

## Effect of a domain wall on conductance quantization in a ferromagnetic nanowire

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The effect of the domain wall (DW) on the conductance in a ballistic ferromagnetic nanowire (FMNW) is revisited by exploiting a specific perturbation theory which is effective for a thin DW; the thinness is often the case in currently interested conductance measurements on FMNW's. Including the Hund coupling between carrier spins and local spins in a DW, the conductance of a FMNW in the presence of a very thin DW is calculated within the Landauer-Büttiker formalism. It is revealed that the conductance plateaus are modified significantly, and the switching of the quantization unit from  $e^2/h$  to about  $2e^2/h$  is produced in a FMNW by the introduction of a thin DW. This accounts well for recent observations in a FMNW.

Owing to technical development in nanofabrication and spin-controlled measurement, much interest has attracted recently to the transport phenomena in ferromagnetic nanowires (FMNW's) and ferromagnetic nanocontacts (FMNC's). Whether the effect of the magnetic domain walls (DW's) on the resistivity in a ferromagnetic wire is positive or negative is a problem which has been argued for a long time from both experimental and theoretical sides,<sup>1-15</sup> and still remains a matter of controversy. This controversy stems from the fact that the effect is affected by and entangled with various factors in actual quantum ferromagnetic wires; the presence of impurities, the band structures and the size of the contacts as well as the experimental geometries and conditions. Recently, relating with device technologies, intensive research efforts have been focused on the conductance in FMNW's and FMNC's.<sup>16,17</sup> In most of these FMNW's, the length of the contacts are shorter than the electronic mean free path so that the transport can be regarded as ballistic and the DW is restricted in a very narrow region. Among such works, a recent one of the conductance measurement on a high quality Ni nanocontact, which is stretched into a nanowire,<sup>16</sup> reported that a distinct staircase behavior is observed just before the wire breaks. Further the step height of the staircase changes from  $2e^2/h$  like to  $e^2/h$  by an application of parallel magnetic fields to the wire axis beyond the saturation during this elongation process. It may be understood that this switching would occur when a DW present in the case of lower fields is eliminated by the application of the saturation field and the magnetization is ferromagnetically saturated (FMS) along the wire axis. But it is not so obvious why the quantization unit of the conductance in the presence of a DW becomes "about  $2e^2/h$ ";  $2e^2/h$  is the quantization unit in the degenerate diamagnetic nanowires.

In this paper, being inspired by the these observations, we make a theoretical study on the conductance of a FMNW with a thin DW in the ballistic regime. In the zero-field case of the measurement mentioned above, the conductance looks to follow so perfect  $2e^2/h$  step staircase at the last stage before the wire breaks that the nanowire may be supposed to be in the ballistic regime. Therefore our study in the ballistic regime may fit suitably with the experiment, and is expected to give an explanation to the origin of the observed change in

the quantization unit of the conductance, if the origin ever traces back to the presence of a DW.

The common ingredient of the ballistic electron transport in quantum wires is Landauer-Büttiker formula,<sup>18,19</sup> which gives the conductance  $G$  as

$$G = \frac{e^2}{h} \sum_n \sum_{\sigma} t_{\sigma}(E_{\parallel n}), \quad (1)$$

where  $E_{\parallel n}$  is the energy of the longitudinal motion of conduction electrons in the  $n$ th channel, and  $t_{\sigma}(E_{\parallel n})$  is the corresponding transmission probability of the incident electrons with spin  $\sigma$  ( $= \uparrow, \downarrow$ ). In early studies,<sup>6</sup> the resistance arising from the electronic scattering by a DW of ordinary thickness in a pure magnetic wire was calculated as to be exponentially small although it is positive, and the contribution was shown later in an adiabatic approximation<sup>7</sup> to decrease quadratically in the inverse DW width. In those works, however, the metallic wire is thick enough for the longitudinal energy  $E_{\parallel n}$  to be taken as  $E_F$  (Fermi energy) in most of channels, and the thickness of the DW is large enough so that electrons track adiabatically the exchange field in the DW and therefore the backward scattering by the DW is negligibly small. In nanoscale wires, on the other hand, the confinement of electrons in the transverse direction forces to open only a restricted number of channels, in most of which  $E_{\parallel n}$  could become small. If we assume a perfect confinement, for simplicity,  $E_{\parallel n}$  is given by

$$E_{\parallel n} = E_{\text{tot}} - E_n \equiv E_F - \frac{\hbar^2}{2m} \left( \frac{\pi n}{W} \right)^2, \quad (2)$$

where  $W$  is the transverse dimension of the wire,  $m$  is the mass of electrons, and the total energy  $E_{\text{tot}}$  is equated to  $E_F$ .

We can show, in the following calculation, that  $t_{\sigma}(E_{\parallel})$  is notably spin dependent as well as deviates from unity significantly when  $E_{\parallel}$  goes to the low energy comparable with the exchange energy  $V_0$  between electronic spins and local spins in a DW. Now, in a wire of nanoscale width, the number of opening channels decreases and  $E_{\parallel n}$  in most of channels goes into the low-energy region, where the effect of the electronic scattering by the DW on the conductance becomes relevant. Then the effect is expected to give a signifi-

cant modification to the conductance plateaus. This is our scenario to explain the change in the staircase behavior of the conductance appearing in the presence of a DW.

We begin with the following effective Hamiltonian for electrons of one-dimensional conduction along  $z$  axis across a  $180^\circ$  DW of width  $2\lambda$ ;

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} - V_0 \tanh\left(\frac{z}{\lambda}\right) \sigma_z - V_0 \operatorname{sech}\left(\frac{z}{\lambda}\right) \sigma_x, \quad (3)$$

where the DW is centered at  $z=0$  and  $\sigma_i$  are the Pauli matrices. The second and the third terms are the exchange potential and the spin-flip potential felt by electrons, respectively. This Hamiltonian is the same one which was introduced first by Cabrera and Falicov considering the effective coupling between the electronic spins with the local magnetization in a DW.<sup>6</sup> This is also derived in a recent work<sup>11</sup> as an effective Hamiltonian for electrons interacting with quantum spins in the DW by the Hund coupling. This Hamiltonian mixes the spin channels, so that, to calculate the transmission probabilities  $t_\sigma(E_\parallel)$  for an electron to go from  $z=-\infty$  to  $z=\infty$  with energy  $E_\parallel$  across the DW, we are forced to solve a one-dimensional two component Schrödinger equation

$$H\Psi_\sigma(z) = E_\parallel\Psi_\sigma(z), \quad (4)$$

where the index  $\sigma(=\uparrow, \downarrow)$  denotes the spin state of the incident electron and  $\Psi_\sigma(z)$  is two component column vector such as  $\Psi_\sigma(z) = [\psi_{\uparrow\sigma}(z), \psi_{\downarrow\sigma}(z)]$  for each  $\sigma = \uparrow, \downarrow$ . This coupled Schrödinger equations are difficult to be solved analytically and have been never solved successfully. Recently it is reported that the equation can be solved analytically for the case of the sinusoidal form of potentials.<sup>20</sup> However, the assumption of such a potential form produces artifacts such as oscillatory behaviors in  $t_\sigma(E_\parallel)$ . To avoid this, we like to solve Eq. (4) keeping with the potential forms in Eq. (3) but perturbationally. There are two ways in perturbational approach which are complementary to each other: One is valid for a thick DW where the unperturbed state is that of a electron tracking adiabatically the local field in the DW, so that the perturbation represents the mistracking. This is the usual way employed in literatures.<sup>8,10,13</sup> The other, on the other hand, is valid for a thin DW. There, a state of complete mistracking appears as an unperturbed state. We proceed in the latter way. This specific perturbational method is made possible by having solved exact Green's function  $G_\sigma^0(z, z'; E_\parallel)$  corresponding to the Hamiltonian  $H_0$ , which has a steplike potential  $v_0(z) \equiv -V_0\{\theta(z) - \theta(-z)\}\sigma_z$ ;

$$H_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + v_0(z)\sigma_z. \quad (5)$$

Then we have  $H = H_0 + H_1$  with  $H_1$  given by

$$H_1 = \left\{ -V_0 \tanh\left(\frac{z}{\lambda}\right) - v_0(z) \right\} \sigma_z - V_0 \operatorname{sech}\left(\frac{z}{\lambda}\right) \sigma_x \\ \equiv v_1(z)\sigma_z + v_2(z)\sigma_x. \quad (6)$$

Both of  $v_1(z)$  and  $v_2(z)$  have finite values only in a region  $|z| \lesssim \lambda$ , so that  $H_1$  can be dealt with as a perturbation.

The Schrödinger Eqs. (4) are put into the Lippmann-Schwinger form

$$\Psi_\sigma(z) = \Phi_\sigma(z) + \int_{-\infty}^{\infty} dz' G^0(z, z'; E_\parallel) H_1(z') \Psi_\sigma(z'), \quad (7)$$

where  $\Phi_\sigma(z)$  are scattering solutions of the unperturbed Schrödinger equation with the step-function potential  $[H_0\Phi_\sigma(z) = E_\parallel\Phi_\sigma(z)]$ . The unperturbed Green's function  $G^0(z, z'; E_\parallel)$  is a  $2 \times 2$  diagonal matrix whose diagonal elements are  $G_\uparrow^0(z, z'; E_\parallel)$  and  $G_\downarrow^0(z, z'; E_\parallel)$ ; their explicit forms are given in the Appendix. We solve Eq. (7) up to the second order in  $H_1$ . The perturbation expansion of Eq. (7) is written in terms of dimensionless quantities  $\tilde{z} = z/\lambda$ ,  $\tilde{H}_1$ , and  $\tilde{G}^0$  defined by  $H_1(z) = V_0\tilde{H}_1(z/\lambda)$  and  $G^0(z_2, z_1; E_\parallel) = (\gamma/2iV_0\lambda)\tilde{G}^0(z_2/\lambda, z_1/\lambda; E_\parallel)$  with  $\gamma = (2m\lambda^2V_0/\hbar^2)^{1/2}$ ;

$$\Psi_\sigma(\lambda\tilde{z}) = \Phi_\sigma(\lambda\tilde{z}) + \frac{\gamma}{2i} \int_{-\infty}^{\infty} d\tilde{z}_1 \tilde{G}^0(\tilde{z}, \tilde{z}_1; E_\parallel) \tilde{H}_1(\tilde{z}_1) \Phi_\sigma(\lambda\tilde{z}_1) \\ + \left(\frac{\gamma}{2i}\right)^2 \int_{-\infty}^{\infty} d\tilde{z}_1 \int_{-\infty}^{\infty} d\tilde{z}_2 \tilde{G}^0(\tilde{z}, \tilde{z}_1; E_\parallel) \tilde{H}_1(\tilde{z}_1) \\ \times \tilde{G}^0(\tilde{z}_1, \tilde{z}_2; E_\parallel) \tilde{H}_1(\tilde{z}_2) \Phi_\sigma(\lambda\tilde{z}_2) + \dots \quad (8)$$

Since  $\int_{-\infty}^{\infty} d\tilde{z}' \tilde{G}^0(\tilde{z}, \tilde{z}'; E_\parallel) \tilde{H}_1(\tilde{z}') \approx O(1)$  as  $\tilde{H}_1(\tilde{z}) \approx O(1)$  for  $|\tilde{z}| \lesssim 1$ , the small parameter of the expansion is  $\gamma$ . The transmission and the reflection coefficient  $S_{\sigma\sigma'}$  and  $R_{\sigma\sigma'}$  are obtained from the asymptotic forms

$$\Psi_\uparrow(z) \equiv \begin{pmatrix} \psi_{\uparrow\uparrow}(z) \\ \psi_{\downarrow\uparrow}(z) \end{pmatrix} \xrightarrow{z \rightarrow -\infty} \begin{pmatrix} e^{ik_2z} + R_{\uparrow\uparrow} e^{-ik_2z} \\ R_{\downarrow\uparrow} e^{-ik_1z} \end{pmatrix} \\ \xrightarrow{z \rightarrow +\infty} \begin{pmatrix} S_{\uparrow\uparrow} e^{ik_1z} \\ S_{\downarrow\uparrow} e^{ik_2z} \end{pmatrix}, \quad (9)$$

$$\Psi_\downarrow(z) \equiv \begin{pmatrix} \psi_{\uparrow\downarrow}(z) \\ \psi_{\downarrow\downarrow}(z) \end{pmatrix} \xrightarrow{z \rightarrow -\infty} \begin{pmatrix} R_{\uparrow\downarrow} e^{-ik_2z} \\ e^{ik_1z} + R_{\downarrow\downarrow} e^{-ik_1z} \end{pmatrix} \\ \xrightarrow{z \rightarrow +\infty} \begin{pmatrix} S_{\uparrow\downarrow} e^{ik_1z} \\ S_{\downarrow\downarrow} e^{ik_2z} \end{pmatrix}, \quad (10)$$

where  $\hbar k_1 = \sqrt{2m(E_\parallel + V_0)}$  and  $\hbar k_2 = \sqrt{2m(E_\parallel - V_0)}$ .

The transmission probabilities  $t_\sigma(E_\parallel)$  for the incident electron with spin  $\sigma(=\uparrow, \downarrow)$  to transmit to any final spin state are calculated by relations  $t_\uparrow(E_\parallel) = (k_1/k_2)|S_{\uparrow\uparrow}(E_\parallel)|^2 + |S_{\downarrow\uparrow}(E_\parallel)|^2$  and  $t_\downarrow(E_\parallel) = (k_2/k_1)|S_{\downarrow\downarrow}(E_\parallel)|^2 + |S_{\uparrow\downarrow}(E_\parallel)|^2$ . The results are shown in Fig. 1 for appropriate values of  $\lambda$ . These figures show that (i)  $t_\sigma(E_\parallel)$  deviates from unity significantly only for energies comparable with  $V_0$ , and (ii) the spin-flip transmission probability rises linearly in  $E_\parallel/V_0$  at the threshold  $E_\parallel/V_0 = -1$ , and the gradient is about  $4\pi^2\gamma^2$  for small  $\gamma$ . This means that, the thinner the DW is, the harder the spin-flip transmission occurs. The last point indicates that electron spins become hard to track local spins in a thin DW adiabatically.

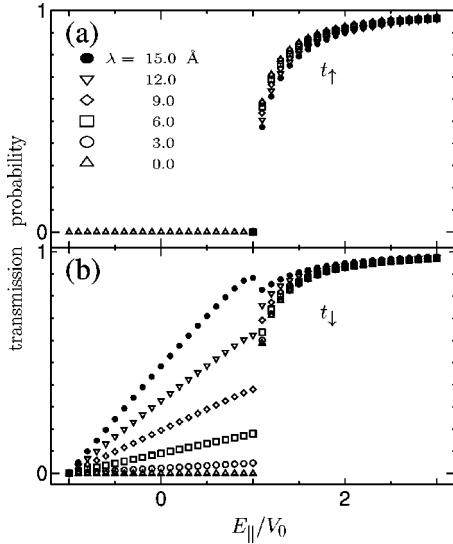


FIG. 1. The transmission probabilities (a)  $t_{\uparrow}$  and (b)  $t_{\downarrow}$  as functions of  $E_{\parallel}/V_0$  with  $V_0=0.001$  eV.

Now we can easily find how the conductance plateaus of a FMNW are modified by the presence of a thin DW. The  $W$  dependence of the conductance is derived from the formula

$$G = \frac{e^2}{h} \left[ \sum_{n=1}^{N_{\uparrow}} t_{\uparrow}(E_{\parallel n}) + \sum_{n=1}^{N_{\downarrow}} t_{\downarrow}(E_{\parallel n}) \right] \equiv G_{\uparrow} + G_{\downarrow}. \quad (11)$$

Numbers  $N_{\uparrow}$  and  $N_{\downarrow}$  are defined by  $N_{\uparrow} = [W\{2m(E_F - V_0)/\pi^2\hbar^2\}^{1/2}]$  and  $N_{\downarrow} = [W\{2m(E_F + V_0)/\pi^2\hbar^2\}^{1/2}]$ , respectively, where the square bracket denotes the Gauss symbol. The curve of  $G$  versus  $W$  in the presence of a single DW (thick solid line) is shown in Fig. 2(a) together with those of  $G_{\uparrow}$  (thin solid line) and  $G_{\downarrow}$  (thin dashed line). In Fig. 2(b), the corresponding curves for the case of FMS are drawn for comparison. In the case of FMS, the exchange energy felt by  $\uparrow$ -spin and  $\downarrow$ -spin electrons differs by  $2V_0$ . Due to this difference, the threshold value of  $W_{\sigma n}$ , at which the  $n$ th chan-

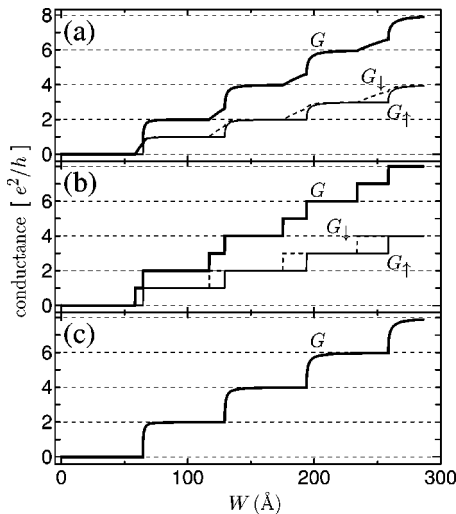


FIG. 2. The conductance as a function of  $W$  in cases; (a) involving a single domain wall, (b) of FMS, and (c) without the spin-flip scattering. There we take  $V_0=0.001$  eV,  $E_F=10V_0$ , and  $\lambda=12.0$  Å.

nel opens, becomes different between the  $\uparrow$ -spin and the  $\downarrow$ -spin channel;  $W_{\downarrow n} = n\{\pi^2\hbar^2/2m(E_F + V_0)\}^{1/2}$  and  $W_{\uparrow n} = n\{\pi^2\hbar^2/2m(E_F - V_0)\}^{1/2}$ . The opening of the channel begins with the first  $\downarrow$ -spin one and is followed by the first  $\uparrow$ -spin one, and so on. This leads to the  $e^2/h$  conductance staircase with clear plateaus in Fig. 2(b). This  $e^2/h$  staircase behavior of the conductance in the case of FMS are observed in conductance measurements on Ni nanowires.<sup>16,17</sup> Now we discuss the result in the presence of a DW shown in Fig. 2(a). There, the conductance curve looks like a staircase with step height of about  $2e^2/h$ . While the step height is well quantized at least up to the third step, steps are gradually inclined as the steps increases although a remnant of  $2e^2/h$  like quantization is still seen. Our curve in Fig. 2(a) resembles one observed recently<sup>16</sup> in this characteristic appearance. Therefore we can say that the switching of the quantization unit from  $e^2/h$  to about  $2e^2/h$  can be produced by the introduction of a thin DW into a FMNW.

Although it is the case, we should make a remark about the origin of the conductance quantization in the unit of about  $2e^2/h$ . It is sometimes said that the presence of a DW makes both spin channels stand on the equal footing, and as a result the spin degeneracy is recovered as it stands in the diamagnetic nanowire. Precisely speaking, it is not exactly the case. By looking at curves  $G_{\uparrow}$  and  $G_{\downarrow}$  in Fig. 2(a), we see that they are quite different from each other. By comparing  $G_{\uparrow}$  and  $G_{\downarrow}$  in Fig. 2(a) with the correspondings in Fig. 2(b), we notice the following: (i)  $G_{\uparrow}$  jumps by an amount  $e^2/h$  at the same value of  $W_{\uparrow n}$  as  $G_{\uparrow}$  does in the FMS case, although the corners of the staircase are rounded by the scattering effect by the DW. (ii) The  $n$ th channel of  $G_{\downarrow}$  opens also at the same value of  $W_{\downarrow n}$  as in the FMS case. There, however,  $G_{\downarrow}$  does not jump up as in the FMS case, since only the slowly increasing spin-flip transmission contributes first to  $G_{\downarrow}$  [see Fig. 1(b)]. When  $W$  reaches the threshold value of the spin-conserving transmission in the same channel,  $G_{\downarrow}$  starts to increase steeply by this contribution. This threshold coincides with  $W_{\uparrow n}$  of  $G_{\uparrow}$ , so that the total conductance  $G$  looks to jump up by about  $2e^2/h$  at  $W_{\uparrow n}$ . Speaking in another way, since the Hamiltonian (3) without the third spin-flip term is invariant under the reflection  $z \rightarrow -z$  and the  $\pi$  rotation about the  $x$  axis in the spin space, we can easily find that the spin-conserving transmission probability for  $\uparrow$  spins and  $\downarrow$  spins become exactly the same. Further, both of  $W_{\sigma n}$  becomes equal to  $n\{\pi^2\hbar^2/2m(E_F - V_0)\}^{1/2}$ , so that the total conductance realizes a staircase of exact  $2e^2/h$  steps. In fact, our perturbational calculation for this case [Fig. 2(c)] shows an exactly quantized behavior with fine plateaus. In such case, therefore, we can say that the perfect quantization in the unit of  $2e^2/h$  precisely comes from the spin degeneracy. From these considerations, we understand that the about  $2e^2/h$  staircase behavior in the presence of a thin DW does not indicate precisely the recovery of the spin degeneracy. We can even claim that the deviation of the curve in Fig. 2(a) from the perfect  $2e^2/h$  staircase shows clearly a distinct effect of the spin-flip forward scattering by a DW.

In summary, we studied theoretically the effect of a thin DW on the conductance quantization in a FMNW in the ballistic regime. The calculations are made by exploiting a

specific perturbational technique which is valid for thin DW case. We point out that notable effects due to the DW scattering can be observed owing to the nanoscale width of the wire. We also find that the conductance quantization in the unit of about  $2e^2/h$  is realized by the introduction of a thin  $180^\circ$  DW while the quantization unit is  $e^2/h$  in the saturated ferromagnetic nanowire as ordinarily expected. This explains well the switching in the quantization unit from about  $2e^2/h$  to  $e^2/h$  observed recently in measurements on Ni nanowires.<sup>16</sup> It is emphasized that, in the deviation of the  $2e^2/h$ -like conductance staircase from the perfect  $2e^2/h$  one

in lack of the spin-flip scattering, we can find an interesting effect of the spin-flip scattering by the DW, from which we can deduce useful informations for the ferromagnetic material. In this sense, the conductance measurement in a FMNW may provide a powerful probe for the magnetotransport in ferromagnetic materials.

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#### APPENDIX A:

The unperturbed Green's function  $G_\alpha^0(z_2, z_1; E_\parallel)$  can be obtained by using some mathematics as

$$G_\uparrow^0(z_2, z_1; E_\parallel) = \frac{m}{i\hbar^2} \times \begin{cases} \frac{1}{k_2} e^{ik_2 z_2} (e^{-ik_2 z_1} - R e^{ik_2 z_1}); & z_2 > z_1 > 0 \\ \frac{1}{k_2} (e^{-ik_2 z_2} - R e^{ik_2 z_2}) e^{ik_2 z_1}; & z_1 > z_2 > 0 \\ \frac{2}{k_1 + k_2} e^{ik_2 z_2} e^{-ik_1 z_1}; & z_2 > 0 > z_1 \\ \frac{2}{k_1 + k_2} e^{-ik_1 z_2} e^{ik_2 z_1}; & z_1 > 0 > z_2 \\ \frac{1}{k_1} (e^{ik_1 z_2} + R e^{-ik_1 z_2}) e^{-ik_1 z_1}; & 0 > z_2 > z_1 \\ \frac{1}{k_1} e^{-ik_1 z_2} (e^{ik_1 z_1} + R e^{-ik_1 z_1}); & 0 > z_1 > z_2, \end{cases} \quad (\text{A1})$$

$$G_\uparrow^0(z_2, z_1; E_\parallel) = G_\uparrow^0(-z_1, -z_2; E_\parallel), \quad (\text{A2})$$

where  $R = (k_1 - k_2)/(k_1 + k_2)$ .

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