Frequency-dependent admittance of a two-dimensional quantum wire

Jian Wang

Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong

Hong Guo

Centre for the Physics of Materials and Department of Physics, McGill University, Montréal, Québec, H3A 2T8 Canada
(Received 19 June 1996; revised manuscript received 7 August 1996)

The frequency-dependent conductance of a two-dimensional quantum wire is computed using a current-conserving formalism. The correction to the dc conductance due to a time-dependent potential is related to the local partial density of states, which we compute numerically. The current conservation is explicitly confirmed by computing the global density of states and comparing it with a quantity that is related to the electron dwell time. Our calculation clearly reveals the physical meaning of the various partial densities of states. [S0163-1829(96)52940-1]

The physics associated with quantum conduction in various low-dimensional systems has been a major focus in current solid state research. Due to advances in controlled crystal growth and lithographic techniques, it is now possible to fabricate various two-dimensional submicrometer structures where accurate experimental measurements can be made.[1] On the theoretical side, the understanding of quantum transport in these very small systems has been advanced by the Landauer theory[2] of one-dimensional transport. In cases where multiprobes are attached to the conductor, Büttiker has provided a useful formula for computing various conductances.[3] The Landauer-Büttiker formalism has been applied to a large class of quantum transport problems in the mesoscopic and ballistic regimes where the external potential is static. On the other hand, when the external potential has a time-dependent oscillating component, the Landauer-Büttiker formalism cannot be directly applied. As shown by Büttiker and his co-workers,[4] a direct application of the original approach of the Landauer-Büttiker formalism, where the internal electric potential distribution is not needed, cannot yield electric current and charge conservation. Hence the coherent quantum transport theory for mesoscopic and ballistic conductors must be extended when time-varying external potentials are to be included. Clearly the problem of computing frequency-dependent conductance for mesoscopic and ballistic conductors is a very important subject from both theoretical and application points of view.

Recently in a series of articles, Büttiker and co-workers[4–7] have developed a theoretical formalism for investigating frequency-dependent coherent quantum transport for mesoscopic and ballistic conductors when electric potential in the leads far away from the scattering region of the conductor is time varying. This is an important advance in the theory of mesoscopic physics and warrants further development of the theory and application. In simple one-dimensional systems such as a δ-function potential, a perfect quantum wire, or a 1D quantum well, the frequency-dependent admittance can be explicitly calculated since the scattering matrix can be obtained analytically.[7] However, in truly 2D systems the application of the formalism is less straightforward. This is due partly to technical difficulties of computing certain quantities

such as the various partial density of states (PDOS, see below). These quantities, which appear naturally in the theoretical formulation of the problem,[4] have a deep physical meaning which is not obvious and needs to be revealed. To the best of our knowledge, there are so far no studies and direct calculations[8] of the various partial density of states in 2D. But these quantities must be obtained if the frequency-dependent admittance is to be computed from first principles. The purpose of this paper is to report our investigations on the dynamic transport properties of a 2D quantum wire system.

In particular, we consider a T-shaped quantum wire structure as shown in Fig. 1. The two probes extend to $x = \pm\infty$ while the scattering region is provided by the T-shaped junction as shown being bounded by the two dotted lines. This 2D quantum wire has been studied by many authors[9,10] for the case of static transport. While this is a simple 2D system, we found that much physical intuition about various quantities can be obtained for the dynamic transport (see below). We have computed the frequency-dependent admittance for this system using the current conserving formalism of Ref. 4. The correction to the dc conductance due to a time-dependent potential is related to the local partial density of states, which we compute numerically. The current conservation is explicitly confirmed by computing the global density of states and comparing it with a quantity which is related to the electron dwell time. Our direct calculation clearly reveals the physical meaning of the partial density of states, which plays an essential role in the dynamic transport theory.

For the sake of presentation we briefly review the current conserving dynamic transport formalism of Büttiker, Thomas, Prêtre, Gasparian, and Christen.[4,7] Their theory proceeds in three steps. The first step is to determine
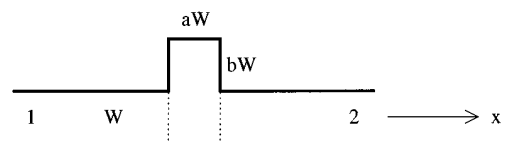

FIG. 1. Schematic plot of the T-shaped quantum wire. The wire width is W, the side-stub width and height is aW and bW. The two dotted lines separate the scattering region from the two probes.
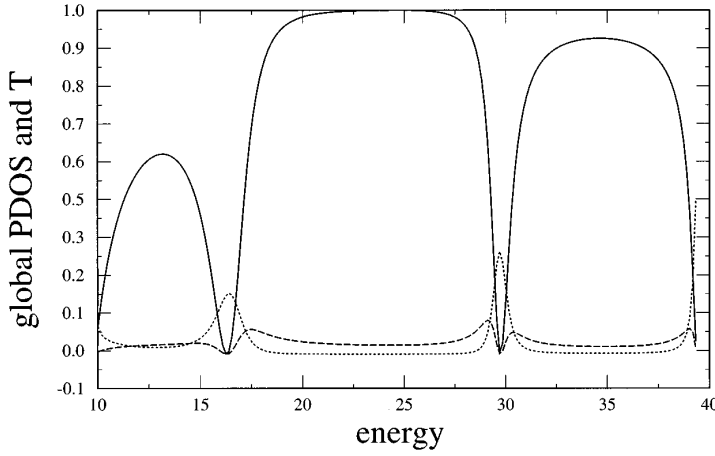
FIG. 2. Global partial density of states and the transmission coefficient as functions of electron energy E. Solid line: transmission coefficient T_{21}; dotted line: dN_{11}/dE; dashed line: dN_{21}/dE. Unit of energy is $\hbar^2/(2mW^2)$.

the current and charge density response of the system to the time variation of the external potential. This leads to an admittance matrix with elements given by, to first order in ω,

$$g^e_{\alpha\beta}(\omega) = g^e_{\alpha\beta}(0) - i\omega e^2 (dN_{\alpha\beta}/dE), \qquad (1)$$

where the first term on the right hand side is the admittance (conductance) when frequency $\omega = 0$ and this term is given by the usual Büttiker multiprobe conductance formula.[3] The second term gives a correction due to the time dependence of the external potential, and is determined by the global partial density of states[7] (global PDOS), $dN_{\alpha\beta}/dE$. Here the indices $\alpha\beta$ denote scattering from a probe labeled by β to that labeled by α. This admittance matrix $g^e_{\alpha\beta}(\omega)$ does not conserve current, since $\Sigma_\alpha g^e_{\alpha\beta}(\omega) \neq 0$. To correct this problem, one must consider the internal potential distribution induced by the external perturbation. This is computed in the second step of the theory,[4] and the result is rather simple if only Thomas-Fermi linear screening is included. In the final step, one computes the currents in the probes induced by this internal potential distribution, which leads to an additional term in the admittance matrix. Thus the total admittance is given by $g^I = g^e + g^i$, with

$$g^i_{\alpha\beta} = i\omega e^2 D_{\alpha\beta} \qquad (2)$$

and

$$D_{\alpha\beta} \equiv \int d\mathbf{r} \left[\frac{dn(\alpha,\mathbf{r})}{dE} \right] \left[\frac{dn(\mathbf{r})}{dE} \right]^{-1} \left[\frac{dn(\mathbf{r},\beta)}{dE} \right]. \qquad (3)$$

In Eq. (3) the quantity $dn(\mathbf{r},\alpha)/dE$ is the *injectivity*, which measures the additional local charge density brought into the sample by the oscillating chemical potential at probe α. Without a magnetic field, the *emissivity* $dn(\beta,\mathbf{r})/dE$ equals to the injectivity. It was shown[7] that these quantities could be computed from the electron dwell time or the scattering Green function. Finally, the total local density of states is $dn(\mathbf{r})/dE = \Sigma_\alpha dn(\alpha,\mathbf{r})/dE$. With these expressions, we obtain the final formula for the frequency-dependent admittance to linear order in ω,

$$g^I_{\alpha\beta}(\omega) = g^e_{\alpha\beta}(\omega=0) - i\omega e^2 \left(\frac{dN_{\alpha\beta}}{dE} - D_{\alpha\beta} \right). \qquad (4)$$

It is now straightforward to prove that current is conserved since the admittance matrix g^I satisfies $\Sigma_\alpha g^I_{\alpha\beta}(\omega) = 0$. This

can be seen by realizing that $\Sigma_\alpha dN_{\alpha\beta}/dE \equiv d\bar{N}_\beta/dE$ is the injectance which is identical to $\Sigma_\alpha D_{\alpha\beta}$.

Let us apply this formalism to the T-shaped 2D conductor. The incident electron comes from probe 1, it scatters at the T junction, and then reflects back to probe 1 or transmits to probe 2. To be concrete we have fixed the wire width to be W; the width and height of the side stub are fixed at aW and bW with $a=b=1$. The units are fixed by $\hbar^2/2m=1$ with m the effective mass of the electron, and lengths measured in terms of W. For simplicity we have focused on the first *transport* subband only, thus the incoming electron energy is restricted: $(\pi/W)^2 < E < (2\pi/W)^2$. In this case elements of the scattering matrix $\mathbf{s}_{\alpha\beta}$ are simple complex numbers. With more than one subband they become matrices in the subband space. However, the computation proceeds in a similar fashion with one or more than one subband. We have solved the quantum scattering problem using a mode matching method,[10] where the wave function in the scattering region was expanded using a suitable basis set and in particular 50 modes were included. We have checked the convergence that including more modes in the scattering region essentially does not change the results. The scattering probabilities were obtained by matching the wave functions and their derivatives at the boundaries between the scattering region and the probes.

To compute the admittance we need to know various partial density of states. These quantities turn out to have very interesting and physically clear properties once they are plotted. The global PDOS is related to the scattering matrix, and is approximately given by[4,7]

$$\frac{dN_{\alpha\beta}}{dE} = \frac{1}{4\pi i} \left(s^\dagger_{\alpha\beta} \frac{ds_{\alpha\beta}}{dE} - \frac{ds^\dagger_{\alpha\beta}}{dE} s_{\alpha\beta} \right). \qquad (5)$$

For a finite scattering volume there are corrections to this expression of the order $O(\lambda/L)$ where λ is the electron wavelength and L the system size.[7] For large system sizes or large energies, Eq. (5) is adequate. Later when we check the current conservation, the correction term will be added. Since in 2D the expression for the scattering matrix cannot be written down analytically, we have decided to perform the energy derivatives of (5) numerically. In particular we computed $s_{\alpha\beta}(E)$ at various values of energy E and used a five-point numerical derivative to find $ds_{\alpha\beta}/dE$. The behavior of
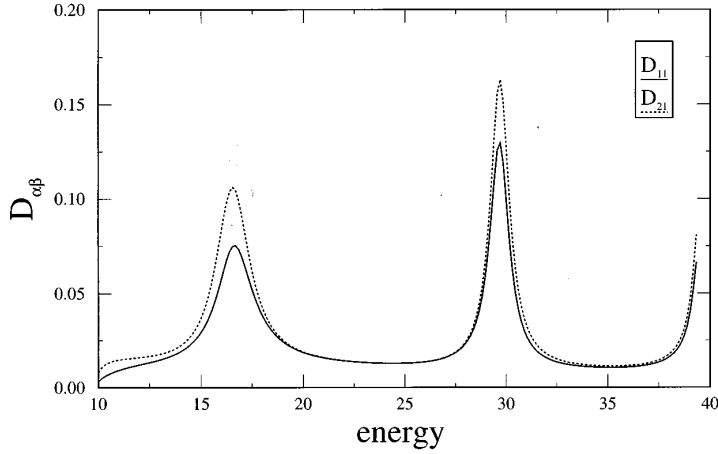
FIG. 3. The current response to the internal potential, $D_{\alpha\beta}$, as a function of energy E. Solid line: D_{11}; dotted line: D_{21}.

the global PDOS is plotted in Fig. 2 together with the transmission coefficient $T_{21}(E)$. As our quantum wire system is very transmissive, T_{21} has large values in general except at the two resonance levels where $T=0$. In a previous work we have shown that the energies where $T=0$ correspond to the quasibound states located in the T junction.[10] The behavior of the global partial density of states coincides well with that of the transmission coefficients. In particular, dN_{11}/dE, which is the global PDOS for reflection, peaks at the energies where the transmission coefficient is minimum or reflection maximum. On the other hand, dN_{21}/dE, which is the global PDOS for transmission, takes minimum value when T is minimum. Indeed, a general discussion for a one-dimensional system with a symmetric scatterer[7] reveals that $dN_{11}/dE \sim R \, dN/dE$ while $dN_{21}/dE \sim T \, dN/dE$ with R and T the reflection and transmission coefficients, and dN/dE the global DOS. Hence these quantities have vivid physical meaning.

The next quantity of interest is $D_{\alpha\beta}$ given by Eq. (3). To compute this quantity, we first find the injectivity which is given by the scattering wave function[4] in the T junction. At zero temperature this is given by

$$\frac{dn(\mathbf{r},\alpha)}{dE} = \frac{1}{hJ}|\psi(\mathbf{r})|^2, \qquad (6)$$

where J is the incoming particle flux. Clearly a spatial integration of this quantity gives the electron dwell time[11,10]

τ_α. In general $D_{\alpha\beta}$ is obtained with two calculations of the wave function for particles coming from the left and from the right. Figure 3 shows this quantity as a function of the electron energy. Both $D_{11}(E)$ and $D_{21}(E)$ peak at the energies where the transmission takes the minimum values. This is understandable since these special energies correspond to the scattering states[10] where the electron dwell time takes maximum value, and the injectivity represents essentially the electron dwelling in an area $d\mathbf{r}$ at position $\mathbf{r}$ irrespective of where it is finally scattered.

With the global partial density states and the quantity $D_{\alpha\beta}$ calculated, we have thus obtained the admittance $g^I_{\alpha\beta}(\omega)$ from Eqs. (1), (2), and (4). Figure 4 shows the ω-dependent part of g^I, $\hat{g}_{\alpha\beta} \equiv dN_{\alpha\beta}/dE - D_{\alpha\beta}$, as a function of energy E. Apart from the prefactor ωe^2, this quantity $\hat{g}$ is the imaginary part of the admittance, and is called *emittance*. At the quasibound state levels where transmission coefficient $T_{21}(E)$ takes minimum values, $\hat{g}_{\alpha\beta}(E)$ also takes extremal values. It is interesting to observe that the transmissive part $\hat{g}_{21}$ takes minimum value where $T(E)=0$, while the reflective part $\hat{g}_{11}$ takes maximum value at the same energy. Thus in this sense, the dynamic part of the admittance $\hat{g}_{\alpha\beta}$ has the same behavior as the static admittance $g_{\alpha\beta}(\omega=0)$ as a function of energy. Furthermore, $\hat{g}_{\alpha\beta}$ changes sign as energy is varied: the system responds either capacitively when $\hat{g}_{11}=-\hat{g}_{21}=-\hat{g}_{12}>0$, or inductively otherwise. Hence at the resonance (where $T\approx 0$ for our system) $\hat{g}_{21}$ and $\hat{g}_{11}$ are
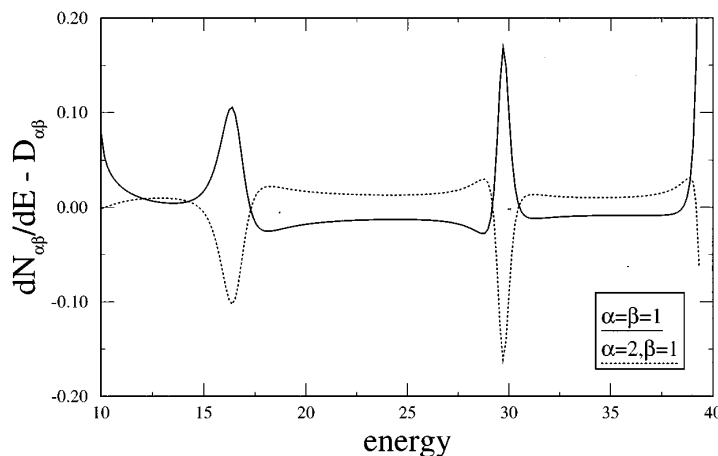

FIG. 4. The imaginary part (dynamic part) of the admittance, $\hat{g}_{\alpha\beta} \equiv dN_{\alpha\beta}/dE - D_{\alpha\beta}$, as a function of energy.
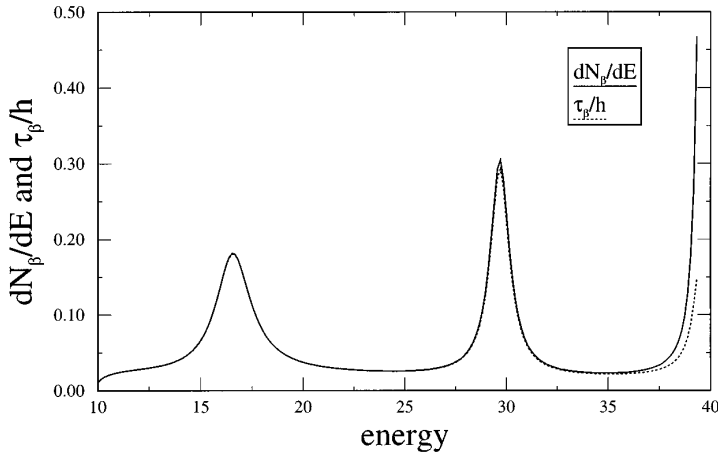
FIG. 5. Explicit confirmation of the current conservation, Eq. (8). Solid line: dN_β/dE given by Eq. (7) and $\beta=1$; dotted line: $\tau_\beta/h = \Sigma_\alpha D_{\alpha\beta}$ with $\beta=1$.

capacitive. Figure 4 shows the clear crossover between the capacitive and inductive responses for this 2D quantum wire as energy is changed.

We can now explicitly confirm the current conservation by summing up the admittance matrix elements and check whether or not $\Sigma_\alpha g^I_{\alpha\beta}=0$. Since the global PDOS obtained using Eq. (5) is not exact, a correction should be added. For a 1D system Gasparian *et. al.*[12] have shown that

$$\frac{dN_\beta}{dE} \equiv \sum_\alpha \frac{dN_{\alpha\beta}}{dE} + \text{Im}\left(\frac{s_{\beta\beta}}{4\pi E}\right), \qquad (7)$$

where E is the electron energy. Unfortunately for a 2D system such as ours, the Green's function cannot be written down analytically, hence how to derive a similar correction term to that in (7) is unclear. However, since we have numerical results of all the quantities, a reasonable correction term can easily be obtained. We found that the same form as (7) led to almost perfect current conservation, provided we use the *transport* energy k^2 as the energy E in (7). Our data in Fig. 5 clearly and unambiguously show that the following is established:

$$\sum_\alpha \frac{dN_{\alpha\beta}}{dE} + \text{Im}\left(\frac{s_{\beta\beta}}{4\pi k^2}\right) = \sum_\alpha D_{\alpha\beta}. \qquad (8)$$

With this result, we have thus explicitly shown[13] the current conservation $\Sigma_\alpha g^I_{\alpha\beta}=0$. Since the correction term is inversely proportional to k^2, it plays a role only at small k. This can already be seen in Fig. 4 where the two curves add up to zero except at low energies.

In summary we have implemented the current conserving dynamic conductance formalism for 2D metallic conductors. In the simple case of applying Thomas-Fermi linear screening for the interacting electrons (hence the analysis is more suitable for metallic samples), the current response to the internal potential can be computed from the electron dwell time using the scattering wave functions. The frequency-dependent admittance of a T-shaped 2D quantum wire is calculated to linear order in frequency. We have explicitly confirmed the electric current conservation and found that a correction to the total density of states is needed at low energies, in the same fashion as that of 1D case. It is very interesting to clarify the physical meaning of the partial DOS. These quantities provide information on the density of carriers *and* the transmission of carriers from one contact to another. At quantum resonances these quantities take extremal values. There are many further applications of this important theoretical formalism, to situations involving multimode, magnetic fields, and nonlinear screening. Another very challenging extension is to push the theory to higher order in frequency[7] and formulate the theory in a way that permits a computational implementation. We hope to be able to report these results in the future.

[1] See, for example, articles in *Nanostructure Physics and Fabrication*, edited by Mark A. Reed and Wiley P. Kirk (Academic Press, New York, 1989).

[2] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957).

[3] M. Büttiker, Phys. Rev. B **38**, 9375 (1988); Phys. Rev. Lett. **57**, 1761 (1986).

[4] M. Büttiker, H. Thomas, and A. Prêtre, Z. Phys. B **94**, 133 (1994).

[5] M. Büttiker, A. Prêtre, and H. Thomas, Phys. Rev. Lett. **70**, 4114 (1993); M. Büttiker and H. Thomas, in *Quantum-Effect Physics, Electronics and Applications*, edited by K. Ismail *et al.*, Institute of Physics Conference Series No. 127, Bristol, 1992 (IOP, Bristol, 1992), p. 19.

[6] T. Christen and M. Büttiker, Phys. Rev. B **53**, 2064 (1996); and (unpublished).

[7] V. Gasparian, T. Christen, and M. Büttiker, Phys. Rev. A **54** (to be published).

[8] Liu *et al.* have investigated dynamic magnetoconductance of a quasi-1D dirty wire using a phenomenological constant to account for the self-consistent internal potential response, rather than using the full theory by computing the local density of states. See D.Z. Liu, Ben Yu-Kuang Hu, C.A. Stafford, and S. Das Sarma, Phys. Rev. B **50**, 5799 (1994).

[9] F. Sols, M. Macucci, U. Ravaioli, and K. Hess, Appl. Phys. Lett. **54**, 350 (1989).

[10] Jian Wang, Yongjiang Wang, and Hong Guo, Appl. Phys. Lett. **65**, 1793 (1994).

[11] M. Büttiker, Phys. Rev. B **27**, 6178 (1983).

[12] V. Gasparian *et al.*, Phys. Rev. B **51**, 6743 (1995).

[13] Near the second subband threshold, there seems to be a small but systematic deviation to the equal sign of Eq. (8). This deviation could be due to the fact that the transmission probability has sharp changes in its value near the onset of the second subband and Eq. (8) does not include multipropagating modes.