Mesoscopic Rectifiers Based on Ballistic Transport:
Playing off Classical against Quantum Mechanics

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Abstract

Recent experiments on symmetry-broken mesoscopic semiconductor structures \cite{1,2} have exhibited an amazing rectifying effect in the transverse current-voltage characteristics with promising prospects for future applications. We present a simple microscopic model, which takes into account the energy dependence of current-carrying modes and explains the rectifying effect by an interplay of fully quantized and quasi-classical transport channels in the system. It also suggests the design of a ballistic rectifier with an optimized rectifying signal and predicts voltage oscillations which may provide an experimental test for the mechanism considered here.

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FIG. 1: (a) Geometry of the experimental setup used in Ref. [1]. The leads at S and D are approx. 400nm wide, corresponding to approx. 20 to 22 modes at the equilibrium Fermi energy (about 18meV). The leads at U and L are approx. 3.2µm wide, corresponding to about 180 – 200 modes. (b) A scheme of a voltage probe. (c) A rectifier consisting of a combination of two such probes with two or three channels. (d) Suggested geometry of an optimized ballistic rectifier.

The decreasing size of nanofabricated structures opens up new possibilities for mesoscopic semiconductor devices by exploiting ballistic transport in the 2-dimensional electron gas and quantization of confined electrons. Details of the geometry are crucial for the functioning of such devices. In the geometry of Fig. 1a, which was used in an experiment by Song et al. [1], the symmetry was broken on purpose by introducing a triangle as shown. When current is injected at the source (S) and drawn out at the drain (D), a majority of charge carriers is deflected towards the lower voltage probe (L). Naively thinking and in the spirit of the Hall effect one might expect that a voltage difference builds up between the upper (U) and lower (L) voltage probe. Since the sample is symmetric with respect to the exchange of source and drain, the same voltage difference would arise on reversing the current and the sample would work as a rectifier.

On second thought, however, our physical understanding of mesoscopic systems leads us not to expect any voltage drop from top to bottom at all. As will be argued in detail below, symmetry considerations and the Landauer-Büttiker formalism [3] in its most common linear form do not allow for such a voltage drop. It thus came as a surprise, when the experiment by Song et al. [1] revealed a rectifying effect. An interpretation of the experimental result
FIG. 2: (A-D): Transverse current-voltage characteristics for various models of a ballistic rectifier as described in the text calculated for temperature $T = 4K$ and Fermi energy $\mu_F = 18\text{meV}$. (Exp.): Experimental curve after Ref. [1] shown for comparison.

In Refs. [1, 2] was based on the assumption of dissipation within the sample leading to self-consistent electric fields and a current dependence of the transmission probabilities through the sample. A phenomenological ansatz was made, as this current dependence would be exceedingly complicated to calculate in a microscopic model.

In the present letter we present a microscopic explanation of the rectifying effect which explicitely takes into account the energy dependence of the number of transverse modes for a system of two voltage probes. It does not require the existence of dissipation in the leads, instead the rectifying effect here originates in the interplay between purely quantized and quasi-classical transport in different channels of the system, which exhibit different energy dependences. A calculation of the tranverse current-voltage characteristics involving this mechanism shows good agreement with the experimental observations. This mechanism also leads to a prediction for the design of a ballistic rectifier with an optimized rectifying signal. For strong currents it predicts a reversal and even oscillations of the transverse voltage, which may provide a test for the explanation presented here.

Transport in mesoscopic systems like the one in Fig. 1a is typically described by the linear
Landauer-Büttiker-formalism \[3\]

\[ I_i = \frac{2e}{h} \left[ (M_i - R_i) \mu_i - \sum_{j \neq i} T_{ij} \mu_j \right]. \quad (1) \]

Here \( I_i \) is the net current in lead \( i \) connecting the sample to a reservoir (contact) with chemical potential \( \mu_i \). The leads are assumed to be ideal quantum leads with \( M_i \) modes. \( R_i = T_{ii} \) is the reflection coefficient, which describes back-scattering from the sample into lead \( i \) and \( T_{ij} \) are the transmission coefficients form lead \( j \) into lead \( i \). Transport across the sample is assumed to be purely elastic and dissipation and equilibration only take place in the reservoirs.

A prominent result of the Landauer-Büttiker formalism is the \emph{reciprocity relation}

\[ R_{ij,kl}(B) = R_{kl,ij}(-B). \quad (2) \]

Here \( R_{ij,kl} = V_{kl}/I_{ij} \) is the resistance obtained by dividing the voltage \( V_{kl} \) measured between contact \( k \) and \( l \) by the current \( I_{ij} \) flowing from contact \( j \) to \( i \). For the system of Fig. 1a at zero magnetic field we thus have

\[ R_{UL,SD} = R_{SD,UL}. \quad (3) \]

Because of the symmetry of the system there can be no voltage build-up between \( S \) and \( D \) if the current is flowing from \( L \) to \( U \). Thus \( R_{UL,SD} = 0 \) and hence by means of Eq. (3) we would expect \( V_{UL} \) to vanish identically – in contrast to the experimental findings. (We would of course obtain the same results by solving the Eqs. (1) directly.) To overcome this apparent contradiction Song et al. \[1, 2\] suggested to include a phenomenological current dependence of the transmission coefficients due to dissipation inside the sample. In our treatment the necessary nonlinearity arises in the transport equations, if we allow for varying numbers of modes in the leads. We will show below that one needs not give up the conceptually attractive assumption of purely elastic transport inside the sample, that was so very successful in describing a wide range of experiments on transport in mesoscopic system (for reviews see e.g. \[4, 5, 6\]).

To achieve this aim we use the Landauer-Büttiker formalism in a more general form \[7\]. The current per unit energy (a quantity, which we will call \emph{current density} in the following for simplicity) injected into the sample from reservoir \( i \) through lead \( i \) at energy \( E \) is

\[ i_i^+(E, \mu_i, T) = \frac{2e}{h} M_i(E) f_i(E). \quad (4) \]
Here \( f_i(E) = f(E, \mu_i, T) \) is the Fermi-distribution in reservoir \( i \) at temperature \( T \). The outgoing current density in lead \( i \) is

\[
i_i^-(E, \{\mu_l\}, T) = \frac{2e}{\hbar} \left[R_i(E)f_i(E) + \sum_{i \neq j} T_{ij}(E)f_j(E)\right].
\]  

(5)

If we assume, that the transmission probabilities \( T_{ij} \) are independent of energy and the mode number, we can write \( T_{ij}(E) = T_{ij} M_j(E) \) and Eq. (5) becomes

\[
i_i^-(E, \{\mu_l\}, T) = \sum_j T_{ij} i_j^+(E, \mu_j, T).
\]  

(6)

The incoming and outgoing currents are, respectively,

\[
I_i^\pm = \int_{\mu_0}^{\infty} i_i^\pm(E) dE,
\]

(7)

where \( \mu_0 \) is an auxiliary quantity that is small enough so that \( f(\mu_0, \mu_i, T) \approx 1 \) holds for all \( i \), but is otherwise arbitrary and will not show up in any measurable quantity. The balance equation for the current source with net current \( I \) then is \( I_S^+ - I_S^- = I \) and for the drain \( I_D^+ - I_D^- = -I \). A voltage probe is characterized by zero net current, i.e. \( I_i^+ = I_i^- \).

The number of modes \( M_j(E) \) can be written as

\[
M_j(E) = \sum_n \Theta(E - \varepsilon_{j,n}),
\]

(8)

where the \( \varepsilon_{j,n} \) are the energy eigenvalues of the transverse modes in lead \( j \) and \( \Theta(x) \) denotes the Heaviside step function. For leads with a hard wall (i.e. box-like) cross section of width \( W_j \) and for electrons of effective mass \( m^* \) we have

\[
\varepsilon_{j,n} = \frac{(h\pi n)^2}{2m^*W_j^2}.
\]

(9)

In this case the number of modes can also be expressed as

\[
M(E) = \text{Int} \left[ \frac{W_j}{\lambda(E)/2} \right] = \text{Int} \left[ \frac{W_j\sqrt{2m^*E}}{h\pi} \right],
\]

(10)

where \( \text{Int}[\cdot] \) denotes the integer part and \( \lambda(E) = h/\sqrt{2m^*E} \) is the de Broglie-wavelength of the electron at energy \( E \). The incoming currents can be expressed as

\[
I_j^+(\mu_j, T) = \frac{2e}{\hbar} \sum_n \left\{ kT \ln \left[e^{(\varepsilon_{j,n} - \mu_j)/kT} + 1\right] + \mu_j - \varepsilon_{j,n} \right\},
\]

(11)
and the outgoing currents accordingly by integrating Eq. (6). These formulas were used in obtaining the numerical results presented below.

Let us now examine the very simple setup of Fig. 1b. A voltage probe reservoir (P) is connected via two identical ideal leads to source and drain. To simplify the calculations let us assume zero temperature, i.e. \( f(E, \mu_i, 0) = \Theta(\mu_i - E) \). Let us further assume \( \mu_S \geq \mu_P \geq \mu_D \geq \mu_0 \), where \( \mu_S \) and \( \mu_D \) are given and \( \mu_P \) is to be determined, and let us distinguish the cases of narrow and wide leads.

(a) If \( M(E) = M = \text{constant} \) in the range between \( \mu_0 \) and \( \mu_S \) (this corresponds to narrow leads), the outgoing and incoming current densities from and to the probe reservoir are simply given by:
\[
i^+_{P}(E) = 2(2e/h)M \Theta(\mu_P - E) \quad \text{(the factor 2 arises because two leads are connected to the same reservoir)} \quad \text{and} \quad i^\pm_{P}(E) = (2e/h) \left[ \Theta(\mu_S - E) + \Theta(\mu_D - E) \right].
\]
These are trivially integrated and the current balance of the voltage probe \( I^+_P = I^-_P \) reads
\[
\frac{4e}{h}M(\mu_P - \mu_0) = \frac{2e}{h}M(\mu_S + \mu_D - 2\mu_0)
\]
and thus the chemical potential \( \mu_P \) of the voltage probe is independent of \( M \) and given by
\[
\mu_P = (\mu_S + \mu_D)/2.
\]

(b) If the leads are assumed to be wide compared to the Fermi wavelength \( \lambda_F \), the number of modes will increase even under small changes in energy. In the case of a hard wall channel of width \( W >> \lambda_F \) we can approximate Eq. (10) by a smooth function, i.e.
\[
M(E) = \text{Int} \left[ \frac{W}{\lambda(E)/2} \right] \approx \frac{\sqrt{2m^*W}}{\pi \hbar} \sqrt{E}.
\]
Since \( M(E) \) grows as \( \sqrt{E} \), the channels described in this approximation may be called \textit{quasi-classical}, because the classical energy surface likewise increases as the square-root of the energy. The current densities are \( i^\pm_P(E) = 2Q\sqrt{E} \Theta(\mu_P - E) \) and \( i_P^\pm = Q\sqrt{E}[\Theta(\mu_S - E) + \Theta(\mu_D - E)] \) with \( Q = \sqrt{16m^*eW/\hbar^2} \). The current balance now reads
\[
\frac{4Q}{3} \left( \frac{\mu_P^{3/2}}{\mu_0^{3/2}} - \frac{\mu_0^{3/2}}{\mu_0^{3/2}} \right) = \frac{2Q}{3} \left( \frac{\mu_S^{3/2}}{\mu_S^{3/2}} + \frac{\mu_D^{3/2}}{\mu_D^{3/2}} - 2\frac{\mu_0^{3/2}}{\mu_0^{3/2}} \right),
\]
and we find
\[
\mu_P = \sqrt[3]{\left( \frac{\mu_S^{3/2}}{\mu_D^{3/2}} \right)^2} > (\mu_S + \mu_D)/2,
\]
FIG. 3: Current balance in the voltage probe P and adjustment of the chemical potential $\mu_P$ at zero temperature. Current enters P from S in the energy interval $[\mu_P, \mu_S]$ and exits from P to D in the interval $[\mu_D, \mu_P]$. The total current $I^+_P - I^-_P$ is determined by the shaded areas and must balance to zero. (a) For narrow leads $(M(E) = \text{const.})$ this obviously determines $\mu_P$ as the mean $(\mu_D + \mu_S)/2$. (b) In the quasi-classical case $\mu_p$ must shift to higher values to counterbalance the increase of $M(E)$ with energy.

i.e. the potential $\mu_P$ deviates from the mean Eq. (13). As illustrated in Fig. 3 this is because the net current is transported from S to P by a larger number of modes in the energy interval $[\mu_P, \mu_S]$ than from P to D in the energy interval $[\mu_D, \mu_P]$ and thus $\mu_P$ raises above the mean to compensate for the additional current.

Equations (13) and (16) suggest how to create a rectifier based on ballistic transport: As sketched in Fig. 1c let us consider two separate pathways from source to drain, each via a voltage probe as in the above example (ignoring the third dotted pathway for the moment). If on both paths the number of modes is constant, the voltage probes will each be at the mean chemical potential between source and drain, i.e. there will be no voltage drop from top to bottom (this is what we showed based on the reciprocity relation in the beginning). The same holds true, if the current density grows identically with energy in both channels, e.g. for two quasi-classical channels. If on the other hand one path is narrow, i.e. has constant mode number $M_1$, whereas the other is wide with an increasing number of modes $M_2(E)$, we can observe a voltage drop between the probes, as indicated by the interval marked by the fat line in Fig. 3. Reverting the current yields the same voltage drop due to symmetry and thus we achieve the rectification of the signal.
In order to explain the experimental results of Ref. [1] we need to assume a third channel connecting the probes U and L in Fig. 1c (dotted lines) with \( M_3(E) \) modes, since there is a direct connection between U and L in Fig. 1a. Now we consider finite temperatures again and choose \( M_1 = 1 = \text{const.} \) in the energy window, whereas for \( M_2(E) \) and \( M_3(E) \) we use the quasi-classical Eq. (14) with \( M_2(E_F) = 20 \) and \( M_3(E_F) = 15 \). These mode numbers were estimated by classical numerical calculations of the transmission coefficients \( T_{US} \) and \( T_{LS} \) in the geometry of Fig. 1a modeling the experiment. Curve A in Fig. 2 shows the resulting rectifying signal of this setup. If we give up the quasi-classical approximation for the wide channels and use the explicit sums instead, we obtain curve B, which nicely agrees with the experimental result (note that the experimental curve is not entirely symmetric due to an unintentional slight asymmetry of the sample about the vertical axis).

Based on the above mechanism we can now suggest the design of a ballistic rectifier with an optimized rectifying signal. If one manages to suppress the third channel between U and L, the voltage drop \( V_{UL} \) can be enhanced. This is shown by curve C of Fig. 2 for the model of Fig. 1c without the dotted channel and using the quasi-classical approximation for the wide channel. Note that this curve can easily be calculated analytically for \( T=0 \). Using Eq. (13) and (16) one obtains \( \mu_U \) and \( \mu_L \), and hence the voltage difference, as a function of \( \mu_S \), while leaving \( \mu_D \) constant. The total current \( I \) is given by the sum of the individual currents from the source S to U and to L, i.e.

\[
I = 2Q/3 (\mu_S^{3/2} - \mu_L^{3/2}) + 2e/h (\mu_S - \mu_U),
\]

which is the current-voltage characteristics in analytic form. If again we give up the quasi-classical approximation for the wide leads, we find an even stronger rectifying signal as shown in curve D. As a realization of such a system which suppresses the third channel we suggest the geometry shown in Fig. 1d.

An interesting phenomenon arises in these structures, which combine narrow and wide leads, when the narrow channel opens up a new mode within the energy window: the voltage \( V_{UL} \) undergoes a change in sign! This is demonstrated in Fig. 4, where the dotted line again shows curve D from Fig. 2. The solid line corresponds to slightly wider leads in the upper channel whereby \( \mu_S \) becomes larger than \( \varepsilon_2 \) of the narrow leads. This curve will eventually turn back to negative voltages as \( I \) (following \( \mu_S \)) increases and shoot up again, when the third mode opens in the upper channel. This change in sign or even oscillations should be observable in an appropriate experiment, which would provide a test for the mechanism of ballistic rectifiers presented in this paper.
FIG. 4: The voltage \( V_{UL} \) undergoes a change in sign as a second mode opens up in the narrow channel of Fig. 1c.

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