yielding a nonzero current, and are normalized to carry a constant current flux $\varphi_{u,k}(y)=|hv_{u,k}|^{-1/2}f_{u,k}(y)$, where $v_{u,k}=(1/\hbar)dE_{u,k}/dk$ is the (nonzero) velocity. We set

$\hat{a}_u(E):=\hat{a}_u^{(+)}(E)$ and $\hat{b}_u(E):=\hat{a}_u^{(-)}(E)$. The operator $\hat{a}_u^{(\sigma)}(E)$ annihilates a carrier in the state $|\varphi_{u,E}^{(\sigma)}\rangle$ and has the anticommutation rules $[\hat{a}_u^{(\sigma)}(E),\hat{a}_w^{(\sigma')\dagger}(E')]_+ = \delta_{\sigma\sigma'}\delta_{uw}\delta(E-E')$. A similar normalization is necessary in order for relation (2) between incident and outgoing amplitudes to hold.

The operator of the particle current flowing through the cross section C_x situated at x is $\hat{I}(x,t)=\int_{C_x}dy\hat{j}_x(\mathbf{r},t)$, where

$$\hat{j}_x(\mathbf{r},t)=\frac{e}{2m}[\hat{\Psi}(\mathbf{r},t)^\dagger P_x(\mathbf{r})\hat{\Psi}(\mathbf{r},t)+\text{H.c.}] \tag{B3}$$

is the x component of the current-density operator at point $\mathbf{r}$, with $\hat{\Psi}(\mathbf{r},t)$ designating the field operator and $P_x(\mathbf{r})=-i\hbar\partial/\partial x-eA_x(\mathbf{r})$ designating the kinetic longitudinal momentum at $\mathbf{r}$. We find

$$\hat{I}(x;t)=\sum_{uu'\sigma\sigma'}\int dE\int dE'\hat{a}_u^{(\sigma)\dagger}(E)I_{uu'}^{\sigma\sigma'}(x;E,E') \times\hat{a}_{u'}^{(\sigma')}(E')e^{i(E-E')t/\hbar}, \tag{B4}$$

$$\begin{aligned}I_{uu'}^{\sigma\sigma'}(x;E,E')&=\frac{e}{2m}\int_{C_x}dy[\varphi_{u,k}^*(\mathbf{r})P_x(\mathbf{r})\varphi_{u',k'}(\mathbf{r})\\&\quad+\varphi_{u',k'}(\mathbf{r})P_x^*(\mathbf{r})\varphi_{u,k}^*(\mathbf{r})]\\&=\frac{e\hbar}{2m}e^{i(k'-k)x}\int dy\chi_{u,k}^*(y)\chi_{u',k'}(y)\\&\quad\times\left[k+k'+\frac{2y}{l_B^2}\right].\end{aligned} \tag{B5}$$

Making use of the reduced Schrödinger equation to calculate the eigenvalue difference $(E_{u',k'}-E_{u,k})$, one finds an expression relating the current-matrix elements $I_{uu'}^{\sigma\sigma'}(x;E,E')$ to the energy difference $(E'-E)$:

$$\hbar(k'-k)I_{uu'}^{\sigma\sigma'}(x;E,E')=\frac{e}{h}\frac{E'-E}{|v_{u,k}v_{u',k'}|}e^{i(k'-k)x}\mathcal{U}_{uk,u'k'} \tag{B6}$$

with the overlap integral $\mathcal{U}_{uk,u'k'}=\int dyf_{u,k}^*(y)f_{u',k'}(y)$. Equation (B6) yields well-known exact relations in two particular cases:

(i) If $B=0$, then for $u\neq u'$ the transverse functions are orthogonal, and for $u=u'$ one has $E'-E=(k'^2-k^2)\hbar^2/2m$; hence[38]

$$I_{uu'}^{\sigma\sigma'}(x;E,E')\cong\frac{e}{h}e^{i(k'-k)x}\frac{(v_{u,k}+v_{u',k'})}{2|v_{u,k}v_{u',k'}|^{1/2}}\delta_{uu'} \quad \text{for } B=0. \tag{B7}$$

(ii) If $B\neq 0$ and $E=E'$, then[9]

$$I_{uu'}^{\sigma\sigma'}(x;E,E)=\sigma\frac{e}{h}\delta_{uu'}\delta_{\sigma\sigma'} \quad \text{for any } B. \tag{B8}$$

For a linear-response calculation, whether directly as in Sec. III or more formally as in Appendix A, the matrix elements (B5) have to be evaluated for $E'-E=\hbar\omega$. We concentrate on a range of low frequencies. In particular, we require $\hbar\omega$ to be far smaller than the typical subband spacing ΔE between neighboring channels, so that in Eq. (B6) $k\neq k'$ if $u\neq u'$. To present specific estimates, two types of confining potentials will be considered. We first treat the case of a semiconductor (GaAs) with a small effective mass $m=0.07m_e$ and a wire width of 700 Å. This corresponds to a subband spacing of the order of 2 meV in the absence of a magnetic field. Below we show that for these parameters Eq. (17) has a range of validity for frequencies up to 10^{11} s^{-1}.

Furthermore, for $kT\ll\Delta E$ corresponding to $T\ll$ 10K, the matrix elements are evaluated at the Fermi surface. For a typical Fermi energy of 20 meV, the carriers at the Fermi surface in the lower subbands have longitudinal velocities $v_F\approx 0.3\times 10^8$ cm/s. In the highest occupied subband, on the other hand, the longitudinal velocity v_F of the carriers at the Fermi surface is much smaller, and tends to zero when the Fermi energy approaches the channel threshold. It is clear that expression (17) of the current operator does not hold for subbands with thresholds close to the Fermi energy. However, in reality, these subbands are susceptible to the smallest amount of disorder and might in fact be localized. It is, therefore, reasonable to estimate the accuracy of Eq. (17) for subbands with relatively high longitudinal velocities (here we consider 0.7×10^7 cm/s $<v_F<0.3\times 10^8$ cm/s) and to neglect the contribution of the subbands with lower v_F (''low-velocity cutoff''). This point will be discussed in more detail at the end of this appendix.

We now show that all off-diagonal current-matrix elements $I_{uu'}^{\sigma\sigma'}$, $(u,\sigma)\neq(u',\sigma')$, may be neglected for frequencies up to 10^{11} s^{-1}. We make use of the Schwartz inequality $|\int dyf_{u,k}^*(y)f_{u',k'}(y)|<1$ and of the fact that the subbands become flatter for increasing magnetic field, $\hbar|k|/m\geq v_F$, where v_F is an average longitudinal Fermi velocity of the subbands u,u' in the presence of an arbitrary B. In the case $\sigma'=-\sigma$ of opposite k vectors, $|k'-k|\approx 2k_F\geq 2mv_F/\hbar$, for the magnitude of the matrix elements in Eq. (B6), we obtain

$$|I_{uu'}^{\sigma,-\sigma}|<\frac{e}{h}\frac{\hbar\omega}{2mv_F^2}, \tag{B9}$$

which is less than 1–2 % of e/h for frequencies $\omega=(E'-E)/\hbar$ up to 10^{11} s^{-1}, where the low-velocity cutoff has been used. In the case $\sigma'=\sigma$, we evaluate the integral in Eq. (B6) for a parabolic confining potential $V(y)=m\omega_y^2y^2/2$, where ω_y is taken to be 0.3×10^{13} s^{-1}. This potential yields eigenfunctions and eigenvalues

$$f_{u,k}(y)=f_u^{(\Omega)}\left(y+\frac{\omega_c}{\Omega^2}\frac{\hbar k}{m}\right), \tag{B10}$$

$$E_{u,k}=(u+\tfrac{1}{2})\hbar\Omega+\left(\frac{\omega_y}{\Omega}\right)^2\frac{\hbar^2k^2}{2m}, \tag{B11}$$

and a velocity $v_{u,k}=(\omega_y/\Omega)^2\hbar k/m$. Here $\omega_c=|eB|/m=(\hbar/ml_B^2)$ is the cyclotron frequency and $\Omega^2=\omega_c^2+\omega_y^2$. The harmonic-oscillator eigenfunctions $f_u^{(\Omega)}$ form an orthonormal set $\langle f_u^{(\Omega)}|f_{u'}^{(\Omega)}\rangle=\delta_{uu'}$ with spatial width $(\langle\Delta y^2\rangle_u)^{1/2}=l^{(\Omega)}(u+1/2)^{1/2}$, where $l^{(\Omega)}=(\hbar/m\Omega)^{1/2}$ is the zero-point amplitude of the oscillator with frequency Ω. From the dispersion relation (B11), one obtains the wave-number difference $k'-k=\sigma[(u-u')\Omega+\omega]/v_F$.

The current-matrix element for $\sigma=\sigma'$, $u\neq u'$ may for $\omega\ll\Omega$ be written as

$$I^{\sigma\sigma}_{uu'}(x;E,E+\hbar\omega)\approx\sigma\frac{e}{h}\frac{\omega}{(u-u')\Omega}e^{i(k'-k)x}\mathcal{U}_{uu'}\left(\frac{a_{k'-k}}{l^{(\Omega)}}\right), \quad \text{(B12)}$$

where $\mathcal{U}_{uu'}(a/l^{(\Omega)})=\mathcal{U}_{uk,u'k'}$ is the overlap integral of the eigenfunctions of two harmonic oscillators located at a distance a, and $a_{k'-k}=(\omega_c/\Omega^2)\hbar(k'-k)/m\approx\sigma(u-u')\hbar\omega_c/(\Omega m v_F)$. Since the overlap integral satisfies $|\mathcal{U}_{uu'}|<1$, this matrix element is also less than 1–2 % of e/h for frequencies ω up to 10^{11} s^{-1}.

For the diagonal current matrix element, $u=u',\sigma=\sigma'$, one finds

$$I^{\sigma\sigma}_{uu}(x;E,E+\hbar\omega)=\frac{e}{h}e^{i(k'-k)x}\frac{(v_{u,k}+v_{u,k'})}{2|v_{u,k}v_{u,k'}|^{1/2}}\mathcal{U}_{uu}\left(\frac{a_0}{l^{(\Omega)}}\right), \quad \text{(B13)}$$

with $a_0=-\sigma(\omega\omega_c/\Omega^2)\hbar/(mv_F)$. Since f_u is normalized, $\mathcal{U}_{uu}(0)=1$. Hence $\mathcal{U}_{uu}(a_0/l^{(\Omega)})=1$ for $B=0$, and $\mathcal{U}_{uu}(a_0/l^{(\Omega)})\rightarrow 1$ for high magnetic fields, because in this limit the distance $a_0\propto 1/B$ vanishes more strongly than the width $l^{(\Omega)}\propto 1/B^{1/2}$. For intermediate magnetic fields, an algebraic evaluation of the integral $\mathcal{U}_{uu}$ shows that always $|\mathcal{U}_{uu}(a_0/l^{(\Omega)})-1|\leqslant 0.01$. This holds even in the worst case of a minimal longitudinal Fermi velocity $v_F=0.7\times 10^7$ cm/s and a maximal band number $u=10$. Thus we obtain the same result as for zero magnetic field, see Eq. (B7). Further, the phase factor $e^{i(k'-k)x}$ may be replaced by unity, because for longitudinal Fermi velocities of at least 0.7×10^7 cm/s, the phase $(k'-k)x\approx\sigma(\omega/v_F)x$ (Ref. 4) is practically constant over the typical dimension of a mesoscopic conductor for frequencies up to 10^{11} Hz. Thus the asymptotic x dependence of the phase factors can be dropped. Similarly $(v_{u,k}+v_{u,k'})(2|v_{u,k}v_{u',k'}|^{1/2})^{-1}\cong\sigma$ owing to the low-velocity cutoff.

Let us next consider the case of hard-wall confining potential. To be specific we take a lead width of 300 Å and use the free-electron mass. A Fermi energy of 5 eV is used. For simplicity we treat the wire as two dimensional. The lowest subband has a longitudinal velocity $v_F\approx 1.2\times 10^8$ cm/s. We omit the current contribution of states with $v_F\lesssim 0.7\times 10^7$ cm/s (low-velocity cutoff). In the case $\sigma'=-\sigma$ of opposite k vectors, we then obtain, according to (B9), $|I^{\sigma,-\sigma}_{uu'}|<0.01e/\hbar$ for frequencies ω up to 10^{12} s^{-1}. In the case $\sigma'=\sigma$, $u\neq u'$, the condition $\hbar\omega\ll\Delta E$ implies $(k'-k)^{-1}\approx(E_{u,k_F}-E_{u',k_F})^{-1}\hbar v_F$, where k_F and v_F are an average k vector and an average longitudinal velocity of the two subbands at the Fermi energy. Then

$$I^{\sigma\sigma}_{uu'}(x;E,E+\hbar\omega)\approx\sigma\frac{e}{h}e^{i(k'-k)x}\hbar\omega\frac{\mathcal{U}_{uk,u'k'}}{(E_{u,k_F}-E_{u',k_F})} \quad \text{(B14)}$$

for $u\neq u'$, and

$$I^{\sigma\sigma}_{uu}(x;E,E+\hbar\omega)=\frac{e}{h}e^{i(k'-k)x}\frac{(v_{u,k}+v_{u,k'})}{2|v_{u,k}v_{u,k'}|^{1/2}}\mathcal{U}_{uk,uk'} \quad \text{(B15)}$$

for the diagonal elements. The transverse eigenfunctions for hard walls with infinite potential steps vanish beyond the lead edges $y=\pm w/2$ and satisfy Eq. (B2) with $V(y)=0$ for $-w/2<y<w/2$. The exact solution for this confining potential are parabolic cylinder functions. However for our purpose more insight is gained by working in the WKB approximation. The energy eigenvalues $E_{u,k}$ are determined by quantization conditions on the action integral $\oint p(y;y_0,E)dy$ extended over the classical paths, where $p(y;y_0,E)=\pm[2mE-(m\omega_c(y-y_0))^2]^{1/2}$ and $y_0=-kl_B^2$ are the classical momentum and the center of the classical orbit, respectively. In the (E,y_0) plane there are three different regions delimited by $E=E_\pm(y_0)=m\omega_c^2(y_0\pm w/2)^2/2$: (i) if $E<E_\pm(y_0)$, the electron does not feel any wall, and from $\oint pdy=(u+\frac{1}{2})\hbar$ we find $E_{u,k}=\hbar\omega_c(u+\frac{1}{2})$; (ii) if $E_-<E<E_+$ or $E_+<E<E_-$, then the electron feels one of the walls, and $E_{u,k}$ has to be determined numerically from $\oint pdy=(u+\frac{3}{4})\hbar$; if in particular $y_0=\pm w/2$ then $E_{u,k}=\hbar\omega_c(2u+\frac{3}{2})$; and (iii) if $E>E_\pm(y_0)$, the electron feels both walls, and $E_{u,k}$ has to be determined numerically from $\oint pdy=(u+1)\hbar$; in this region a WKB approximation $f_{u,k}(y)\propto p^{-1/2}\sin[\int_{-w/2}^{y}pdy']$ is well defined and for $E\gg E_\pm(y_0)$ tends to the solution of a free particle in a box of width w. The WKB energy levels are quite accurate except around the discontinuities at the borders between regions (i), (ii), and (iii). The results show that the distance between the subbands is minimal at the subband bottoms and increases with increasing magnetic field and subband quantum number. Those parts of the bands corresponding to region (i), which are completely flat in the WKB approximation, contribute a negligible amount to the current in virtue of the low-velocity cutoff. In the higher subbands $(u\gtrsim(w/l_B)^2/2)$ corresponding to region (iii), the overlap integrals satisfy in good approximation $\mathcal{U}_{uk,u'k'}=\delta_{uu'}$. More caution is needed for the lower subbands which are strongly influenced by the magnetic field. Particularly critical for the evaluation of (B14) and (B15) are those parts of the subbands corresponding to the transition from region (i) to region (ii), where the energy starts to deviate from the band bottom at $E_{u,k}=(u+1/2)\hbar$, because for $u\neq u'$ they give rise to the smallest denominators $|E_{u,k_F}-E_{u',k_F}|$, and for $u=u'$ to the smallest overlap $\mathcal{U}_{uk,uk'}$. A transverse eigenfunction of subband u in region (ii) is typically proportional to $f^{(\omega_c)}_{2u+1}(z\mp w/2)$ if $z_0\approx\pm w/2$ is near the wall, and is well approximated by $f^{(\omega_c)}_u(z-z_0)$ when approaching region (i). With these trial functions and the WKB solution in (iii), we have estimated the overlap integrals for the worst cases. In general we find $|\mathcal{U}_{uk,u'k'}|/|E_{u,k_F}-E_{u',k_F}|\leqslant 1/(4\Delta E)$ for $u\neq u'$, and $||\mathcal{U}_{uk,uk'}|-1|\leqslant 0.02$. Here $\Delta E=3(\hbar^2/2m)\times(\pi/w)^2=$ 1.5 meV is the minimal subband spacing. By the same reasoning as for light carriers, the matrix element [(B14) and (B15)] is further reduced to $I^{\sigma\sigma}_{uu'}=\sigma(e/h)\delta_{uu'}$ within 1–2 % for arbitrary magnetic field and frequencies ω up to 10^{11} s^{-1}.

In conclusion, one can neglect all off-diagonal matrix elements $I^{\sigma\sigma'}_{uu'}(x;E,E')$, $(u,\sigma)\neq(u',\sigma')$, for frequencies up to 10^{11} s^{-1}. For any magnetic field we recover the asymptotic current operator in Eq. (17), with matrix elements of the form

$$I^{\sigma\sigma'}_{uu'}(E,E')\cong\sigma\frac{e}{h}\delta_{uu'}\delta_{\sigma\sigma'}. \tag{B16}$$

This conclusion, however, is valid only if the low-velocity states can be considered to be weakly coupled to the mesoscopic structure. This avoids any divergence arising for longitudinal velocities tending to zero (Fermi energies tending to a channel threshold). On the one hand, one can say that the cutoff of all longitudinal velocities below a $v_{\rm min}$ while taking into account longitudinal velocities at the Fermi energy up to a $v_{\rm max}\gtrsim 5v_{\rm min}$ corresponds to neglecting in average less than 4% of the active channels relevant to the current. This is so because the subbands are equally spaced in the worst case, while the longitudinal energy is approximately quadratic in the longitudinal velocity. On the other hand, according to the microscopic expression we have derived, the current displays considerable fluctuations as the Fermi energy approaches a channel threshold. But we expect the prediction of these fluctuations not to be reliable. In fact we expect the phase of a carrier in a low-velocity state to be more easily randomized, because the lower the velocity, the shorter the effective dephasing/inelastic length, and the more difficult it is to fulfill the coherence condition for such a slow carrier inside the mesoscopic sample. In this sense we consider low-velocity carriers as being weakly coupled to the mesoscopic transport.

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