Weakly nonlinear quantum transport: an exactly solvable model

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We have studied the weakly non-linear quantum transport properties of a two-dimensional quantum wire which can be solved exactly. The non-linear transport coefficients have been calculated and interesting physical properties revealed. In particular we found that as the incoming electron energy approaches a resonant point given by energy $E = E_r$, where the transport is characterized by a complete reflection, the second order non-linear conductance changes its sign. This has interesting implications to the current-voltage characteristics. We have also investigated the establishment of the gauge invariance condition. We found that for systems with a finite scattering region, correction terms to the theoretical formalism are needed to preserve the gauge invariance. These corrections were derived analytically for this model.

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1 Introduction

Non-linear quantum transport in mesoscopic systems has been a very active research field in recent years. Taboryski et al. have reported observations of non-linear and asymmetric conductance oscillations of quantum point contacts at a small bias voltage. They found that the non-Ohmic and asymmetric behavior causes a rectified dc signal as the response to an applied ac current. On the theoretical side, Wingreen et al. have presented a general formulation to deal with the situation of a non-linear and time-dependent current going through a small interacting region where electron energies can be changed by time-dependent voltages. At the same time, Büttiker and his co-workers have advanced a current conserving theory for the frequency dependent transport. Recently, this current conserving formalism has been applied to a two dimensional mesoscopic conductor. This theory can also be applied to discuss the non-linear behavior of mesoscopic samples and the theory is gauge invariant. It has been recognized that in non-linear coherent quantum transport, it is essential to consider the internal self-consistent potential in order to satisfy the gauge invariant condition. This condition demands that all physical properties predicted by a theory can not change if there is a global voltage shift. Obviously this is a fundamental requirement.

Recently, Christen and Büttiker have investigated the rectification coefficient of a quantum point contact and the non-linear current-voltage characteristic of a resonant level in a double barrier structure using the theory of gauge invariant non-linear conductance. Another important application of this theory is to investigate two-dimensional (2D) mesoscopic and ballistic quantum devices which can now be routinely fabricated in many laboratories. Unfortunately due to a particular technical difficulty, namely the evaluation of a quantity called sensitivity (see below), so far little is known for the non-linear conductance in 2D. Clearly an understanding of 2D situation is very much needed in order to gain further intuition to the coherent transport and to predict the non-linear characteristics of the variety of 2D nanostructures. The purpose of this paper is to investigate the gauge invariant non-linear transport in a specific two dimensional system which can be solved exactly. Hence we were able to obtain various relevant physical quantities. Although a general study for an arbitrary 2D system seems difficult, our perspective is that an exactly solved model is valuable since it clearly and unambiguously reveals the physical properties of the non-linear transport coefficients.
To be specific, we have considered a very simple 2D model which is a quasi-1D ballistic conductor with a $\delta$-potential confined inside, as shown in figure (1a). Because 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. In a previous work we have used this model to study the electric current conservation of the AC-transport formalism at the linear conductance level, and calculated the important physical quantities such as the global and local partial density of states. In the following we shall extend our calculation to explicitly calculate the second order non-linear conductance $G_{111}$ and $G_{112}$. Due to the gauge invariant condition (see below), we should have $G_{111} + G_{112} = 0$. It turns out that for systems with a finite scattering volume, as those of any numerical calculations, we found that a correction term must be added to satisfy this condition. For this system there is a resonant state with energy $E_r$ characterized by a complete reflection, i.e. the reflection coefficient $R = 1$. Our results showed that the second order non-linear conductance $G_{111}$ changes sign near the resonant point $E_r$. This leads to interesting current-voltage characteristics of this system.

The paper is organized as the following. In the next section we shall briefly review the gauge invariant theory for non-linear transport set out by Böttiker. In section III we will present the solution of the 2D scattering problem. Some of the technical details of section III have been put into the Appendix. Our results are presented in section IV. The last section serves as a brief summary.

2 Gauge invariant formalism

To be complete, we shall first briefly review the gauge invariant formalism of Christen and Böttiker and set out our calculation procedure for the 2D system. For a multi-probe mesoscopic system, the current through probe $\alpha$ is given by

$$I_\alpha = \frac{2e}{h} \sum_\beta \int dEf(E - E_F - eV_\beta)A_{\alpha\beta}(E, \{V_\gamma\}),$$

where $f(E)$ is the Fermi distribution function, and

$$A_{\alpha\beta}(E, \{V_\gamma\}) = Tr[1_{\alpha\delta} - s^\dagger_{\alpha\beta}(E, \{V_\gamma\})s_{\alpha\beta}(E, \{V_\gamma\})]$$

are the screened (negative) transmission functions. For the weakly non-linear transport, Eq.(1) can be expanded with respect to the voltages $V_\beta$,

$$I_\alpha = \sum_\beta G_{\alpha\beta}V_\beta + \sum_{\beta\gamma} G_{\alpha\beta\gamma}V_\beta V_\gamma + ...,$$

(3)
where
\[ G_{\alpha \beta} = \frac{2e^2}{h} \int dE (-\partial_E f) A_{\alpha \beta} \]  \hspace{1cm} (4)
is the linear conductance and
\[ G_{\alpha \beta \gamma} = \frac{e^2}{h} \int dE (-\partial_E f) (\partial f A_{\alpha \beta} + \partial f A_{\alpha \gamma} + e\partial_E A_{\alpha \beta \delta}) \]  \hspace{1cm} (5)
is the second order non-linear conductance. In Eqs.(4) and (5), the \( A_{\alpha \beta} \) are evaluated at \( \{V_\gamma\} = 0 \). The requirements that the current is conserved and be independent of a global voltage shift (gauge invariance) yield
\[ \sum_{\alpha} G_{\alpha \beta} = \sum_{\beta} G_{\alpha \beta} = 0 \]
and
\[ \sum_{\alpha} G_{\alpha \beta \gamma} = \sum_{\beta} G_{\alpha \beta \gamma} = \sum_{\gamma} G_{\alpha \beta \gamma} = 0 \ . \]
From this equation and Eq.(5), the gauge invariance condition for \( A_{\alpha \beta} \) is
\[ e\partial_E A_{\alpha \beta} + \sum_{\gamma} \partial f A_{\alpha \beta} = 0 \ . \]  \hspace{1cm} (6)
The derivative \( \partial f A_{\alpha \beta} \) can be expressed in terms of functional derivative of \( A_{\alpha \beta} \) with respect the electric potential \( U \) and the characteristic potential \( u_\gamma \) which satisfies \( \sum_{\gamma} u_\gamma = 1 \)
\[ \partial f A_{\alpha \beta} = \int d^3r \frac{\delta A_{\alpha \beta}}{\delta U(r)} u_\gamma(r) \ . \]  \hspace{1cm} (7)
To gain further insight on Eq.(6), let’s consider a two probe system. Eq.(6) can be written as
\[ I_1 = G_{11} V_1 + G_{12} V_2 + G_{111} V_1^2 + 2G_{112} V_1 V_2 + G_{122} V_2^2 \]
Obviously, \( G_{12} = -G_{11} \) due to the conservation of electric current. From Eqs.(4), (5), and (7) and using the fact that \( u_1 + u_2 = 1 \), we have \( G_{111} = -G_{112} = G_{122} \). Therefore the current depends only on the voltage differences which is the direct consequence of the gauge invariant condition Eq.(6). We obtain,
\[ I_1 = G_{11}(V_1 - V_2) + G_{111}(V_1 - V_2)^2 \ . \]  \hspace{1cm} (8)
To calculate the transmission functions \( A_{\alpha \beta} \) and their functional derivatives, we need the characteristic potential \( u_\gamma \). This, in turn, needs the solution of the Poisson equation with a nonlocal screening term. To actually carry
out this procedure is very complicated. However if we can use the Thomas-Fermi approximation, which is more appropriate for metallic conductors, the characteristic potential is simplified and is found to be related to the local partial density of states. Within Thomas-Fermi screening, we obtain

\[ u_\gamma(r) = \frac{dn(r, \gamma)}{dE} \frac{dn(r)}{dE} , \tag{9} \]

where the partial local density of states \( dn(r, \gamma)/dE \) is called the injectivity and is given by

\[ \frac{dn(r, \gamma)}{dE} = \sum_n |\Psi_{\gamma n}|^2 \frac{v_{\gamma n}}{\hbar v_{\gamma n}} , \tag{10} \]

where \( v_{\gamma n} \) is the channel velocity and \( \Psi_{\gamma n} \) is a scattering state. Finally the term \( dn(r)/dE = \sum_\alpha dn(r, \alpha)/dE \) is the total local density of states. Substituting Eqs. (2) and (9) into Eq.(7), we obtain

\[ \partial V_\gamma A_{\alpha \beta} = - \int d^3r \eta_{\alpha \beta} \frac{dn(r, \gamma)}{dE} \frac{dn(r)}{dE} \tag{11} \]

where

\[ \eta_{\alpha \beta} = s_{\alpha \beta}^\dagger \frac{\delta s_{\alpha \beta}}{\delta U(r)} + s_{\alpha \beta} \frac{\delta s_{\alpha \beta}^\dagger}{\delta U(r)} \tag{12} \]

is called sensitivity\(^{10}\). We are aware of two ways of calculating the sensitivity\(^{10}\). The first is to evaluate \( \delta s_{\alpha \beta}/\delta U \) directly by introducing a \( \delta \)-function of infinitesimal strength \( \delta U \) inside the scattering region. Alternatively, one can calculate it using the retarded Green’s function. For a 2D system, in general the Green’s function can not be obtained explicitly, hence we shall use the first method by directly compute the sensitivity. After obtaining the sensitivity, we can then compute \( \partial V_\gamma A_{\alpha \beta} \) from Eq. (11), and obtain \( G_{\alpha \beta \gamma} \) from Eq. (5).

### 3 Model and Analysis

As mentioned in the introduction, figure (1a) 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, i.e. the potential \( V = \infty \) at the walls. Inside the conductor, the potential is zero everywhere except that a \( \delta \) function potential \( V(x, y) = \gamma \delta(x) \delta(y - y_0) \) is placed at position \( r = (0, y_0) \). 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.
The transmission and reflection amplitudes have been calculated using a mode matching method\[12, 11\]. When the incident electron is in the first subband, in an earlier work we have explicitly obtained these amplitudes\[13\]. The evaluation was straightforward but quite tedious, we refer interested reader to Ref. \[13\] for details of this algebra. Here we only quote the results: for reflection the amplitude is

\[ b_n = \frac{-i\Gamma_{n1}}{2k_n\alpha}, \tag{13} \]

and for transmission it is

\[ c_n = \delta_{n1} + b_n \tag{14} \]

Here \( \alpha = 1 + i \sum_n \Gamma_{nn}/(2k_n); \Gamma_{nm} = \gamma \chi^*(y_0)\chi_n(y_0), \) and \( \chi_n(y) \) is the wave function of the \( n \)-th subband along \( y \)-direction. \( k_n = E - (n\pi/a)^2 \) is the longitudinal momentum for the \( n \)-th mode; \( i = \sqrt{-1} \). Note that for electron traveling in the first subband, \( k_n \) with \( n > 1 \) is purely imaginary. For our coordinate system the scattering matrix elements \( s_{\alpha\beta} \) are given by \( s_{11} = b_1 \exp(ik_1L) \) and \( s_{12} = c_1 \exp(ik_1L) \).

As mentioned in the last section, to calculate the non-linear conductance of our 2D sample, it is necessary to find the sensitivity \( \eta_{\alpha\beta} \). Hence according to Eq. (12) we must evaluate \( \delta s_{\alpha\beta}/\delta U(x_1, y_1) \) where the pair \((x_1, y_1)\) is an arbitrary location in the scattering volume. For a general 2D sample a direct calculation of this functional derivative is very difficult if not impossible. Fortunately for our model this can actually be done exactly. As a first step we shall introduce an additional \( \delta \)-potential of infinitesimal strength \( \delta U \) at position \((x_1, y_1)\) inside the scattering volume. Thus our system becomes to that shown in figure (1b). Then we shall solve the scattering matrix formally as a functional of \( \delta U \). Obviously being able to carry out this step is crucial. Finally the functional derivative is performed. To proceed we again use the mode matching method\[12, 11, 13\]. We will assume \( x_1 < 0 \) in the following calculation. The calculation for \( x_1 > 0 \) can be done in a similar fashion. The electron wave functions are written as follows. For region I (see figure. (1b)):

\[ \Psi_I = \sum_n \chi_n(y)(a_n e^{ik_n x} + b_n e^{-ik_n x}) \]

where \( a_n \) is the incoming wave amplitude and taken as an input parameter; \( b_n \) is the reflection amplitude. Similarly for region II

\[ \Psi_{II} = \sum_n \chi_n(y)(e_n e^{ik_n x} + f_n e^{-ik_n x}) \]
and for region III

\[ \Psi_{III} = \sum_n \chi_n(y)c_ne^{ik_nx}, \]

where \( c_n \) is the transmission amplitude. We shall match the wavefunctions and their x-derivatives at the positions \( x = x_1 \) and \( x = 0 \). We obtain, at \( x = x_1 \)

\[
a_n e^{ik_nx_1} + b_n e^{-ik_nx_1} = e_n e^{ik_nx_1} + f_n e^{-ik_nx_1},
\]

(15)

and

\[
\begin{align*}
  ik_n(e_n e^{ik_nx_1} - f_n e^{-ik_nx_1}) &= ik_n(a_n e^{ik_nx_1} - b_n e^{-ik_nx_1}) \\
  &= \sum_m \tilde{\Gamma}_{nm}(e_m e^{ik_mx_1} + f_m e^{-ik_mx_1})
\end{align*}
\]

(16)

where \( \tilde{\Gamma}_{nm} = \delta U \chi_n^*(y_1)\chi_m(y_1) \).

At \( x = 0 \), the matching gives

\[ e_n + f_n = c_n, \]

and

\[ ik_n c_n - ik_n(e_n - f_n) = \sum_m \Gamma_{nm}c_m. \]

To simplify the notation, from now on \((x_1, y_1)\) is replaced by \((x, y)\). From the last two equations, we solve for \( e_n \) and \( f_n \)

\[
2ik_n e_n = - \sum_m P_{nm} c_m,
\]

(17)

and

\[
2ik_n f_n = \sum_m \Gamma_{nm}c_m,
\]

(18)

where \( P_{nm} = \Gamma_{nm} - 2ik_n \delta_{nm} \). Eliminating \( b_n \) from Eqs. (13) and (16), we obtain

\[
2ik_n e_n e^{ik_nx} = 2ik_n a_n e^{ik_nx} + \sum_m \tilde{\Gamma}_{nm}(e_m e^{ik_mx} + f_m e^{-ik_mx})
\]

Taking the limit \( \delta U \to 0 \), we have

\[
2ik_n \frac{\delta e_n}{\delta U} = \sum_m \tilde{\Gamma}_{nm}(a_m e^{ik_mx} + b_m e^{-ik_mx}),
\]

(19)
where \( \bar{\Gamma}_{nm} = \tilde{\Gamma}_{nm}/\delta U \). To arrive at the above result we have used the fact that as \( \delta U \to 0 \), \textit{i.e.} when the extra \( \delta \) function vanishes, we must have \( e_m = a_m \) and \( f_m = b_m \). From Eq.(17),

\[
2ik_n \frac{\delta \epsilon_n}{\delta U} = -\sum_m P_{nm} \frac{\delta c_n}{\delta U}.
\]

From Eqs.(19) and (20), we arrive at

\[
-\sum_m P_{nm} \frac{\delta c_m}{\delta U} e^{i k_n x} = \sum_m \bar{\Gamma}_{nm} (a_m e^{i k_m x} + b_m e^{-i k_m x}) = \chi^*_n \Psi.
\]

where \( \Psi = \Psi_I \) for \( x < 0 \). From Eq.(21), we have

\[
\frac{\delta c_l}{\delta U} = -\sum_n (P^{-1})_{ln} e^{-i k_n x} \chi^*_n \Psi.
\]

The matrix \( P^{-1} \) has been obtained in Ref. [13], and we quote

\[
(P^{-1})_{ln} = \frac{i}{2k_l} \left( \delta_{ln} - \frac{i \Gamma_{ln}}{2k_n \alpha} \right).
\]

From this equation and Eq.(14) we see that for \( l = 1 \), \textit{i.e.}, the first subband, \( (P^{-1})_{1n} = ic_n/(2k_1) \) provided that \( \chi_n \) is real which is true in our case. This yields

\[
\frac{\delta c_1}{\delta U} = \frac{1}{2ik_1} \sum_n c_n \chi_n e^{-i k_n x} \Psi.
\]

Similarly, from Eqs. (15), (17), (18), (20), and (21), we obtain

\[
\frac{\delta b_n}{\delta U} = \frac{\delta \epsilon_n}{\delta U} e^{2ik_n x} + \frac{\delta f_n}{\delta U} = -\frac{e^{2ik_n x}}{2ik_n} \sum_m P_{nm} \frac{\delta c_m}{\delta U} + \frac{1}{2ik_n} \sum_m \bar{\Gamma}_{nm} \frac{\delta c_m}{\delta U} = \frac{\sin(k_n x)}{k_n} \chi_n \Psi + \frac{\delta c_n}{\delta U}
\]

When \( n = 1 \), \( \delta b_1/\delta U \) becomes,

\[
\frac{\delta b_1}{\delta U} = \frac{1}{2ik_1} (\chi_1 e^{ik_1 x} + \sum_n b_n \chi_n e^{-i k_n x}) \Psi = \frac{1}{2ik_1} \Psi^2.
\]
Because the scattering matrix elements $s_{11} \sim b_1$ and $s_{12} \sim c_1$ as mentioned above, with the functional derivatives Eqs. (23) and (22) we can evaluate $\delta s_{\alpha\beta}/\delta U$ trivially thus obtaining the sensitivity $\eta_{\alpha\beta}$ of Eq. (12). Then using the prescription discussed at the end of Section 2, we obtain all the weakly non-linear conductances and other quantities of interest. Our results will be presented in the next section.

To end this section of the theoretical analysis, we mention that to check the result of functional derivatives, in the Appendix we shall explicitly calculate a quantity called emissivity using these functional derivatives. In the absence of a magnetic field, it is known that emissivity equals to the injectivity defined in Eq. (11) which we can compute using the wavefunctions. Indeed we confirm in the Appendix that these two equal thus providing a necessary check to the calculations presented here.

4 Results

To obtain numerical results from our analytical formula, for the system of figure (1a) we consider incident electron coming from probe 1 and set $a = L = 1$, $y_0 = 0.3$, and $\gamma = -1$. Although we have restricted the incoming electron energy to the first subband, quantum scattering at the $\delta$-function potential leads to mode mixing. Thus in our numerical calculations we have included 50 modes in the scattering volume. We have checked that this is enough to obtain good numerical convergence.

As a first result we plot the sensitivity $\eta_{11}(r, E)$ as a function of the electron incident energy $E$ at several positions $r$. This is shown in figure (2). As discussed in Section 2, $\eta_{\alpha\beta}$ appears naturally in the theoretical formalism, and it essentially describes the local electric current response of the scattering problem when there is a small local potential change. It is related to the real part of the diagonal elements of the Green’s function. figure (2) not only shows interesting behavior of this quantity, but also gives vivid intuition about the local current response. As shown in our earlier work and mentioned above, the quantum wire studied here has a resonant state at energy $E = E_r = 36.65$ where we have a complete reflection (reflection coefficient $R = 1$). Not surprisingly, the sensitivity has a large peak at this resonance energy because the system response is most sensitive to potential perturbations at resonance. On the other hand, this peak is larger when we are closer to the $\delta$-function scatterer located at $x = 0$: this indicates that the local perturbation has larger effects when it is closer to the scattering.
center. Although figure (2) shows $\eta_{11}$ at positions to the left of the scatterer, we have checked that its behavior is exactly the same for positions $x > 0$ as our system is symmetric.

Adding up all the local responses according to Eq. (11), we can explicitly examine the gauge invariant condition Eq.(6). Using Eqs.(2) and (7) and the fact that $u_1 + u_2 = 1$, Eq.(3) reduces to

$$2 \text{Re}(s_{\alpha\beta}^1 \frac{ds_{\alpha\beta}}{dE}) + 2 \int d^3 r \text{Re}(s_{\alpha\beta}^1 \frac{\delta s_{\alpha\beta}}{\delta U(r)}) = 0 .$$

It is straightforward to evaluate the left hand side of this equation. Using the functional derivatives obtained in the last section, as well as the energy derivatives of Eqs. (13) and (14), we found that the left hand side of the above equation is nonzero, and is given by

$$\text{correction} = \left| s_{12} \right|^2 k_1^2 \text{Re}(s_{11}) + \text{Re}\left( \sum_{n=2}^\infty \frac{b_1|b_n|^2}{k_1k_n} (e^{ik_nL} - 2) \right) .$$

(24)

Thus in order to have precise gauge invariance, this correction must be included. From this result, we notice that the first correction term is only significant near the first subband threshold where $k_1 \approx 0$ and is negligible for larger incoming electron energies. For the second correction term, let’s examine its behavior near the $n$-th subband with $n > 1$. From Eq.(13) we see that as the incoming electron momentum $k \to k_n$, $b_1 \to k_n$ and $b_n$ is finite. Therefore, the second correction term remains finite when electron energy approaches the $n$-th subband ($n > 1$).

This is different from the AC-transport where the correction diverges near the $n$-th subband with $n > 1$. We emphasize that the correction term is due to the fact that we are considering a finite scattering volume. As the scattering volume or the incident energy become larger, the effect of these correction terms diminishes. This can be seen clearly due to the factor $k_1$ in the denominator, and the exponentially decaying factor $\exp(ik_nL)$ as $k_n$ is purely imaginary for all $n > 1$.

Now we present numerical evaluations of the analytical formula derived in the last section for the second order non-linear conductance $G_{\alpha\beta\gamma}$. In figure (3) for a comparison the solid line shows the linear conductance $G_{21}$ which is proportional to the transmission coefficient by the Landauer formula. The dotted line shows the second order non-linear conductance $G_{111}$. In the presence of an attractive $\delta$-function scatterer, there exists a quasi-bound state at $E = E_r = 36.65$. As a result, we observe the complete reflection indicated by $G_{21}=0$.

As expected, the non-linear coefficient $G_{111}$ also vanishes at $E_r$. Furthermore
$G_{111}$ changes its sign as the incoming electron energy passes through the resonant energy. This has important implications on the current-voltage characteristics if we recall the I-V relation Eq. (8). The I-V curves of this quantum wire system is shown in figure (4) for several different electron energies. We can clearly see that when $E$ is smaller than $E_r$, e.g. for $E = 10.91$ and $36.22$, since both $G_{21}$ and $G_{111}$ are positive, the current $I_1$ increases with potential difference of the two probes $\Delta V = V_1 - V_2$. However when $E = 37.11$ which is just above $E_r$, $I_1$ is a decreasing function of $\Delta V$ due to the negative non-linear conductance $G_{111}$. For this case the quantum wire has a negative differential resistance. Finally at a even larger energy $E = 39.03$, while $G_{111} < 0$, the value of $G_{21}$ is large enough such that the linear contribution dominates at small $\Delta V$ and the non-linear term is larger at larger $\Delta V$. This behavior is shown in the dash-dotted line in figure (4).

To numerically demonstrate the gauge invariance, we have also computed the non-linear conductance $G_{112}$ according to Eq. (5) and it is shown in figure (5) as the dotted line. For comparison we have re-plotted the non-linear conductance $G_{111}$ (solid line). Note that near the resonant region, these two non-linear conductances are very close to each other. This is a surprising result, because if the gauge invariant condition is precisely satisfied we should have $G_{111} = -G_{112}$. Thus without the correction term discussed above, the gauge invariance could not even be satisfied up to a sign! Hence it is important, in any numerical calculations, to have a large scattering volume[9]. Indeed, when we add the correction term of Eq. (24) to $G_{112}$, (dashed line in figure (5)), we obtain the expected perfect agreement to the gauge invariance.

5 Summary

To summarize, we have solved exactly the weakly non-linear transport characteristics of a two-dimensional quantum wire model. To the best of our knowledge this is the first exact solution for a truly two-dimensional ballistic model. The second order non-linear conductances are derived analytically. We found that as the incoming electron energy crosses the resonant point, the non-linear conductance changes its sign. This leads to interesting current-voltage behavior when the incoming electron energy changes. We have also examined the gauge invariant condition which is obtained by the global voltage shift. We found that for systems with a finite scattering volume, correction terms are needed to preserve the gauge invariant condition. We have derived these corrections analytically for our
model. The correction term consists of two parts. The first part dominates when
the incident energy $E$ is near the first subband threshold. On the other hand
the second part is given by the amplitudes of the non-propagating modes and
is significant near the resonant point. Finally, our exact calculation reveals the
interesting behavior of the sensitivity which describes the local electric current
response to a potential perturbation.

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Appendix

To check our result of the functional derivatives, i.e. Eqs. (22) and (23), in this
Appendix we compute the emissivity defined as\cite{1}

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

It has been shown\cite{9} that in the absence of a magnetic field the emissivity is equal
to the injectivity defined in Eq.(10). We shall explicitly perform the functional
derivatives to confirm this fact, hence provide the necessary check to our algebra.

Using Eqs.(22) and (23), we have

$$
s_{11} \frac{\delta s_{11}}{\delta U} + s_{12} \frac{\delta s_{12}}{\delta U} = c_1 \frac{\delta c_1}{\delta U} + b_1 \frac{\delta b_1}{\delta U}
$$

$$
= \frac{1}{2ik_1} (c_1^* \chi_1 e^{-ik_1 x} + c_1^* \sum_n b_n \chi_n e^{-ik_n x} + b_1^* \chi_1 e^{ik_1 x} + b_1^* \sum_n b_n \chi_n e^{ik_n x}) \Psi
$$

$$
= \frac{1}{2ik_1} (b_1^* \chi_1 e^{ik_1 x} + \chi_1 e^{-ik_1 x} + (1 + 2b_1^*) \sum_{n=2} b_n \chi_n e^{-ik_n x}) \Psi
$$

where the relation $c_1 = 1 + b_1$ has been used. Before we proceed further, let
us derive a useful relation from the unitary condition of the scattering matrix,
namely

\[ 1 + 2b_1^* = -\frac{b_1^*}{b_1} = \frac{\alpha}{\alpha^*}. \] (26)

The first equality comes from the unitary condition \( c_1^* b_1 + c_1 b_1^* = 0 \) or \( b_1^* + (1 + 2b_1^*)b_1 = 0 \); and the second equality is from Eq. (13). Since the incoming electron is in the first subband, we have \( k_n^* = -k_n \) for \( n > 1 \). Hence for \( n > 1 \),

\[ \frac{b_n}{b_n^*} = \frac{\alpha^*}{\alpha}. \] (27)

Substituting Eqs. (26) and (27) into Eq. (25), we obtain

\[ s_{11}^* \frac{\delta s_{11}}{\delta U} + s_{12}^* \frac{\delta s_{12}}{\delta U} = \frac{1}{2ik_1} |\Psi|^2, \] (28)

which is equivalent to Eq. (10). Notice that the imaginary part of left hand side of Eq. (28) is proportional to the emissivity. Its real part gives the sensitivity \( \eta_{11} + \eta_{12} \). From the unitary condition we have \( \eta_{11} + \eta_{12} = 0 \) which agrees with Eq. (28).
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Figure Captions

Figure 1. Schematic plot of the quantum wire system. (a). The quantum wire system we have studied: 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 \( \gamma = -1.0 \). (b). To compute the functional derivatives of the scattering matrix with respect to a local potential change, we add another \( \delta \) function potential at the position \((x_1, y_1)\). In this case the system is divided into three regions by the dotted lines for the boundary matching solution of the Schrödinger equation.

Figure 2. The sensitivity \( \eta_{11}(r, E) \) as a function of energy \( E \) at three different positions \( x = -L/2, -L/4, 0 \) with the same \( y = 0.5 \). For different \( y \) the curve \( \eta_{11} \) as a function of \( E \) will be multiplied by a constant. Other system parameters are the same as those of figure (1). Here the unit of energy is \( \hbar^2/(2ma^2) \).

Figure 3. The conductances \( G_{21} \) and \( G_{111} \) as functions of energy \( E \). Solid line: \( G_{21} \); dotted line: \( G_{111} \). Other system parameters are the same as those of figure (1). Here the unit of energy is \( \hbar^2/(2ma^2) \).

Figure 4. The current-voltage characteristics as calculated from Eq. (8) at several different electron energies \( E = 10.91, 36.22, 37.11, 39.03 \). \( \Delta V = V_1 - V_2 \). Other system parameters are the same as those of figure (1).

Figure 5. A numerical check of the gauge invariant condition. Solid line is \( G_{111} \), dotted line is \( G_{112} \), dashed line is the \( G_{112} + \text{correction} \) where \( \text{correction} \) is given by Eq. (24). Clearly \( G_{112} + \text{correction} = -G_{111} \). Here the unit of energy is \( \hbar^2/(2ma^2) \).
Figure (1a)
Figure (1b)
Figure (2)
Figure (3)
Figure (4)
Figure (5)