Formalism of nonlinear transport in mesoscopic conductors

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We study nonlinear transport in mesoscopic conductors using the scattering approach. Extended multiterminal Landauer-Büttiker formulas are presented in conditions such as at zero/finite temperatures and in the weakly/strongly nonlinear regimes and are shown to be gauge invariant. As an example, we model the ballistic rectification effect recently observed in a symmetry-breaking microjunction. We are then able to provide an analytical description of the rectification effect, which is in remarkably good agreement with the experimental observations. [S0163-1829(99)04815-8]

When the characteristic sizes of semiconductor devices are small in comparison with the elastic mean free path of carriers, the carrier transport becomes ballistic.[1] The Landauer-Büttiker formalism, which treats transport as a transmission problem for carriers at the Fermi level, is widely used to describe the linear transport behavior of these conductors.[2,3] There is increasing attention paid to nonlinear ballistic transport.[4–11] Nonlinearity is important in mesoscopic conductors because of the small device feature sizes and the fact that, in principle, nonlinearity starts at any nonzero current. Much effort has been made to extend the Landauer-Büttiker formalism to nonlinear regime. In particular, Bagwell and Orlando presented a theory to treat two terminal devices at finite temperatures and finite applied voltages,[5] and recently Christen and Büttiker developed a self-consistent gauge-invariant theory for multiterminal devices.[8]

In this paper, we study nonlinear transport in mesoscopic conductors using the scattering approach. Extended Landauer-Büttiker formulas are obtained at zero/finite temperatures and in the weakly/strongly nonlinear regimes and are shown to be gauge invariant. We find that even in the nonlinear regime, four-terminal resistances can still be expressed as simple functions of transmission coefficients. Thus the formalism makes it possible to analyze nonlinear transport problems in a direct and convenient way, similar to that of using the standard Landauer-Büttiker formula in the linear regime. As an example, we model the ballistic rectification effect recently observed in a semiconductor microjunction.[12] The model provides an analytical description of the effect with no adjustable parameters, which thus allows for an unambiguous comparison with the experimental observations.

Consider a mesoscopic conductor that is connected via perfect leads to a number of carrier reservoirs. The electrons deep inside the reservoirs are assumed to maintain a Fermi-Dirac distribution at temperature T, $f(E-\mu_\alpha)=\{\exp[(E-\mu_\alpha)/k_BT]+1\}^{-1}$, where μ_α is the chemical potential of reservoir α. The total transmission coefficient for carriers from lead α to lead β at energy E and magnetic field B, $T_{\beta\leftarrow\alpha}(E,B,\{\mu_\gamma\})$, is determined by the electric potential $U(\boldsymbol{x},\{\mu_\gamma\})$ in the conductor, which is a function of the position $\boldsymbol{x}$ and the chemical potentials of all the reservoirs $\{\mu_\gamma\}$. As emphasized by Landauer,[13] $U(\boldsymbol{x},\{\mu_\gamma\})$ is a self-consistent field, which mainly exists at the geometric narrowing or spreading including the entrances and exits of the leads. In principle, the determination of $U(\boldsymbol{x},\{\mu_\gamma\})$ and thus $T_{\beta\leftarrow\alpha}(E,B,\{\mu_\gamma\})$ requires a self-consistent calculation that, however, is considerably difficult to be performed in a practical device.

Using the scattering approach, the current through lead α is written as

$$I_\alpha=\frac{2e}{h}\sum_{\beta\neq\alpha}\int[f(E-\mu_\alpha)T_{\beta\leftarrow\alpha}(E,B,\{\mu_\gamma\})-f(E-\mu_\beta)T_{\alpha\leftarrow\beta}(E,B,\{\mu_\gamma\})]dE. \tag{1}$$

Considering that $\Sigma_{\beta\neq\alpha}T_{\beta\leftarrow\alpha}(E,B,\{\mu_\gamma\})=\Sigma_{\beta\neq\alpha}T_{\alpha\leftarrow\beta}(E,B,\{\mu_\gamma\})$ holds for an arbitrary magnetic field B, Eq. (1) becomes

$$I_\alpha=\frac{2e}{h}\sum_{\beta\neq\alpha}\int[f(E-\mu_\alpha)-f(E-\mu_\beta)]T_{\beta\leftarrow\alpha}(E,B,\{\mu_\gamma\})dE. \tag{2}$$

In the following we examine Eq. (2) at different experimental limits where it reduces to simplified forms that are similar to that of the standard Landauer-Büttiker formula. At $k_BT=0$, Eq. (2) becomes

$$I_\alpha=\frac{2e}{h}\sum_{\beta\neq\alpha}\overline{T}_{[\beta,\alpha]}(\{\mu_\gamma\})(\mu_\alpha-\mu_\beta). \tag{3}$$

Here $\overline{T}_{[\beta,\alpha]}(\{\mu_\gamma\})$ depends on the sign of $(\mu_\alpha-\mu_\beta)$ and is equal to $\int_{\mu_\beta}^{\mu_\alpha}T_{\beta\leftarrow\alpha}(E,B,\{\mu_\gamma\})dE/(\mu_\alpha-\mu_\beta)$ and $\int_{\mu_\alpha}^{\mu_\beta}T_{\alpha\leftarrow\beta}(E,B,\{\mu_\gamma\})dE/(\mu_\beta-\mu_\alpha)$ when μ_α is higher and lower than μ_β, respectively. This means that only the transmissions of carriers above the lowest chemical potential of the reservoirs contribute to the net lead currents and therefore determine the resistances of the conductor.

We now further restrict ourselves to the case in which $|\mu_\alpha-\mu_\beta|$ is so small that within the energy interval between μ_α and μ_β the dependences of $T_{\beta\leftarrow\alpha}(E,B,\{\mu_\gamma\})$ and $T_{\alpha\leftarrow\beta}(E,B,\{\mu_\gamma\})$ on E can be neglected, i.e., in the *weakly* nonlinear transport regime. It is easy to obtain from Eq. (3)

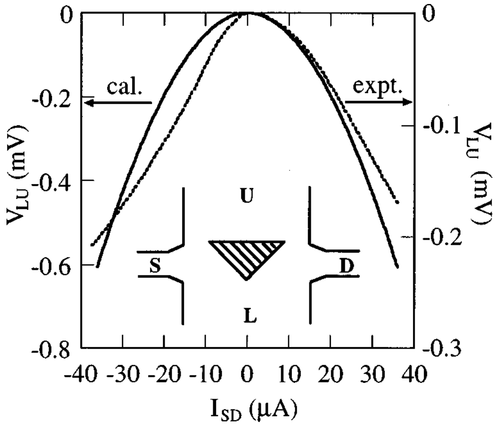

FIG. 1. Experimental (dashed line) and theoretical (solid line) V_{LU} vs I_{SD} curves (note the different scales) of the ballistic rectifier, which is schematically shown by the inset. The hatched area in the inset represents an antidot. The widths of the four leads (denoted as *S*, *D*, *U*, and *L*) and the size of the triangular antidot are smaller than the electron mean free path. These curves show that the device outputs negative voltages between leads *L* and *U*, independent of the direction of the input current through leads *S* and *D*.

$$I_\alpha \approx \frac{2e}{h}\sum_{\beta\neq\alpha} T_{[\beta,\alpha]}\left(\frac{\mu_\alpha+\mu_\beta}{2},B,\{\mu_\gamma\}\right)(\mu_\alpha-\mu_\beta)$$
$$\approx \frac{2e}{h}\sum_{\beta\neq\alpha} T_{[\beta,\alpha]}(\{\mu_\gamma\})(\mu_\alpha-\mu_\beta). \tag{4}$$

Here $T_{[\beta,\alpha]}(\{\mu_\gamma\})$ is the transmission coefficient at the chemical potential of the reservoirs at equilibrium (before the conductor is biased), $\mu^{\rm eq}$. $T_{[\beta,\alpha]}(\{\mu_\gamma\})$ is equal to $T_{\beta\leftarrow\alpha}(\{\mu_\gamma\})$ if $\mu_\alpha>\mu_\beta$ or $T_{\alpha\leftarrow\beta}(\{\mu_\gamma\})$ otherwise, which reflects the direction of net flow of carriers.

In principle, nonlinear ballistic transport starts at any nonzero current. Nevertheless, one can define a linear transport regime where $(\mu_\alpha-\mu_\beta)\rightarrow 0$ and the dependence of $T_{\beta\leftarrow\alpha}(E,B,\{\mu_\gamma\})$ on $\{\mu_\gamma\}$ is neglected. At $k_BT=0$, it is easy to find that Eq. (1) reduces to the standard Landauer-Büttiker formula $I_\alpha=(2e/h)\Sigma_{\beta\neq\alpha}T_{\alpha\leftarrow\beta}(\mu_\alpha-\mu_\beta)$.

We point out that Eqs. (1)–(4) are all gauge invariant, i.e., any result of which is invariant under a global potential shift and depends only on the differences of the voltages applied to the carrier reservoirs.

In the following, we shall apply Eq. (4) to model the rectification effect recently realized in a semiconductor microjunction.[12] We show that in the weakly nonlinear transport regime, the changes of transmission coefficients $T_{[\beta,\alpha]}(\{\mu_\gamma\})$ with applied voltages can be approximately evaluated directly from the lead currents rather than from a self-consistent calculation.

The inset of Fig. 1 schematically illustrates the central part of the ballistic rectifier, which was fabricated on a GaAs/Al_xGa_{1-x}As heterostructure. The hatched area represents a triangular antidot. The elastic mean free path $l_e \approx 6$ μm at 4.2 K is much larger than the width of the source (denoted as *S*) and drain (*D*) channels ($W_{SD}\approx 0.4$ μm) and the width of the lower (*L*) and upper (*U*) channels ($W_{LU} \approx 2.9$ μm). Negative voltages were observed between the *L* and *U* probes V_{LU} independent of the direction of the source-drain current I_{SD} as shown by the dashed line in Fig. 1. The curve is not perfectly symmetric with respect to the zero I_{SD} axis because of the imperfection of the device fabrication. The mechanism of this ‘‘ballistic rectifier’’ is entirely different from that of a normal diode since no doping junction or barrier structure was used along the current direction in this device.

To model the rectification effect, the dependence of $T_{\beta\leftarrow\alpha}(\{\mu_\gamma\})$ on the applied voltages should be calculated first. In general, $T_{\beta\leftarrow\alpha}(\{\mu_\gamma\})$ is mainly determined by the angular distribution of the carriers ejected from lead α, $P_\alpha(\theta)$ (θ being the angle with respect to the channel axis x). $P_\alpha(\theta)$ is determined by the self-consistent field $U(\boldsymbol{x},\{\mu_\gamma\})$ in the device. However, it is considerably difficult to perform a self-consistent calculation to obtain this self-consistent field in practical devices such as the ballistic rectifier. Instead, we note that $P_\alpha(\theta)$ is closely related to the lead current I_α. The reason is that if a lead current I_α is applied, the velocity component of an electron along the channel direction x, v_x, will approximately increase/decrease by the amount of the excess velocity Δv depending on the direction of Δv with respect to that of v_x. Here we refer the excess velocity Δv to the mean velocity of electrons in the lead, which, as mentioned before, the electrons gain from the self-consistent field. On the other hand, we may assume that the velocity component in the perpendicular direction v_y is not affected. Therefore, the angle of ejection of the electron changes from $\arctan(v_y/v_x)$ at $I_\alpha=0$ to $\arctan[v_y/(v_x\pm\Delta v)]$. This means that the self-consistent field in the device causes a kind of *collimation/decollimation* effect, the extent of which can be determined by the magnitude of the excess velocity or the lead current. Note that the self-consistent field mainly exists at the entrances and the exits of the leads as shown by Ref. 11, and the measured V_{LU} ($|V_{LU}|<0.2$ mV) suggests that the self-consistent field in the center of the junction is weak. Therefore, one can write $T_{\beta\leftarrow\alpha}(\{\mu_\gamma\}) \approx T_{\beta\leftarrow\alpha}(I_\alpha)$ and avoid to perform a self-consistent calculation. Equation (4) thus becomes

$$I_\alpha \approx \frac{2e}{h}\sum_{\beta\neq\alpha} T_{[\beta,\alpha]}\left(\frac{\mu_\alpha+\mu_\beta}{2},I_{[\beta,\alpha]}\right)(\mu_\alpha-\mu_\beta),$$
$$\approx \frac{2e}{h}\sum_{\beta\neq\alpha} T_{[\beta,\alpha]}(I_{[\beta,\alpha]})(\mu_\alpha-\mu_\beta), \tag{5}$$

where $T_{[\beta,\alpha]}(I_{\{\beta,\alpha\}})$ is the transmission coefficient for carriers at $\mu^{\rm eq}$, and equal to $T_{\beta\leftarrow\alpha}(I_\alpha)$ if $\mu_\alpha>\mu_\beta$ or $T_{\alpha\leftarrow\beta}(I_\beta)$ otherwise.

The V_{LU} vs I_{SD} characteristic is calculated via the four-terminal resistance $R_{SD,LU}(I_{SD})\equiv V_{LU}/I_{SD}$ derived from Eq. (4) or (5). If a negative source-drain current is applied ($\mu_S > \mu_D$), one obtains

$$R_{SD,LU}=(h/2e^2D_t)[T_{L\leftarrow S}(I_S)T_{D\leftarrow U}(I_U)$$
$$-T_{D\leftarrow L}(I_L)T_{U\leftarrow S}(I_S)], \tag{6}$$

where $I_S=-I_{SD}$ and $I_L=I_U=0$, which means that $T_{D\leftarrow U}(I_U)$ and $T_{D\leftarrow L}(I_L)$ can be approximately treated as constants. In Eq. (6), D_t is a subdeterminant of the matrix defined by Eq. (5), and is found from its expression to be insensitive to lead currents.

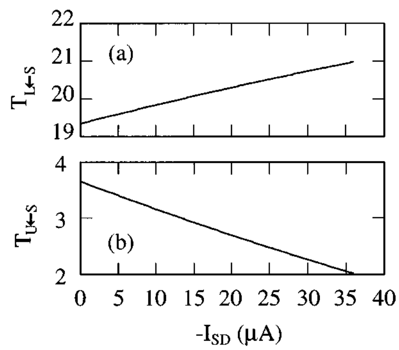

FIG. 2. The calculated transmission coefficients $T_{L\leftarrow S}$ (a) and $T_{U\leftarrow S}$ (b) as functions of the negative source-drain current. For negative source-drain currents, the electrons ejected out of lead *S* will be collimated as discussed in the text. Therefore, the probability for these electrons to be scattered into lead *L* by the triangular antidot is increased, while the probability for them to transfer into lead *U* is reduced.

At $I_{SD}=0$, the angular distribution of the ballistic electrons ejected from the *S* and *D* channels is given by $P(\theta)=\frac{1}{2}\cos\theta$, where θ lies in the interval $(-\pi/2,\pi/2)$.[14] Therefore, $T_{L\leftarrow S}(0)=T_{L\leftarrow D}(0)=\int_{-\pi/2}^{\theta_0}(N_{SD}/2)\cos\theta d\theta$ and $T_{U\leftarrow S}(0)=T_{U\leftarrow D}(0)=\int_{\theta_0}^{\pi/2}(N_{SD}/2)\cos\theta d\theta$, where $N_{SD}=k_F W_{SD}/\pi$ is the number of propagating modes in the *S* and *D* channels for a Fermi wave vector k_F. This means that the electrons ejected out of the *S* or *D* channel with angles smaller than θ_0 ($\theta_0\approx\pi/4$ for this device geometry) will transmit into the *L* channel, whereas the electrons with angles between θ_0 and $\pi/2$ will go into the *U* channel.[15]

When a negative source-drain current is applied, as mentioned above, the electrons ejected out of the *S* channel will be collimated. Therefore, these electrons will have more chance to be scattered into lead *L* by the triangular antidot and less chance to transfer into lead *U*. Thus, $T_{L\leftarrow S}$ will increase and $T_{U\leftarrow S}$ will decrease, as expressed by

$$T_{L\leftarrow S}(I_S)-T_{L\leftarrow S}(0)=N_{SD}(\sin\theta_e-\sin\theta_0)/2,$$

$$T_{U\leftarrow S}(I_S)-T_{U\leftarrow S}(0)=-N_{SD}(\sin\theta_e-\sin\theta_0)/2, \quad (7)$$

where $\theta_e=\theta_0+\arcsin[(\Delta v/v_F)\sin\theta_0]$. It is noticed that the total number of electrons ejected out of lead *S* is increased. This is because the electrons that move from the junction into lead *S* with velocities between zero and $-\Delta v$ will now be driven back to the junction due to the self-consistent field, without transmitting into reservoir *S*. Since these electrons *originally* are not coming from reservoir *S* but from other reservoirs, they should not be taken into account in the calculation of $T_{L\leftarrow S}(I_S)$ or $T_{U\leftarrow S}(I_S)$.

The curves in Figs. 2(a) and 2(b) display the dependences of $T_{L\leftarrow S}$ and $T_{U\leftarrow S}$ on I_{SD}. From $I_{SD}=0$ to -37 μA, $T_{L\leftarrow S}$ increases by about 6.4% while $T_{U\leftarrow S}$ decreases by about 34%. From Eq. (6), this indicates that although the magnitude of the transmission from *S* to *U* is much less than that from *S* to *L*, it has a much stronger influence on $R_{SD,LU}$ and therefore contributes much more to the observed negative V_{LU}. For the transmission coefficients $T_{D\leftarrow L}$ and $T_{D\leftarrow U}$, according to the time-reversal invariance at zero magnetic field, we take $T_{D\leftarrow L}(0)=T_{L\leftarrow D}(0)$ and $T_{D\leftarrow U}(0)=T_{U\leftarrow D}(0)$.[3]

To calculate D_t in Eq. (6), we make use of $T_{S\leftarrow D}=T_{D\leftarrow S}=0$ because the direct path between *S* and *D* is blocked by the antidot at zero magnetic field. We find $D_t=N_{SD}^2[N_{LU}(1-W_t/W_{LU})-N_{SD}(1-\sin\theta_0)^2/2]$, where $W_t\approx\frac{2}{3}W_{LU}$ is the upper sidelength of the triangular antidot. Thus, $R_{SD,LU}$ is finally written as

$$R_{SD,LU}=\frac{3}{2}\frac{h}{e^2}\frac{\sin\theta_e-\sin\theta_0}{2N_{LU}-3N_{SD}(1-\sin\theta_0)^2}. \quad (8)$$

The obtained V_{LU} vs I_{SD} curve together with the case of $I_{SD}>0$ is plotted using the solid line in Fig. 1. From the different scales of the V_{LU} axes, we find that the obtained voltages V_{LU} are about 3 times as high as the experimental values shown by the dashed line. So far, we have neglected the elastic scatterings from the impurities in the microjunction, which will certainly reduce the transmission coefficients in Eq. (6) and therefore the output voltage V_{LU}. Indeed, the length of the *L* and *U* channels $l=5$ μm is comparable to the elastic mean free path. Therefore, the impurities will reduce the transmission coefficients in Eq. (6) approximately to $(\frac{1}{2})^{l/l_e}\approx 56\%$, and V_{LU} just to $(0.56)^2\approx 30\%$. Thus, after taking the finite length of the leads into account, we find that the theoretical result is in remarkably good agreement with the experimental data although no adjustable parameters have been used.

We notice that the deviation of the theoretical curve from the experimental data increases at higher currents I_{SD}. This is expected since in this model we have restricted ourselves only to the weakly nonlinear regime, where the excess velocity Δv is small in comparison with the Fermi velocity v_F. In the strongly nonlinear regime, Eq. (3) should be employed instead of Eq. (5). In addition, the self-consistent field, which is built up in the center of the cross junction, might become not negligible, so that a self-consistent calculation is needed for the case of large currents.

It was argued that the ballistic rectifier has no intrinsic threshold since the nonlinear ballistic transport, on which the device relies, starts at any nonzero current.[12] To verify this prediction, we write Eq. (8) in the limit of $|I_{SD}|\to 0$ as

$$\frac{V_{LU}}{I_{SD}}\approx-\frac{h}{e^2}\frac{3\hbar}{4eE_FN_{SD}}\frac{\sin 2\theta_0 I_{SD}}{2N_{LU}-3N_{SD}(1-\sin\theta_0)^2}. \quad (9)$$

Although Eq. (9) shows that the rectification efficiency V_{LU}/I_{SD} decreases *linearly* with decreasing the magnitude of the applied current, we point out that indeed no intrinsic threshold is expected. The reason is that any nonzero current will lead to a finite excess velocity and therefore result in the (de-)
collimation effect of carriers and changes of the transmission coefficients.

Equation (9) also indicates a parabolic *I*-*V* curve at low source-drain currents, which is supported by the experimental observations. This means that the ballistic rectifier is also favorable for second harmonic generation, because unlike a normal nonlinear device, ideally this device will not produce third or higher harmonics.

So far, we have not included in the model the geometric collimation effect of the horn-shape openings of the *S* and *D* channels. In the presence of a geometric collimation, the angular distribution of the ejected electrons becomes $P(\theta) = \frac{1}{2} f \cos\theta$, where $-\arcsin(1/f) < \theta < \arcsin(1/f)$ and $f > 1$ is a factor determined by the geometry.[1] However, we emphasize that the influence of the geometric collimation on the transmission coefficients does not change with lead current, and the horn-shape openings alone will never induce a negative voltage V_{LU} as shown by Eq. (6). To observe the rectification effect, nonlinear transport is necessary, where the transmission coefficients change with lead currents. Therefore, the geometric collimation is not expected to have a significant influence on the rectification effect. Furthermore, to include the geometric collimation effect, certain assumptions will be needed for the potential profile of the horn-shape openings, which is very complex. We have also neglected the spatial (y direction) distribution of ballistic electrons in the *S* and *D* channels, which we expect to have no obvious influence on $R_{SD,LU}$ in this case.

It is very easy to use Eq. (9) to predict the highest efficiency V_{LU}/I_{SD}, for this type of sample geometry, which turns out to be more than two orders of magnitude higher than that of the present device. The easiest and most effective approach is to use a top gate, to which negative voltages are applied to lower the Fermi energy E_F and reduce N_{SD} and N_{LU}. A lower Fermi energy corresponds to a lower Fermi velocity, so that for the same excess velocity Δv a better collimation effect can be reached. Motivated by this prediction, we recently performed an experiment on a similar device with a top gate.[16] By applying a negative gate voltage, the observed V_{LU}/I_{SD} was found to be about 100 times higher than that of the present device at a given current I_{SD}, which has confirmed the theoretical prediction.

In summary, we have developed a formalism of nonlinear transport in multiterminal mesoscopic conductors. We show that even in the nonlinear regime, four-terminal resistances can still be expressed as simple functions of transmission coefficients. Using the formula of weakly nonlinear transport, we have provided an analytical description of the ballistic rectification effect, which is in remarkably good agreement with the experimental observations.

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[15] Like the case of modeling the quenched Hall effect (Ref. 14), only classical billiard scattering is considered in the present model, i.e., assuming that the lateral confinement in the *S* and *D* channels is not strong enough for the wave nature of the carriers to dominate the transport. This is also supported by the experiment result, which showed that the device even worked at 77 K (Ref. 12).
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