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Ballistic transport in nanowire through junctions of narrow–wide–narrow geometry

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ABSTRACT

We investigate ballistic transport phenomena through a region containing a cavity in a quasi-one-dimensional quantum wire. Conductance curve calculated as a function of a structure parameter shows very narrow periodic dips, which are due to anti-resonances. The nature of the virtual bound state appearing around the cavity is studied in detail. Transport phenomena through a small dilute magnetic semiconductor are also investigated.

1. Introduction

The development of the semiconductor microprocessing technology has made it possible to fabricate two-dimensional ballistic quantum systems, in which the scattering of electrons by disorders can be eliminated. In these systems, the quantum mechanical nature of electrons plays an essential role, since the dimension of the system is comparable to the wavelength of electrons. The sample structures and the positions of artificial impurities are important for the quantum interference effects on transport phenomena in this regime [1,2], because of very few scattering of electrons by artificial disorders. Recently, various sample structures such as bent [3], kinked, stubbed [4] and superlatticed nanowires [5], the sample structures of which had been experimentally synthesized, were studied numerically using the recursive Green's function method and the Landauer–Büttiker formula [6,7] by Wang et al. [8]. They calculated ballistic conductances and Seebeck coefficients in order to evaluate the dimensionless figure of merit (ZT), *i.e.*, $ZT = GS^2T/\kappa$, with G being the electrical conductance, S the Seebeck coefficient, T the absolute temperature, and κ the thermal conductance. The value ZT characterizes the energy conversion efficiency of solid-state thermoelectric (TE) materials. Wang et al. indicated that the value of the conductance and the Seebeck coefficient were controlled by the structure parameters such as bend angle, inter-bend length, stub height and potential barrier height [8]. Zhou and Yang also studied the ballistic TE transport properties of double-bend quantum wires in the ballistic regime [9]. They showed that the geometric confinement induced quantum interference effects, which resulted in a large Seebeck coefficient, and that the geometry-controlled ballistic TE effect could be potentially explored to design TE devices such as thermocouples at nanoscale [9]. Moreover, ballistic TE properties in double-bend graphene nanoribbons (GNRs) were investigated using the nonequilibrium Green's function by Li et al. [10]. They suggested that the maximum value of ZT ($ZT_{\max}$) was able to be controlled by modulating the length or width of double-bend GNRs [10].

So far, we have studied the quantum interference effects on the transport in the linear response regime, making use of the modal expansion [11], the Lippmann–Schwinger equation [12–15], and the transfer matrix methods [16] for various sample structures. In those works, we reported the results of investigation for the interference effects in quantum wires including disk-shaped obstacles with negative potentials [13], a ring-shaped barrier with a positive potential [15] in magnetic fields, and so forth [14,16].

In this Letter, we demonstrate the results of our examination of the interference effects on the transport properties through a quantum wire containing a single cavity. We show the conductance as a function of the size of cavity using the Landauer Formula with the calculated transmission matrix. We consider the quantum wire including the cavity in terms of an abrupt narrow–wide (NW) and wide–narrow (WN) junctions confined by infinite potential barriers without screening potentials. The results calculated show sharp dips (very narrow gaps) in the conductance, which are due to the resonant reflections (anti-resonances) by the virtual bound states around the cavity. These resonant reflections were also reported in various geometries of normal conductor [8–10,17]

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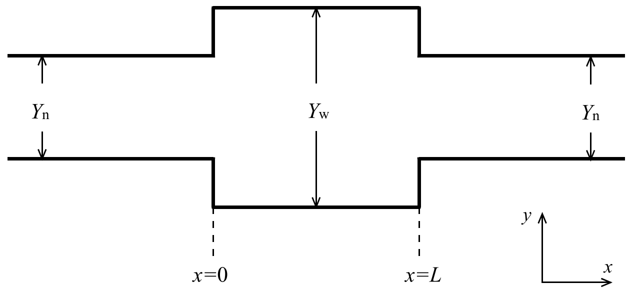

Fig. 1. Schematic figure of the system. Y_n and Y_w denote the widths of the region ($0 > x$, $L < x$) and $0 < x < L$, respectively.

and the geometries of normal conductor–superconductor composite systems [16]. In this work, we have payed attention to the variation of the interference effects as changing geometry, and therefore, we have calculated the conductance as a function of the size of cavity instead of the Fermi energy. We have also investigated the transport phenomena in the case where the cavity consisted of a small dilute magnetic semiconductor. Realizing ferromagnetic interactions in dilute magnetic semiconductor quantum dots is an important subject to the development of next-generation spin-based information technologies [18].

2. Model and method

To examine the conductance in the quasi-one-dimensional case, we have employed the modal expansion method. In the system considered, only two junctions (*i.e.*, the NW and WN junctions) are included, and hence, this method is advantageous for the calculation of the scattering matrix. We consider a quantum wire, which is assumed to be infinitely long in the x-direction, but to be finite in the y-direction as illustrated in Fig. 1. In this case, along the x-direction, the system consists of three parts; a semi-infinite lead for $-\infty < x < 0$, a finite central region (*i.e.*, cavity) for $0 < x < L$, and a semi-infinite lead for $L < x < +\infty$. The wave function $\psi_\ell(x, y)$ for the ℓth mode is described as

$$\psi_\ell(x,y) = \begin{cases} e^{ik_\ell x} f_\ell^{Y_n}(y) + \sum_m R_{m\ell} e^{-ik_m x} f_m^{Y_n}(y) \quad (x<0) \\ \sum_m \{T'_{m\ell} e^{ik'_m x} + R'_{m\ell} e^{-ik'_m (x-L)}\} f_m^{Y_w}(y) \\ \quad (0<x<L) \\ \sum_m T_{m\ell} e^{ik_m (x-L)} f_m^{Y_n}(y) \quad (L<x) \end{cases}, \quad (1)$$

where

$$f_\ell^Y(y) = \sqrt{\frac{2}{Y}} \sin\left(\frac{\ell \pi y}{Y}\right) \quad (2)$$

with Y being the width of the wire. The quantities Y_n and Y_w denote the widths of the wire for the regions ($0 > x$, $L < x$) and $0 < x < L$, respectively. We use the condition $Y_n \le Y_w$ in the following calculation. The value ℓ and the wave vector k are related to the Fermi Energy E_F by the dispersion relation

$$E_F = \frac{h^2 k_\ell^2}{8\pi^2 m^*} + \frac{h^2}{8m^*}\left(\frac{\ell}{Y}\right)^2, \quad (3)$$

where m^* is the effective mass of conduction band in GaAs. Each junction is divided into N regions uniformly along the y-direction. Evanescent modes are also included in transmitted and reflected waves. The coefficients R_{ml}, R'_{ml}, T_{ml}, and T'_{ml} are calculated by the imposition of the continuity of the wave function and its derivative at $x = 0$ and $x = L$, using the technique described in Ref. [11]. We

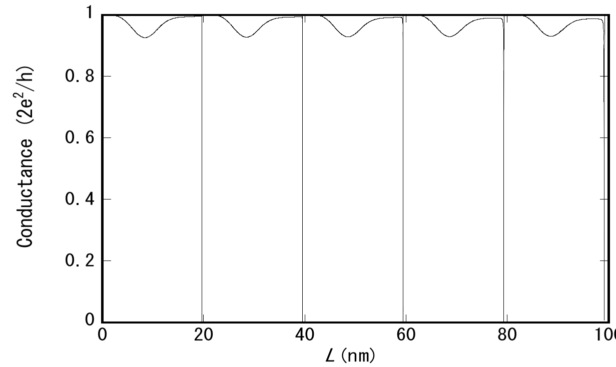

Fig. 2. Conductance plotted as a function of L.

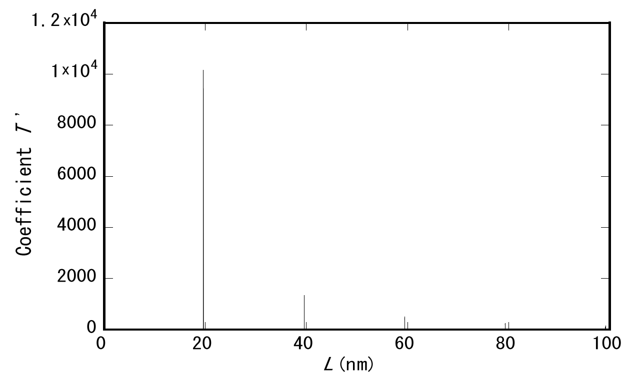

Fig. 3. Transmission coefficient T' plotted as a function of L.

can evaluate the transmission amplitudes from the normalization of the velocity to obtain the conductance G as

$$G = (2e^2/h) \sum_{m\ell} \frac{k_m}{k_\ell} |T_{m\ell}|^2. \quad (4)$$

3. Numerical results and discussion

Now, we discuss the transport phenomena through the cavity (wide region). We have calculated the conductance numerically as a function of length L of the cavity, instead of changing Fermi energy, in order to clarify the geometrical effects on the transport. The parameters used in the following calculation are chosen to be $E_F = 0.14$ eV, $N = 80$, $Y_n = 10$ nm, and $Y_w = 20$ nm. Fig. 2 shows the conductance calculated as a function of L in the case where the number of propagating mode of the incident wave is unity. In what follows, only the first mode (lowest subband in leads) for the incident wave is considered to simplify the discussion. As can be seen from Fig. 2, the conductance shows oscillating structures clearly by the interference effects. In Fig. 2, we also notice extremely narrow dips in the conductance curve. These narrow dips take place periodically with a period 19.88 nm. The conductance dips as a function of the Fermi energy were reported with different calculations [8,17]. The dips occurring with increasing size L in Fig. 2 are considered to be due to the anti-resonances by the local electronic states around the cavity. We also show the transmission coefficient T' $(= \sum_{m\ell} (k'_m/k_\ell)|T'_{m\ell}|^2)$ in Fig. 3. We can see sharp peaks at the same positions of the dips in Fig. 2. The amplitudes of peaks are very large compared with the transmission coefficient T $(= G/2e^2/h)$, the maximum of which is unity. Multiple scatterings occur at the NW and WN junctions, when the coefficient T' shows a peak value in Fig. 3, so that the value T' goes well beyond the number of propagating modes of the incident wave. Here, we show the modulus squared of the wave function in