Nonlinear voltages in multiple-lead coherent conductors

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(Received 1 April 1992)

We use the generalized S-matrix approach to study multiple-lead coherent conductors in the case of finite applied voltages. In this framework we discuss the transverse voltage arising in a four-lead conductor with two symmetric biased leads.

Recently a great number of experiments have shown the possibility of investigating the coherent electron transport.[1,2] In the regime of very small applied voltages and currents (linear regime) coherent transport can be described in terms of the Landauer-Büttiker formula for conductance.[3,4] However, in different situations nonlinear corrections to the Landauer-Büttiker formula may become important. Some authors[5–7] have noticed that in two-lead devices nonlinear phenomena occur for applied voltages greater than a critical value. In this paper we show that nonlinear effects can arise in a multiple-lead conductor for *arbitrarily small* values of the applied voltage when certain geometrical symmetries exist.

The Landauer-Büttiker formula for multiple-lead conductors[8,9] has been recently extended to account for temperature changes in the reservoirs and heat fluxes in the leads.[10] We propose a similar extension which accounts for a nonlinear dependence of the conductance on the applied voltages.

Let us consider a general three-dimensional conductor with N ideal leads (see Fig. 1 for a two-dimensional four-lead schematic picture). Let $V(x,y,z)$ be the potential function inside the conductor when $M<N$ leads are connected to voltage sources which keep them to constant potential V_i, $i=1,\ldots,M$. When electron inelastic scattering is neglected, the potential values in the open leads, V_i, $i=M+1,\ldots,N$, can be calculated by considering the related coherent quantum-mechanical transmission problem. Let (x_i,y_i,z_i) be a reference frame associated to the ith lead with x_i parallel to the lead itself. The electron eigenfunctions inside the ith lead can be expressed in terms of plane waves in the x_i direction and localized states in the (y_i,z_i) plane

$$\sqrt{\frac{m}{2\pi\hbar^2 k_i}}\,e^{\pm ik_i x_i}\phi_\nu(y_i,z_i), \tag{1}$$

where $k_i=\sqrt{2m(\epsilon-V_i)/\hbar^2}$ is the ith lead wave vector at the longitudinal energy ϵ and ν is the index of the transverse state with energy ϵ_ν. The longitudinal plane waves are chosen normalized to an energy δ distribution. In this way any relevant physical quantity is related to the longitudinal energy distribution of the electrons inside the leads. When an electron is injected inside the conductor through the ith lead in the state (ϵ,ν) its wave function is scattered in all the other leads. In the stationary regime we have

$$\psi_i=\sqrt{\frac{m}{2\pi\hbar^2 k_i}}\,e^{-ik_i x_i}\phi_\nu(y_i,z_i)+\sum_{\nu'}\sqrt{\frac{m}{2\pi\hbar^2 k_i'}}\,e^{ik_i' x_i}\phi_{\nu'}(y_i,z_i)r_{i\nu,i\nu'}(\epsilon,\epsilon';[V]), \tag{2}$$

$$\psi_j=\sum_{\nu'}\sqrt{\frac{m}{2\pi\hbar^2 k_j'}}\,e^{ik_j' x_j}\phi_{\nu'}(y_j,z_j)\;t_{i\nu,j\nu'}(\epsilon,\epsilon';[V]),\qquad j\neq i, \tag{3}$$

where ϵ' and ν' are fixed by the energy conservation relation for elastic scattering: $\epsilon+\epsilon_\nu=\epsilon'+\epsilon_{\nu'}$. The transmission and reflection amplitudes, t and r, depend on the potential function $V(x,y,z)$ inside the conductor. The electric current per unit longitudinal energy flowing into the jth lead due to the quantum state (ϵ,ν) follows the usual current rule

$$\frac{dI^{i\to j}(\epsilon,\nu)}{d\epsilon}=-e\int dy_j dz_j\;\frac{\hbar}{2mi}\left(\psi_j^*\frac{\partial\psi_j}{\partial x_j}-\psi_j\frac{\partial\psi_j^*}{\partial x_j}\right)=-\frac{e}{h}\sum_{\nu'}|t_{i\nu,j\nu'}|^2. \tag{4}$$

The total electric current $I^{i\to j}$ flowing into the jth lead from the ith lead is obtained summing this contribution over all the ith lead electrons. If the energy distribution of the electrons inside the leads is $n[(\epsilon-eV_i-\mu)/k_B\theta]$ for each ν transverse state where $n(x)\equiv[\exp(x)+1]^{-1}$ is the Fermi function and θ and μ are the relevant temperature and chemical potential, respectively, we get

$$I^{i\to j}=-\frac{2e}{h}\int d\epsilon\;n[(\epsilon-eV_i-\mu)/k_B\theta]\;T_{ij}(\epsilon), \tag{5}$$

where spin degeneracy has been accounted for explicitly. The transmission coefficients $T_{ij}(\epsilon) = \sum_{\nu,\nu'} |t_{i\nu,j\nu'}|^2$ are functionals of $V(x,y,z)$. However, in most cases, for small applied potentials the dependence of $T_{ij}(\epsilon)$ on V is weak and they can be calculated with good approximation by setting $V = 0$. Making use of the probability flux conservation and the symmetry relations $T_{ij} = T_{ji}$, we write the total current I_j flowing into the jth lead from the inside of the conductor as

$$I_j = \sum_{i \neq j} (I^{i\to j} - I^{j\to i}) = \frac{2e}{h} \sum_{i\neq j} \Gamma_{ij}, \tag{6}$$

where

$$\Gamma_{ij} = \int d\epsilon \, \{ n[(\epsilon - eV_j - \mu)/k_B\theta] - n[(\epsilon - eV_i - \mu)/k_B\theta]\} \, T_{ij}(\epsilon). \tag{7}$$

From this equation we can determine the potentials generated into the open leads by the current flowing into the leads kept at fixed external voltages. Due to the energy dependence of the transmission coefficients $T_{ij}(\epsilon)$ the condition $I_j = 0$ for the open leads represents a system of nonlinear equations. As a consequence the unknown potentials V_j, $j = M+1,\ldots,N$ are nonlinear functions of the fixed voltages V_j, $j = 1,\ldots,M$.

At sufficiently low temperature Γ_{ij} can be developed in a series of even powers of $k_B\theta$:

$$\Gamma_{ij} = \int_{eV_i}^{eV_j} T_{ij}(\mu + x)\, dx + \frac{\pi^2}{6}(k_B\theta)^2 [T'_{ij}(\mu + eV_j) - T'_{ij}(\mu + eV_i)] + \ldots, \tag{8}$$

where $T'_{ij}(\epsilon) \equiv dT_{ij}(\epsilon)/d\epsilon$. If we make the ansatz that

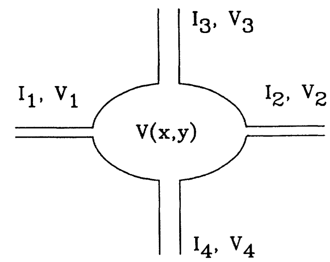

FIG. 1. Schematic picture of a four-lead two-dimensional conductor with the relevant potentials and currents.

the transmission coefficients are linearly varying functions near the chemical potential, i.e.,

$$T_{ij}(\epsilon) = T_{ij}(\mu) + T'_{ij}(\mu)\, (\epsilon - \mu) \tag{9}$$

the temperature-dependent term in Eq. (8) cancels out and Γ_{ij} is quadratically dependent on the lead potentials:

$$\Gamma_{ij} \simeq (eV_j - eV_i)T_{ij}(\mu) + \tfrac{1}{2}(e^2V_j^2 - e^2V_i^2)T'_{ij}(\mu). \tag{10}$$

The above approximation is well suited to investigate analytically some definite situations in the limit of small but finite applied voltages. Here we study the case of a four-lead conductor (see Fig. 1). Two leads of the conductor (leads 1 and 2 of Fig. 1) are open and $I_1 = I_2 = 0$. A current $I = I_4 = -I_3$ flows between the other two leads due to a voltage source V which keeps them at potentials $V_4 = -V_3 = V/2$. The presence of the current I induces a potential difference $V_1 - V_2$ also between the open leads. If a geometrical symmetry $3 \leftrightarrow 4$ between the biased leads exists, $V_1 - V_2$ is a nonlinear function of I for arbitrarily small values of I. Let us analyze in detail this symmetric case. Imposing $T_{13} = T_{14}$ and $T_{23} = T_{24}$ in Eq. (6) for I_1 and I_2 and using approximation (10), we get

$$[T_{12}(\mu) + 2T_{13}(\mu)]V_1 - T_{12}(\mu)V_2 + [\tfrac{1}{2}T'_{12}(\mu) + T'_{13}(\mu)]eV_1^2 - \tfrac{1}{2}T'_{12}(\mu)eV_2^2 = \tfrac{1}{4}T'_{13}(\mu)eV^2, \tag{11}$$

$$[T_{12}(\mu) + 2T_{23}(\mu)]V_2 - T_{12}(\mu)V_1 + [\tfrac{1}{2}T'_{12}(\mu) + T'_{23}(\mu)]eV_2^2 - \tfrac{1}{2}T'_{12}(\mu)eV_1^2 = \tfrac{1}{4}T'_{23}(\mu)eV^2. \tag{12}$$

Due to the symmetry $3 \leftrightarrow 4$ the terms linear in V cancel out. The voltage V is related to the applied current I through Eq. (6) for I_3 and I_4, i.e.,

$$I = \frac{e^2}{h}[T_{13}(\mu) + T_{23}(\mu) + 2T_{34}(\mu)]\, V. \tag{13}$$

Now the quadratic terms cancel out and the Ohm law $V = R_{34}I$ holds. At small applied current the quadratic terms in the left-hand side of Eqs. (11) and (12) can be neglected as well, hence

$$V_1 - V_2 = \frac{e}{8}V^2 \; \frac{T'_{13}(\mu)T_{23}(\mu) - T_{13}(\mu)T'_{23}(\mu)}{T_{13}(\mu)T_{23}(\mu) + T_{12}(\mu)[T_{13}(\mu) + T_{23}(\mu)]/2}. \tag{14}$$

Taking into account the linear dependence of V on I we get a quadratic dependence of the transverse voltage on the applied current. It is worth noting that this transverse voltage crucially depends on the gradients of the transmission coefficients near the chemical potential.

In the case of a not-too-small applied current the quadratic terms in Eqs. (11) and (12) cannot be neglected and the system of nonlinear equations can be solved numerically. The transmission coefficients and their derivatives at the chemical potential are in principle valuable from the geometrical characteristics of the device. In Fig. 2 we assign to these quantities a set of arbitrary but realistic values and we show the behavior of the numerical solution $V_1 - V_2$ as a function of I in comparison with the analytical small-current result.

The example we have discussed may be relevant in the interpretation of two recent experiments.[11,12] In both these experiments the transverse voltage established at the open leads of a four-lead device is interpreted in terms of a pure thermopower effect.[5,13] Due to the current I flowing in the biased channel (channel 3-4 in Fig. 1) the central portion of the device, the region c hereafter, would heat up to a temperature $\theta + \Delta\theta$ while the leads 1 and 2 are held at the lattice temperature θ. If leads 1 and 2 have different thermoelectric conductivity with respect to the region c, a potential difference between them arises proportional to $\Delta\theta$. The region c at potential V_c acts as a reservoir at temperature $\theta+\Delta\theta$ and leads 1 and 2 can be considered separately in relation to c. In this two-lead scheme from Eq. (6) within approximations (8) and (9) we get

$$0 = \int d\epsilon \,\{n[(\epsilon - eV_i - \mu)/k_B\theta] - n[(\epsilon - eV_c - \mu)/k_B(\theta + \Delta\theta)]\}\, T_{ic}(\epsilon)$$
$$\simeq (eV_i - eV_c)T_{ic}(\mu) + \tfrac{1}{2}(e^2V_i^2 - e^2V_c^2)T'_{ic}(\mu) - \frac{\pi^2 k_B^2}{3}\,\theta\,\Delta\theta\, T'_{ic}(\mu), \quad i = 1,2. \tag{15}$$

In the limit of small $\Delta\theta$, i.e., small I, the quadratic terms in the above equation can be neglected and the potential difference between leads 1 and 2 increases linearly with $\Delta\theta$

$$V_1 - V_2 = \frac{\pi^2 k_B^2}{3e}\,\theta\,\Delta\theta\,\frac{T'_{1c}(\mu)T_{2c}(\mu) - T_{1c}(\mu)T'_{2c}(\mu)}{T_{1c}(\mu)T_{2c}(\mu)}. \tag{16}$$

The transverse voltage arising from the thermopower effect and the transverse voltage arising from the multiple-lead effect are, in principle, both present in any experiment involving a multiple-lead device. The question has been already raised by Gusev, Kvan, and Pogosov.[14] In fact, the very current used to create a temperature gradient through a mesoscopic sample may cause a transverse voltage between open leads. In the case of a four-lead device with two symmetric biased leads this effect is quantitatively represented at small applied current by Eq. (14) which has to be compared with the thermopower voltage of Eq. (16).

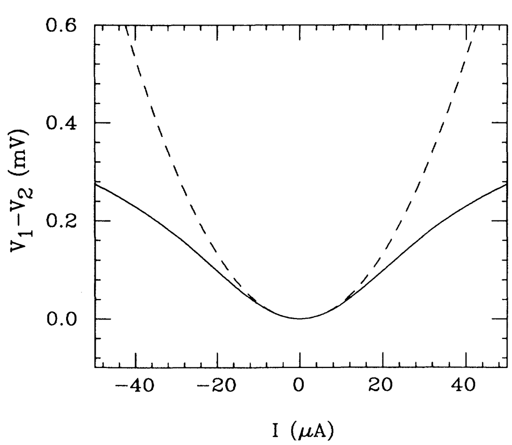

FIG. 2. Example of the nonlinear behavior of the transverse voltage $V_1 - V_2$ as a function of the applied current $I = V/R_{34}$. The dashed line is the small current analytical result of Eq. (14). The solid line is the numerical solution of the system of Eqs. (11) and (12). The parameter values are as follows: $T_{12}(\mu) = 0$, $T_{13}(\mu) = 0.3$, $T_{23}(\mu) = 0.5$, $T'_{12}(\mu) = 200\ \mathrm{eV}^{-1}$, $T'_{13}(\mu) = 200\ \mathrm{eV}^{-1}$, $T'_{23}(\mu) = 200\ \mathrm{eV}^{-1}$, and $R_{34} = 100\ \Omega$.

A comparison between the two effects needs the evaluation of the transmission coefficients for each physical device. However, in the experimental situation described in Ref. 12 a great simplification arises. The open leads 1 and 2 are two quantum point contacts on the sides of the symmetric channel 3-4. In this case the transmission coefficient T_{12} is small with respect to $T_{13} = T_{14}$. The transmission coefficient relevant in the thermopower effect $T_{1c} \simeq T_{12}+T_{13}+T_{14}$ reduces therefore to $T_{1c} \simeq 2T_{13}$. Analogously $T_{2c} \simeq 2T_{23}$. As a consequence the thermopower and the multiple-lead transverse voltages have the same dependence on the transmission coefficients and their ratio can be evaluated without any quantum-mechanical calculation:

$$\frac{(V_1 - V_2)_{\mathrm{th}}}{(V_1 - V_2)_{\mathrm{ml}}} = \frac{8\pi^2 k_B^2}{3e^2}\,\frac{\theta\Delta\theta}{(R_{34}I)^2}. \tag{17}$$

Here $R_{34} = V/I$ is the resistance of the biased channel. In the experiment[12] the channel 3-4 (of width $W = 4\ \mu$m and length $L = 18\ \mu$m) is defined electrostatically in a high-mobility two-dimensional (2D) electron gas in a GaAs-(Al,Ga)As heterostructure. Assuming typical 2D electron mobility $\mu \simeq 100\ \mathrm{m^2\,V^{-1}\,s^{-1}}$ and carrier density $n \simeq 3 \times 10^{15}\ \mathrm{m}^{-2}$ the resistance R_{34} turns out to be around 100 Ω. For a current $I = 5\ \mu$A the authors of Ref. 12 estimate an electron gas heating $\Delta\theta \simeq 2$ K. With these values at a lattice temperature $\theta = 1.65$ K the ratio $(V_1 - V_2)_{\mathrm{th}}/(V_1 - V_2)_{\mathrm{ml}}$ is of the order of unity. Using the words of Büttiker,[9] this is an example that multiple-lead effects are an essential step to understanding transport in small systems.

We thank V. Fal'ko, G. Jona-Lasinio, and F. Marchesoni for useful discussions. One of us (G.B.L.) is indebted to G. Jona-Lasinio and F. Marchesoni for the kind hospitality in the Universities of Roma "La Sapienza" and Perugia where a part of this work has been completed.

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