Magnetoresistance effect in spin-polarized junctions of ferromagnetically contacting multiple conductive paths: Applications to atomic wires and carbon nanotubes

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For spin-polarized junctions of ferromagnetically contacting multiple conductive paths, such as ferromagnet (FM)/atomic wires/FM and FM/carbon nanotubes/FM junctions, we theoretically investigate spin-dependent transport to elucidate the intrinsic relation between the number of paths and conduction, and to enhance the magnetoresistance (MR) ratio. When many paths are randomly located between the two FM's, electronic wave interference between the FM's appears, and then the MR ratio increases with increasing number of paths. Furthermore, at each number of paths, the MR ratio for carbon nanotubes becomes larger than that for atomic wires, reflecting the characteristic shape of points in contact with the FM.

Recently, the magnetoresistance (MR) effect in spin-polarized junctions of a ferromagnetically contacting single conductive path, which is ferromagnet (FM)/path/FM junctions such as Co/carbon nanotube/Co junctions,[1−4] has been reported. When the MR ratio was defined as $(\Gamma^{(P)} - \Gamma^{(AP)})/\Gamma^{(P)}$, with $\Gamma^{(P)}$ and $\Gamma^{(AP)}$ being the conductances of parallel (P) and antiparallel (AP) magnetization configurations of the FM's, its magnitude for Co/carbon nanotube/Co was experimentally observed to be 9%,[1] 23%,[2] and 26% (Ref. 3) at 4.2 K. In the theoretical study based on Green's-function method, the maximum value of the MR ratio was evaluated to be 20%.[4] From the viewpoint of spintronics, however, larger MR ratios than those values are strongly desired, because conventional systems with film spacer, FM/Al-O/FM junctions,[5,6] have much larger MR ratios in spite of using a FM with almost the same spin-polarization rate.[7]

The difference in the MR ratio between the film and the single path systems originates from that in the number of conductive paths connecting the two FM's or that of conductive mechanisms. The former has many conductive paths and tends to exhibit coherent conduction (CC),[8,9] in which the intralayer momentum of the FM's is conserved in the transmission between them, while the latter exhibits incoherent conduction (IC),[10] where the momentum is not conserved.

Our interests are in how the number of paths influences the coherence of conduction and how the coherence contributes to the enhancement of the MR ratio. Microscopic theoretical studies on such questions have not been reported so far. By introducing many paths in the path systems, we may find an intrinsic relation between the paths and the coherence of conduction. Furthermore, if the MR ratio in the path systems is successfully enhanced by many paths, our study will significantly contribute to the development of future nanowire or nanotube MR devices.

In this work, we investigate spin-dependent transport properties of FM/many paths/FM junctions, where many conductive paths are randomly located between the two FM's. Using Green's-function technique,[11] we obtain an expression of conductance having not only the IC term but also the CC term, which appears as a result of electronic wave interference between the two FM's. In applications to atomic wire and carbon nanotube systems, we find that the MR ratios increase with increasing number of paths because of an increase of CC. We will demonstrate that such electronic wave interference brings about the enhancement of MR ratios in path systems.

First, let us derive an expression of the conductance of FM/many paths/FM junctions shown in the left panel of Fig. 1. Here, the FM is an electrode, the path can be, for example, an atomic wire or a nanotube, and many paths are randomly located under the assumption that contact points between their edges and the FM exist parallel to the x axis and at $y = 0$, and current flows in the z direction. Keeping the qualitative discussion in mind, we assume that all parts consist of atoms with a single orbital, and the FM has a simple cubic structure with 100 monolayers. Furthermore, the intralayer direction (xy plane) of the FM is regarded as an infinite system and is set to have the periodic boundary condition. The system is described using a tight-binding model with the nearest-neighbor transfer integral.

Within Green's-function technique,[11] the conductance for spin σ at zero temperature is written as

$$\Gamma_\sigma = \frac{2\pi e^2}{\hbar} \text{Tr}[D_{L,\sigma} T_\sigma^\dagger D_{R,\sigma} T_\sigma], \tag{1}$$
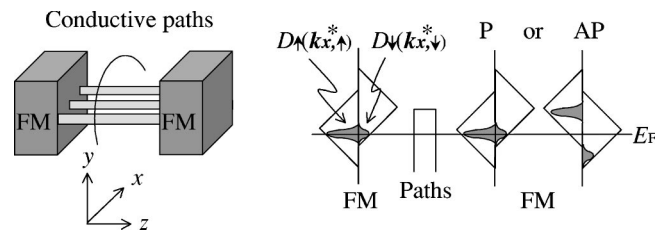

FIG. 1. Left panel: A schematic illustration of FM/many paths/FM junctions. Right panel: A schematic illustration of the local DOS at the interfacial layer of the left and right FM's for the P or AP magnetization configuration. In discussing IC, we focus on the structure of the DOS at E_F. In contrast, for CC, we pay attention to the DOS indexed by $k_{x,\uparrow(\downarrow)}^*$, $D_{\uparrow(\downarrow)}(k_{x,\uparrow(\downarrow)}^*)$, where $k_{x,\uparrow(\downarrow)}^*$ is the FM wave vector in the x direction for up- (down-) spin giving energy levels in the vicinity of E_F for the P configuration, and its dominant component is shown by the shaded region.

with $T_\sigma = V_\sigma + V_\sigma G_\sigma^\dagger V_\sigma$, $G_\sigma = (E_F - H_\sigma + i0^+)^{-1}$, $D_{j,\sigma} = -(1/\pi)\text{Im}(E_F - H_{j,\sigma} + i0^+)^{-1}$, and $H_\sigma = \Sigma_\ell H_{\ell,\sigma} + V_\sigma$, where H_σ is the Hamiltonian for the whole systems, $H_{\ell,\sigma}$ is the Hamiltonian for an ℓ part with ℓ being a suffix for the left FM, paths, or the right FM, V_σ is coupling between the FM and the paths, $D_{j,\sigma}$ ($j = L$ or R) is the density of states (DOS) operator, and E_F is the Fermi level at which conduction electrons exist. The unit of $2\pi e^2/\hbar = 1$ is adopted below.

When the atomic orbital at the contact points between the FM and the paths is represented as $|x,y,z\rangle$ indexed by x,y,z coordinates, the conductance is rewritten as

$$\Gamma_\sigma = \sum_{x,x',x'',x'''} \langle x,0,L|D_{L,\sigma}|x',0,L\rangle\langle x',0,L|T_\sigma^\dagger|x'',0,R\rangle$$

$$\times \langle x'',0,R|D_{R,\sigma}|x''',0,R\rangle\langle x''',0,R|T_\sigma|x,0,L\rangle, \quad (2)$$

where $L(R)$ is the z coordinate at the interfacial layer in the left (right) FM. Transference of state represents the circular propagation, left FM $\rightarrow$ right FM $\rightarrow$ left FM, and T_σ connects the two FM's. Here we use an approximation in which T_σ is finite only for the same x coordinate between the left and right FM's, and it is independent of x. The validity of the approximation will be described in applications. Using the Bloch wave at the interfacial layer in the FM, $|\mathbf{k},L(R)\rangle$, where $\mathbf{k}[=(k_x,k_y)]$ is the intralayer wave vector of the FM, we obtain

$$\Gamma_\sigma = \frac{1}{(N_x N_y)^2}|T_\sigma|^2 \sum_{x,x'} \sum_{\mathbf{k},\mathbf{k}'} e^{-i(k_x-k_x')(x-x')} D_{L,\sigma}(\mathbf{k})$$

$$\times D_{R,\sigma}(\mathbf{k}'), \quad (3)$$

with $D_{L(R),\sigma}(\mathbf{k}) = \langle \mathbf{k},L(R)|D_{L(R),\sigma}|\mathbf{k},L(R)\rangle$, where $|T_\sigma|^2$ denotes the transmission coefficient including information on the paths, $N_{x(y)}$ is the number of atoms on the $x(y)$ axis at the interfacial layer in the FM, and $(k_x - k_x')(x - x')$ corresponds to difference in the phase of the Bloch wave between the left and right FM's.

Now, based on randomly located paths, we average Γ_σ over the distribution of the paths, that is, $\langle\Gamma_\sigma\rangle_{\text{path}}$. We utilize $\langle\Sigma_{x,x'}e^{-i(k_x-k_x')(x-x')}\rangle_{\text{path}} = \langle\Sigma_{x,x'}\delta_{x,x'} + \Sigma_{x\neq x'}e^{-i(k_x-k_x')(x-x')}\rangle_{\text{path}} = N_{\text{path}} + N_{\text{path}}(N_{\text{path}}-1)\delta_{k_x,k_x'}$,[12] where N_{path} is the number of paths. The first term means that the difference in the phase disappears when the electron uses the same path in the circular propagation. The second term represents the propagation with different paths. Correlation of the Bloch wave between the left and right FM's becomes large for $k_x = k_x'$, while it is negligibly small for $k_x \neq k_x'$. It is interpreted just as the result of the interference between the electronic wave in the left FM and that in the right FM. The conductance per N_x becomes

$$\frac{\Gamma_\sigma}{N_x} = \frac{N_{\text{path}}}{N_x}|T_\sigma|^2 D_{L,\sigma}D_{R,\sigma}$$

$$+ \frac{N_{\text{path}}^2 - N_{\text{path}}}{N_x^2}|T_\sigma|^2 \frac{1}{N_x}\sum_{k_x} D_{L,\sigma}(k_x)D_{R,\sigma}(k_x), \quad (4)$$

with $D_{L(R),\sigma} = (1/N_x N_y)\Sigma_\mathbf{k}D_{L(R),\sigma}(\mathbf{k})$ and $D_{L(R),\sigma}(k_x) = (1/N_y)\Sigma_{k_y}D_{L(R),\sigma}(\mathbf{k})$. The first and second terms represent IC with nonconservation of $\mathbf{k}$ and CC with conservation of k_x, respectively. For $N_{\text{path}} = 1$, only the IC term remains, and it results in an expression obtained straightforwardly for the single path systems.[11] With increasing N_{path}, the CC term increases rapidly, meaning that the interference effect is enhanced by an increase of the propagation between the two FM's. Also, using this expression, we calculate the MR ratio, which is defined as $(\Gamma_\uparrow^{(P)} + \Gamma_\downarrow^{(P)} - \Gamma_\uparrow^{(AP)} - \Gamma_\downarrow^{(AP)})/(\Gamma_\uparrow^{(P)} + \Gamma_\downarrow^{(P)})$.

We simply explain the MR ratios for the IC and CC terms by paying attention to only the DOS's (see right panel of Fig. 1). In the case of IC, based on the conductance with the product of DOS's, the MR ratio can be estimated using the Julliere model.[13] The MR ratio for the Co electrode becomes merely about 21%.[1] On the other hand, in the case of CC, the conductance is related to k_x-dependent DOS, as shown by the shaded region in Fig. 1. When DOS with $k_{x,\uparrow}^*$ and $k_{x,\downarrow}^*$ at the left FM is in the vicinity of E_F, the DOS at the right FM is in the vicinity of E_F in the P case and absent in the AP case. Then, the conductance with $k_{x,\uparrow}^*$ and $k_{x,\downarrow}^*$ is finite in the P case, while it is almost zero in the AP case. This obvious difference in the conductance between the P and AP cases leads to a large MR ratio.

As an application to realistic systems, we first consider FM/atomic wires/FM junctions, where the atomic wire consists of n atoms and the z coordinate of the left (right) edge of the atomic wire is indexed by 1 (n). We here obtain an exact expression of T_σ, which finally becomes $\langle x,0,L|T_\sigma|x',0,R\rangle = \langle x,0,L|V_\sigma G_\sigma V_\sigma|x',0,R\rangle = v^2\langle x,0,1|G_\sigma|x',0,n\rangle$ with v being a transfer integral between the FM and the atomic wire, by solving the Dyson equation $G_\sigma = g_\sigma + g_\sigma V_\sigma G_\sigma$, with $G_\sigma = (E_F - H_\sigma + i0^+)^{-1}$ and $g_\sigma = (E_F - \Sigma_\ell H_{\ell,\sigma} + i0^+)^{-1}$, i.e.,

$$\tilde{T}_\sigma = v^2 g_{1n,\sigma}(\tilde{I} + \tilde{\Pi}_\sigma)^{-1}, \quad (5)$$

$$\tilde{\Pi}_\sigma = -v^2(g_{11,\sigma}\tilde{g}_{L,\sigma} + g_{nn,\sigma}\tilde{g}_{R,\sigma}) + v^4(g_{11,\sigma}g_{nn,\sigma}\tilde{g}_{R,\sigma}\tilde{g}_{L,\sigma}$$

$$- g_{1n,\sigma}g_{n1,\sigma}\tilde{g}_{R,\sigma}\tilde{g}_{L,\sigma}), \quad (6)$$

with $g_{ij,\sigma} = \langle x,0,i|g_\sigma|x,0,j\rangle$ for $i,j = 1$ or n, $\tilde{g}_{L(R),\sigma} = \Sigma_{x,x'}|x\rangle(1/N_x N_y)\Sigma_\mathbf{k}e^{-ik_x(x-x')}g_{L(R),\sigma}(\mathbf{k})\langle x'|$, $g_{L(R),\sigma}(\mathbf{k}) = \langle \mathbf{k},L(R)|g_\sigma|\mathbf{k},L(R)\rangle$, and $\tilde{I} = \Sigma_x|x\rangle\langle x|$, where $|x\rangle$ is introduced for a matrix representation about the x coordinate. Here, $\tilde{T}_\sigma$ is a matrix including $\tilde{\Pi}_\sigma$ which has off-diagonal elements between different paths, reflecting the propagation throughout all paths. For $\tilde{g}_{L(R),\sigma}$, we now take into account only the diagonal elements, because those elements are much
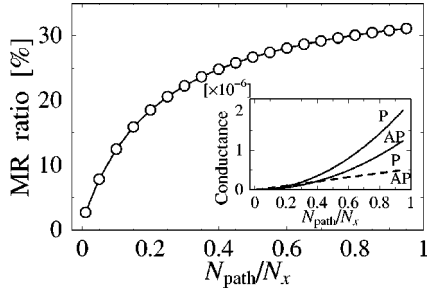
FIG. 2. MR ratio vs N_{path}/N_x for FM/atomic wires/FM junctions. $N_{path}=1$ corresponds to $N_{path}/N_x=0.01$. Inset: The CC and IC terms in $\Sigma_\sigma \Gamma_\sigma /N_x$ vs N_{path}/N_x. The solid (dotted) line represents the CC (IC) term.

larger than the off-diagonal ones owing to the disappearance of the phase factor $k_x(x-x')$. Therefore, $\widetilde{T}_\sigma$ results in a diagonal matrix having an expression for the single path systems as the matrix element, which is independent of x. It should also be mentioned that v is assumed to be smaller than the transfer integrals in the FM and the atomic wire parts for reasons such as differences of types between two orbitals and imperfect lattices matching at the interface. Therefore, the contribution of $\widetilde{\Pi}_\sigma$ is small.

We use the following parameters. The number of atoms in the single wire is 20, the transfer integrals in the FM and the wire parts are t ($t<0$), and the transfer integral between the FM and the wire is $v=0.1t$. When $E_F=0$, the on-site energy of up- (down-) spin for the FM is $3.8|t|$ ($4.2|t|$),[14] and that of the wire is 0, which corresponds to the conductive wire.

Figure 2 shows the MR ratio vs N_{path}/N_x. The MR ratios for $N_{path}>1$ are larger than that for $N_{path}=1$, and it gradually increases with increasing N_{path}. This behavior originates from the contribution of the CC term. As the inset shows, the CC term causes a large difference between the P and AP cases, while the IC term exhibits little difference between them. Furthermore, such a CC term and its difference between the P and AP cases increase with increasing N_{path}.

As the second application, we consider single-walled $(N_{cir},0)$ zigzag carbon nanotubes,[15] where N_{cir} is the number of unit cells in the zigzag edge. Each edge carbon atom of the nanotube is assumed to interact with its nearest atom in the cubic lattice of the FM. The interaction is denoted as the transfer integral v. In a similar way to that in the case of the atomic wire, we obtain the conductance for the nanotube systems. As a characteristic result, conductive processes in the circumferential direction of the nanotube are newly added, reflecting the shape of contact points between the FM and the nanotube edges.

In the parameter set, the nanotube length is of ten zigzag lines, the transfer integrals in the FM and the nanotube parts are t,[16] those between the edge carbon atoms and their nearest FM atoms are $v=0.1t$, the on-site energy of carbon is 0, and the on-site energy of the FM and E_F are the respective ones used in the case of the atomic wire. This carbon nanotube appears to behave nearly as a semiconductor, in which transmission between the two edges of the nanotube is mainly through a small energy gap in the vicinity of E_F. Originally, however, the nanotube is metallic, because it is
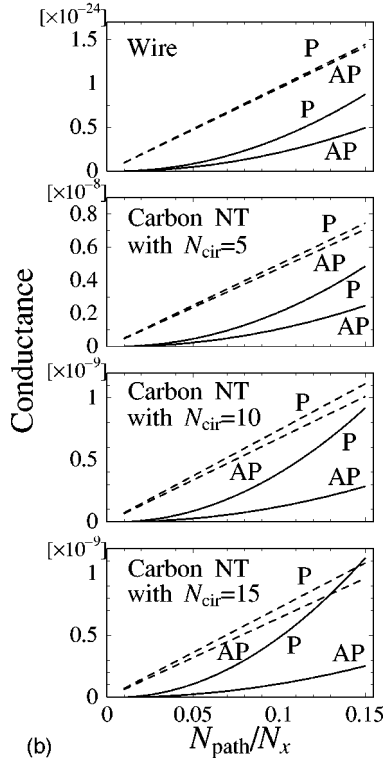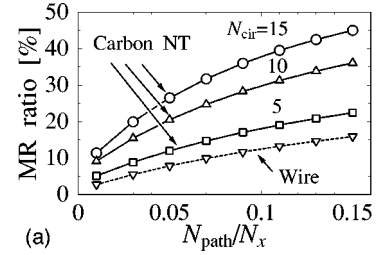

FIG. 3. (a): MR ratio vs N_{path}/N_x for FM/carbon nanotubes (NT)/FM junctions (solid lines) and FM/atomic wires/FM junctions (dotted line). $N_{path}=1$ corresponds to $N_{path}/N_x=0.01$. Furthermore, the range of N_{path}/N_x is determined so as to be less than the system size with $N_{cir}=15(r=3)$. (b): The CC and IC terms in $\Sigma_\sigma \Gamma_\sigma /N_x$ vs N_{path}/N_x for the respective cases. The solid (dotted) line represents the CC (IC) term.

regarded merely as a zigzag ribbon[17] with short periodicity. Since wave functions on E_F localize at the left or right edges of the nanotube,[17] they contribute little to the conduction between the two edges.

In Fig. 3(a), we show the MR ratio vs N_{path}/N_x for the cases of $N_{cir}=5$ $(r=1)$, 10 $(r=2)$, and 15 $(r=3)$. The MR ratios qualitatively exhibit the same dependence on N_{path}/N_x as that in the case of atomic wires. We emphasize that the MR ratio is larger than that for atomic wires, and furthermore, the MR ratio at each N_{path} becomes large as N_{cir} increases. For $N_{path}>1$, the above properties mainly are a result of the contribution of the CC term of the P case, where the magnitude of the CC term based on the IC term becomes obviously large with increasing N_{cir} [see Fig. 3(b)]. In particular, we compare the nanotube case with the wire case. At the points of contact with the FM, the nanotubes have a distribution of atoms also in the y direction, which is not

present in the wires. Then, a new conductive process with consistency of k_y between the left and right FM's becomes predominant, indicating that CC is favored in the y direction as well as in the x direction. In a classical picture, when an electron with a certain momentum goes into the nanotubes, the momentum in the y direction also tends to be conserved, because conduction along the circumference is possible. Of course, such a conduction in the circumferential direction enhances the MR ratio in the $N_{cir}=1$ case, too.

Finally, we give several comments. First, in this study, the spin polarization of the FM electrode comes from only the single orbitals of the FM atoms, although the spin-polarization rate[13] is actually influenced so strongly by interfacial states that even its sign can be altered.[3] We note, however, that if the interface of the FM is uniform, an increase of the magnitude of the MR ratio due to the interference effect can occur. Second, the present phenomena are found for numerous similar systems. For example, MR properties calculated for FM/BN nanotubes/FM junctions with insulating nanotubes are almost the same as those for the junctions with carbon nanotubes.[18] We speculate that when many conductive paths are randomly located in the xy plane,[19] larger MR ratios than the present ones can be expected, because the CC will appear as predominant features in the y direction as well as in the x direction. Third, we mention the Luttinger liquid (LL) behaviors,[20] which are characteristic of one-dimensional conductive systems with electron-electron inter-actions. Actually, the LL behaviors may exert little influence on the MR ratio and its N_{path} dependence, because the present MR effect is mainly realized by the difference in the spin-dependent potential between the two FM's, and also, it does not change without the introduction of spin-polarized paths. The LL behaviors may, rather, be observed in the temperature dependence on the conductance for each magnetization configuration, for example.

In conclusion, the spin-dependent transport in the spin-polarized junctions of ferromagnetically contacting multiple conductive paths was theoretically investigated to elucidate the intrinsic relation between the number of paths and the conduction, and to enhance the MR ratio. When many paths are randomly located between the two FM's, CC appears as a result of electronic wave interference between the two FM's. With increasing N_{path}, CC becomes more marked and the MR ratio increases. Furthermore, the carbon nanotube junctions show larger MR ratio compared with the atomic wire junctions, because the intralayer momentum tends to be well conserved owing to conduction along the circumference of the nanotubes. We expect that the characteristic phenomena will be observed with progress of experimental techniques and will be utilized in nanowire or nanotube MR devices in the future.

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