Current conservation in two-dimensional AC-transport

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The electric current conservation in a two-dimensional quantum wire under a time dependent field is investigated. Such a conservation is obtained as the global density of states contribution to the emittance is balanced by the contribution due to the internal charge response inside the sample. However when the global partial density of states is approximately calculated using scattering matrix only, correction terms are needed to obtain precise current conservation. We have derived these corrections analytically using a specific two-dimensional system. We found that when the incident energy $E$ is near the first subband, our result reduces to the one-dimensional result. As $E$ approaches to the $n$-th subband with $n > 1$, the correction term diverges. This explains the systematic deviation to precise current conservation observed in a previous numerical calculation.

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1 Introduction

The dynamic conductance of a quantum coherent mesoscopic system under a time dependent external field is the subject of recent interests[1, 2, 3, 4, 5]. In contrast to dc-transport where the internal potential distribution inside the sample does not appear explicitly, the AC-response depends sensitively on the internal potential distribution. This internal potential is due to the charge distribution generated by the applied AC-field at the leads and it has to be determined self-consistently[1]. So far there are two approaches to the coherent AC-transport problem. One is to derive a formal linear response to a given potential distribution in the sample[6]. The difficulty with such an approach is that the potential distribution is not known a priori. Another approach is to investigate the AC-response to an external perturbation which prescribes the potentials in the reservoirs only[7, 1]. The external potentials effectively determine the chemical potential of the reservoirs and the potential distribution in the conductor must be considered a part of the response which is to be calculated self-consistently. In this approach, Böttiker and his coworkers[1, 8] have formulated a current conserving formalism for the low frequency admittance of mesoscopic conductors.

In the theory of Böttiker, Prêtre and Thomas[1], it is necessary to consider the Coulomb interactions between the many charges inside the sample, in order to preserve the current conservation. For a multi-probe conductor the low frequency admittance is found to have the form[8, 9] \[ G_{\alpha\beta}(\omega) = G_{\alpha\beta}(0) - i\omega E_{\alpha\beta} + O(\omega^2), \]
where \( G_{\alpha\beta}(0) \) is the dc-conductance, \( E_{\alpha\beta} \) is the emittance[8], and \( \alpha \) (or \( \beta \)) labels the probe. The emittance \( E_{\alpha\beta} \) describes the current response at probe \( \alpha \) due to a variation of the electro-chemical potential at probe \( \beta \) to leading order with respect to frequency \( \omega \). It can be written as[8, 5] \[ E_{\alpha\beta} = \frac{dN_{\alpha\beta}}{dE} - D_{\alpha\beta}, \]
where the term \( \frac{dN_{\alpha\beta}}{dE} \) is the global partial density of states (GPDOS)[10] which is related to the scattering matrix. It describes the density of states of carriers injected in probe \( \beta \) reaching probe \( \alpha \) and is a purely kinetic term. The term \( D_{\alpha\beta} \) is due to the Coulomb interaction of electrons inside the sample and is a term of capacitive nature. \( D_{\alpha\beta} \) can be computed from the local density of states[1, 8] which is related to the electron dwell times. Electric current conservation, namely \( \sum_\alpha G_{\alpha\beta}(\omega) = 0 \), means that \( \sum_\alpha E_{\alpha\beta} = 0 \) or equivalently[1, 11]

\[
\frac{dN_\beta}{dE} = \sum_\alpha \frac{dN_{\alpha\beta}}{dE} = \sum_\alpha D_{\alpha\beta} = \frac{\tau_{d,\beta}}{h}
\]

(1)

where \( dN_\beta/dE \) is the DOS and \( \tau_{d,\beta} \) is the dwell time for particles coming from the probe \( \beta \). Clearly the current conservation is established since one realizes
that $\sum_\alpha dN_{\alpha\beta}/dE$ is the physical quantity called injectance which is identical to $\sum_\alpha D_{\alpha\beta}$.

Applying the above formalism to mesoscopic conductors, one needs to compute various physical quantities such as the partial density of states. These quantities have vivid physical meaning but are not easy to obtain exactly. For a large system, the GPDOS can be expressed approximately in terms of the energy derivative of the scattering matrix elements:

$$\frac{dN_{\alpha\beta}}{dE} = \frac{1}{4\pi i} \left( s_{\alpha\beta}^\dagger ds_{\alpha\beta} - \frac{ds_{\alpha\beta}^\dagger}{dE} s_{\alpha\beta} \right).$$

(2)

Because for a given system one may be able to obtain the scattering matrix, Eq. (2) thus provides a practical means of computing the GPDOS. On the other hand, in order to obtain current conservation precisely, a correction should be added to Eq. (2) which can be neglected for large systems and large energies.

For one-dimensional systems, such a correction has been derived by Gasparian et al. which contains the reflection amplitude divided by the energy,

$$\frac{dN_\alpha}{dE} = \frac{d\tilde{N}_\alpha}{dE} + Im\left\{\frac{s_{\alpha\alpha}}{4\pi E}\right\},$$

(3)

where $d\tilde{N}_\alpha/dE \equiv \sum_\beta dN_{\alpha\beta}/dE$ which is computed from Eq. (2).

We have recently applied the above current conserving formalism to a two-dimensional mesoscopic conductor in the shape of a T-junction. To the best of our knowledge, it was the first 2D calculation with first principles. Among other things, an interesting and we believe useful discovery was that Eq. (3) turned out to be inaccurate in 2D. First of all, energy $E$ in the second term on the right hand side of Eq. (3) has to be replaced by the longitudinal part of the incident energy. Even with this change, there were small but systematic deviations to precise current conservation when the energy is approaching the second subband. In fact it was found that the DOS $d\tilde{N}_\alpha/dE$ as defined above diverges near the onset of the second subband and this led to the observed systematic deviations.

We are not aware of any 2D theory to account for the correction term which should appear in Eq. (3). The purpose of this paper is to investigate such correction terms in two dimensions. This not only provides further theoretical insights to the problem of AC-transport, but is also very helpful from a practical application point of view. From our own experience, numerical AC-transport calculations can be quite tricky and being able to obtain precise electric current conservation often serves as a very stringent check to numerical results. To this
purpose, we have considered the simplest two-dimensional model which is a $\delta$-
potential inside a quasi-1D ballistic conductor\cite{14}. Since quantum scattering in
this system leads to mode mixing which is the basic feature of a two-dimensional
system, it provides answers to our 2D problem. The advantage of this system is
that it can be solved exactly. We have thus derived analytically the correction
term. In particular we found that when the incident energy $E$ is within the first
subband, our result essentially reduces to the one-dimensional result Eq. (3). As
$E$ is increased to approach the $n$-th subband edge with $n > 1$, the correction
term diverges. This explains the systematic deviation observed in our previous
numerical calculation\cite{3}.

The paper is organized as the following. In the next section we present the
solution of the 2D scattering problem and derive the correction term. Section III
contains our numerical tests of the analytical formula. The last section serves as
a summary.

2 Model and results

Figure 1 shows the system where a $\delta$-potential is confined inside a quasi-1D wire
with width $a$. We assume, for simplicity of the calculation, that the boundaries
of the ballistic conductor are hard walls, \textit{i.e.} the potential $V = \infty$. Inside the
conductor, the potential is zero except that a $\delta$ function potential $V(x, y) =
\gamma \delta(x) \delta(y - y_0)$ is placed at $\vec{r} = (0, y_0)$. The scattering region $x_1 < x < x_2$ is
assumed to be symmetric with $x_2 = -x_1 = L/2$. From now on we set $\hbar = 1$ and
$m = 1/2$ to fix our units.

To compute the transmission and reflection amplitudes thus the scattering
matrix, a mode matching method\cite{15} is employed. The electron wave functions
are written as follows. For region I (see figure 1):

$$\Psi_I = \sum_n \chi_n(y) \left( a_n e^{ik_n x} + b_n e^{-ik_n x} \right) ,$$

where $\chi_n(y)$ is the wave function of the $n$-th subband along $y$-direction; $a_n$ is the
incoming wave amplitude and taken as an input parameter; $b_n$ is the reflection
amplitude; and $k_n^2 = E - (n\pi/a)^2$ is the longitudinal momentum for the $n$-th
mode. Note that for electron traveling in the first subband, $k_n$ with $n > 1$ is
purely imaginary. Similarly for region II:

$$\Psi_{II} = \sum_n \chi_n(y) \left( c_n e^{ik_n x} + d_n e^{-ik_n x} \right) ,$$
where $c_n$ is transmission amplitude and $d_n$ is set to zero in our calculation. After matching the boundary conditions at $x = 0$, we obtain

$$a_n + b_n = c_n$$

and

$$ik_n c_n - ik_n (a_n - b_n) = \sum_m \Gamma_{nm} (a_m + b_m),$$

where $\Gamma_{nm} = \gamma \chi^*(y_0) \chi(y_0)$. Eliminating $c_n$, we have

$$\vec{e} = P \vec{b},$$

(4)

where $e_n = -\sum_m \Gamma_{nm} a_m$ and $P_{nm} = \Gamma_{nm} - 2i k_n \delta_{nm}$. To find $\vec{b}$ we need to compute $P^{-1}$. Introducing a new matrix $\tilde{P} \equiv I + M$ with $M_{nm} = i \Gamma_{nm} / (2 k_n)$ so that $\tilde{P}_{nm}(-2i k_n) = P_{nm}$. Expanding $\tilde{P}^{-1}$ in powers of $M$, we have

$$\tilde{P}^{-1} = 1 - M / \alpha$$

(5)

where $\alpha = 1 + i \sum_n \Gamma_{nn}/(2 k_n)$, from which we have $\tilde{P}^{-1} = 1 - M / \alpha$. Finally, we obtain the matrix elements

$$(P^{-1})_{nm} = \frac{i}{2k_n} (\delta_{nm} - \frac{i \Gamma_{nm}}{2k_n \alpha}).$$

We shall specialize to consider the incident electron being in the first subband: $a_n = \delta_{n1}$. Using Eq.(5) the reflection and transmission amplitudes are

$$b_n = \sum_m (P^{-1})_{nm} e_m = -\frac{i \Gamma_{n1}}{2k_n \alpha}$$

(6)

$$c_n = \delta_{n1} + b_n.$$

(7)

For our system the scattering matrix elements $s_{\alpha\beta}$ are given by $s_{11} = b_1 \exp(ik_1 L)$ and $s_{12} = c_1 \exp(ik_1 L)$. The approximate DOS becomes, using Eq. (2),

$$\frac{d \bar{N}_\alpha}{dE} = \frac{1}{4\pi i} \sum_\beta \left( s_{\alpha\beta}^\dagger \frac{ds_{\alpha\beta}}{dE} - \frac{ds_{\alpha\beta}^\dagger}{dE} s_{\alpha\beta} \right)$$

$$= \frac{L}{4\pi k_1} - \text{Im} \left( \frac{b_1}{4\pi k_1^2} \right) - \frac{1}{4\pi} \sum_n \left| b_n \right|^2 \frac{ik_1}{k_n}.$$

(8)

To derive this expression we have used a relation $2b_1^* + 1 = \alpha/\alpha^*$ which follows directly from the unitary condition of the scattering matrix. Next we compute
the dwell time and hence the precise DOS (as opposed to the approximate DOS of Eq. (8)):

\[ \tau_{d1} = \int_{I} |\Psi_I|^2 dx dy + \int_{II} |\Psi_{II}|^2 dx dy \]

\[ = \frac{L}{2k_1} + \text{Re}(b_1 e^{ik_1L} - 1) + \sum n |b_n|^2 e^{ik_nL} - 1 \]

(9)

From Eqs. (1), (8) and (9), we arrive at the following central result of this work,

\[ \frac{dN_\alpha}{dE} = \frac{d\bar{N}_\alpha}{dE} + \text{Im} \left\{ \frac{s_{\alpha\alpha}}{4\pi k_1^2} \right\} + \frac{1}{4\pi} \sum_{n=2}^{\infty} \frac{|b_n|^2}{ik_n^2} e^{ik_nL} \cdot (10) \]

Hence we found that for this 2D system, there are two correction terms to the DOS. Clearly the first correction term, i.e. the 2nd term on the right hand side of Eq. (10), is generic, as it can be written in terms of the scattering matrix element. This term is similar to the corresponding term in Eq. (3) of the 1D case, except that the total energy \( E \) in Eq. (3) is now replaced by the transport energy \( k_1^2 \). In fact this term has been guessed in our earlier work[5]. There is a second correction term (the 3rd term of Eq. (10)) which comes solely due to mode mixing in our 2D system, and understandably it does not exist in 1D cases[13].

For small incident energies, i.e. as \( k_1 \) goes to zero, \( |b_n|^2 \to k_n^2 \) for \( n > 1 \). Therefore the second correction term of (10) is actually negligible at small energies. Indeed, this is the case in our earlier numerical calculations[3] where current conservation was very well satisfied at low energies using Eq. (3). However, as energy is approaching the \( n \)-th subband edge, for small \( k_n \to 0 \) with \( n > 1 \), \( |b_n|^2 \) remains finite. Hence according to Eq. (10) the second correction term diverges at these higher subband edges. This explains the observation of our calculation[3] where systematic numerical errors exist in current conservation near the 2nd subband edge. For energies within the first subband, as mentioned above \( k_n \) are all pure imaginary numbers with \( n > 1 \). Hence with large system size \( L \), the factor \( \exp(i k_n L) \) is very small as long as \( k_n \neq 0 \). However we emphasis that the second correction term becomes dominant very near each subband edge thus must be included in order to obtain precise current conservation.

Finally we note that Eq. (10) is not coordinate independent, so care must be taken when using it. For instance, if we choose \( x_1 \) as the origin in figure 1, the factor \( \exp(i k_n L) \) in the last term of Eq. (10) will be canceled due to the coordinate shift while the second term of Eq. (10) remains the same. In this sense, the new correction term is not generic and must be computed case by case for 2D systems.
3 Numerical test

To gain further intuitive impression of the AC-transport, and in particular to check our analytical formula Eq.(10), we shall first present direct numerical calculations of the admittance for the quantum wire system studied in the last section (Fig.(1)). Obviously since this problem was solved exactly above, agreement is obtained with Eq.(10). We shall then study the validity of Eq.(10) using another more complicated 2D conductor in the shape of a T-junction (see below). Indeed, although Eq.(10) was derived using a specific example of Fig.(1), it dramatically improves the current conservation near the second subband edge for the T-junction as well.

In order to compute the admittance, we have to know \( D_{\alpha,\beta} \) which is related to the dwell time[1, 5]. For a metallic conductor, it is appropriate to use the Thomas-Fermi approximation. Under such an approximation \( D_{\alpha,\beta} \) is given by[1, 8]

\[
D_{\alpha,\beta} = \int \frac{d^3r}{dn(\vec{r})/dE} \left( \frac{dn(\vec{r}, \beta)/dE}{dn(\vec{r})/dE} \right),
\]

where the local density of states \( dn(\vec{r}, \beta)/dE \) is the injectivity which measures the additional local charge density brought into the sample at point \( \vec{r} \) by the oscillating chemical potential at probe \( \beta \). The injectivity can be expressed as[1]

\[
\frac{dn(\vec{r}, \beta)}{dE} = \sum_n \frac{|\Psi_{\beta n}(\vec{r})|^2}{2\pi v_{\beta n}},
\]

where \( v_{\beta n} \) is the velocity of carriers at the Fermi energy at mode \( n \) in probe \( \beta \). \( dn(\alpha, \vec{r})/dE \) is called the emissivity which describes the local density of states of carriers at point \( \vec{r} \) which are emitted by the conductor at probe \( \alpha \). It is defined as

\[
\frac{dn(\alpha, \vec{r})}{dE} = \frac{1}{4\pi i} \sum_{\beta} Tr \left[ s_{\alpha\beta}^\dagger e^{\delta U(\vec{r})} s_{\alpha\beta} - \frac{\delta s_{\alpha\beta}^\dagger}{e\delta U(\vec{r})} s_{\alpha\beta} \right].
\]

It has been shown[4] that in the absence of magnetic field the injectivity is equal to the emissivity. Using Eqs.(8), (11) and (12), we can calculate the emittance.

Specifically, for the system of Fig.(1) we consider incident electron coming from probe 1 and set \( a = L = 1 \), \( y_0 = 0.3 \), and \( \gamma = -1 \). In Fig.(2), we plot the global DOS together with the transmission coefficient \( T \). As expected, the transmission coefficient \( T(E) \) (solid line) has large values for almost all energies \( E \) except at a special energy \( E_r \) where we have complete reflection (reflection coefficient \( R(E_r) = 1 \)) due to the resonant state. This can also be seen from the
behavior of the global partial DOS for reflection $dN_{11}/dE$ (dotted line) which peaks when $T(E = E_r) = 0$. On the other hand, $dN_{21}/dE$ (dashed line), which is the global partial DOS for transmission, takes minimum value at $E = E_r$. This behavior is consistent with that of a 1D system made of a symmetric scatterer [10] where one has $dN_{11}/dE \sim RdN/dE$ and $dN_{21}/dE \sim TdN/dE$. In Fig.(3), the quantities $D_{11}$ (solid line) and $D_{12}$ (dotted line) are shown. Both curves reach maximum values near the resonant point $E_r$, which is expected since $D_{\alpha\beta}$ are proportional to the dwell time or the DOS. The emittance $E_{\alpha\beta}$ is plotted in Fig.(4). Both $E_{11}$ (solid line) and $E_{12}$ (dotted line) reach extremal values at the resonant point. The system responds differently for different energy, either capacitively when $E_{11} = -E_{12} > 0$, or inductively otherwise. From Fig.(4), we observe that near the resonance $E_{11}$ and $E_{12}$ respond capacitively while $E_{12}$ is inductive away from this resonance energy. This behavior, namely being capacitive when at the $T \approx 0$ resonance, is the same as that observed in the 2D T-junction [3]. On the other hand for an 1D tunneling system [1] the response is inductive at its resonance. But in that case the resonance is marked by transmission coefficient being near unity. Finally, to confirm electric current conservation, essentially the two curves of Fig.(4) must add to zero. Clearly these curves do not cancel each other as the figure shows, exactly due to the approximate nature of the partial density of states as obtained using Eq. (2). After including the two corrections to DOS as derived in Eq. (10), however, we did obtain perfect current conservation for the whole energy range. This is not surprising since after all (10) is an exact result for this quantum system.

Our main result Eq.(10) is derived using a specific simple example shown in Fig.(1). There seems no special reason for Eq.(10) to apply to other 2D systems, since the form of the new correction term is given by the amplitudes of the non-propagating modes inside the scattering junction (as oppose to the more general scattering matrix elements), and these evanescent amplitudes probably depend on the scatterer in some fashion. In this sense it is unfortunate that a more general form was not obtained. However since the new correction term does explain, qualitatively, the observed discrepancy of using Eq. (3) as discussed above, it is tempting to test it using the more complicated 2D system of the T-junction studied previously [3]. As the T-junction has been reviewed and studied by many authors [10, 4] at various contexts, here we shall not present the details for its calculation. For this purpose, we have checked the current conservation of the T-junction using Eq.(3) and compared with the result obtained using Eq.(10). In Fig.(5), we have plotted the DOS $d\tilde{N}_1/dE$ given by Eq.(3) (dotted line) and by [17]
Eq. (10) (solid line), and the dwell time $\tau_{d,1}/2\pi$ (dashed line). Although the result Eq. (10) is model dependent, we observe that the agreement is clearly better. This suggests that the new correction term does capture the essential ingredient of the correction, although it is not completely universal as the evanescent amplitudes depend on the peculiarities of a 2D system in some weak way, leading to the small remaining difference.

4 Summary

In summary, we have investigated the electric current conservation in a two-dimensional ballistic conductor under a time dependent field. Similar to that of the 1D case, we found that in order to obtain precise current conservation, certain corrections to the density of states as obtained approximately from the scattering matrix must be included. We have derived these corrections analytically for a specific two-dimensional system and found that there are two correction terms. One of the correction term has the same form as that of the 1D case, while the second correction term is purely due to mode mixing characteristic of 2D quantum scattering. In particular, when the incident energy $E$ is within the first subband, our result essentially reduces to the one-dimensional result if $E$ is not too high. On the other hand as $E$ approaches to the $n$-th subband with $n > 1$, the correction term diverges at the subband edges. Hence in 2D the mode mixing leads to important changes in the global density of states and must be included if precise electric current conservation is desired. Finally, the new correction term found here provides a qualitative explanation for the small but systematic deviation to precise current conservation observed in our previous numerical calculations on a 2D quantum wire in the shape of the T-junction. Indeed, our numerical test has produced better agreement when the new formula derived here is used.

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To apply Eq. (10) for the T-junction, we have substituted the appropriate amplitudes $b_n$ for the T-junction into (10).

**Figure Captions**

Figure 1. Schematic plot of the quantum wire system: a $\delta$ potential $\gamma\delta(\vec{r} - \vec{r}_0)$ is confined inside a quasi-1D quantum wire, with $\vec{r}_0 = (0, y_0)$. The wire width is $a$. The scattering region is between $x_1$ and $x_2$, where $x_2 = -x_1 = L/2$. In our calculations, the parameters are set to $L = a = 1$, $y_0 = 0.3$, and $\gamma = -1.0$.

Figure 2. The global partial density of states and the transmission coefficient as functions of electron energy $E$. Solid line: transmission coefficient $T$; dotted line: $dN_{11}/dE$; dashed line: $dN_{21}/dE$. Unit of energy is $\hbar^2/2ma^2$.

Figure 3. The current response to the internal potential, $D_{\alpha\beta}$, as a function of energy $E$. Solid line: $D_{11}$; dotted line: $D_{21}$.

Figure 4. The dynamic part of the admittance, $E_{\alpha\beta} \equiv dN_{\alpha\beta}/dE - D_{\alpha\beta}$ as a function of energy.

Figure 5. A numerical check of the electric current conservation, Eq. (1), for the T-junction studied in Ref. [5]. Solid line: $dN_1/dE$ as obtained by Eq. (10); dotted line: $\tau_d/\hbar = \sum_\alpha D_{\alpha1}/\hbar$. Agreement of the two curves indicate the conservation. The remaining small differences at high end of the energy between the two curves indicates that the new correction term in Eq. (10) has a weak non-universal dependence on the 2D system shapes.