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Analytical expression for the spin-transfer torque in a magnetic junction with a ferromagnetic insulator

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Analytical expressions for the spin-transfer torque (STT) in magnetic junctions with a ferromagnetic insulator (FI) are derived using the Keldysh formalism. Adopting simple approximations and ballistic transport, both parallel and perpendicular torques are expressed in terms of spin-dependent intersite Green's functions of the insulator. They depend linearly on the bias voltage because of the asymmetry of junctions. The relationship between STT and tunnel magnetoresistance, the difference between the features of the STT obtained in the present and previous works, and effects of the electronic structures of FI and those of impurities on the STT are discussed.

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Magnetic multilayers and magnetic tunnel junctions are widely used in various fundamental physics and technological applications in the field of spintronics. Giant magnetoresistance (GMR) in magnetic multilayers and tunnel magnetoresistance (TMR) in magnetic tunnel junctions are phenomena that are used to control charge current by means of a magnetic field. An inverse effect, the control of magnetism by charge current, that is, current-induced magnetization switching (CIMS), was also predicted contemporaneously with the discovery of GMR and TMR,[1,2] and confirmed experimentally.[3] It is well understood that CIMS is realized by spin-transfer torque (STT) exerted by spin-polarized currents.[4–7] After a breakthrough in TMR using an epitaxial MgO barrier in magnetic tunnel junctions,[8] CIMS in magnetic tunnel junctions has been extensively studied in both experiment[9–12] and theory.[13–19] CIMS has also been applied to magnetoresistive random access memories and spin-torque oscillators.[20,21]

STT exerted on a magnetization $\boldsymbol{M}$ in tunnel junctions is a vector having two components, one parallel ($N_\parallel$) and one perpendicular ($N_\perp$) to the plane of $\boldsymbol{M}$. $N_\parallel$ and $N_\perp$ are called spin-transfer and fieldlike terms, respectively, and are generally nonzero. The magnitude of each component is important for the magnetization dynamics controlled by currents.[6] The dependence of $N_\parallel$ and $N_\perp$ on the bias voltage V has been predicted to be proportional to V and V^2, respectively, for symmetric junctions.[14,17,18] It was also predicted that $N_\parallel$ changes sign with $|V|$, and that $N_\perp$ shows oscillatory dependence on V.[17,19]

Meanwhile, the magnetic tunnel junctions mentioned above comprise transition-metal ferromagnets (FMs) separated by a MgO insulator (I). Recently, half-metallic Heusler alloys and spinel ferrites have attracted interest as spintronic materials. Especially some ferrites such as $CoFe_2O_4$ and $NiFe_2O_4$ are ferromagnetic (or ferrimagnetic) insulators (FI) and are expected to play the role of a spin filter.[22–24] Figure 1(a) shows a schematic of the density of states (DOS) of an FI, in which two types of magnetic atoms A and B are included. The DOS has spin-dependent energy gaps between the occupied and unoccupied states.[25] Because they possess both ferromagnetism with a high Curie temperature and an electrically insulating character, it would be interesting to fabricate tunnel junctions with FIs and to study the STT exerted on $\boldsymbol{M}$ of the FI. Furthermore, in view of recent interest in FIs such as YIG (yttrium iron garnet),[26,27] STT and spin current through FIs would be important subjects.

Hence, the purpose of this Rapid Communication is to derive an analytic expression for the STT, including both $N_\parallel$ and $N_\perp$, for junctions with a FI by using a nonequilibrium Keldysh formalism in the ballistic transport regime. Instead of FM/I/FM-type tunnel junctions, we use FM/NM(or I)/FI/NM-type junctions, shown in Fig. 1(b), in which a thick FM and a thin FI are separated by a thin nonmagnetic metal (NM) or by a thin insulator to decouple any exchange interaction between the FM and FI. We will show that both $N_\parallel$ and $N_\perp$ are proportional to V because of the asymmetry of the junction, and they are expressed in terms of spin-dependent nonlocal Green's functions of the FI. We will discuss the difference between features of the STT obtained in the present Rapid Communication and those in FM/I/FM junctions studied so far.

We formulate the charge and spin currents flowing through the FI layer using the Keldysh formalism.[28] The formalism in general may be applied to a full-orbital tight-binding (TB) model, however, analytical expressions are obtained in a single-orbital TB model. Inelastic scattering by spin waves, etc., and the effects due to magnetic anisotropy are not considered.[6]

A spin-polarized current induced by the magnetization $\boldsymbol{M}_p$ of the FM exerts a STT on the magnetization $\boldsymbol{M}$ of the FI. The direction of $\boldsymbol{M}_p$ is fixed and that of $\boldsymbol{M}$ may be be canted by an angle (θ,φ), as depicted in Fig. 1(c). In the formalism, we divide the junction into three parts by inserting two cleaved layers, an electrode of the left (L) side including a FM and thin NM or I, a FI layer, and an electrode of the right (R) side made of a NM. The cleaved layers are inserted between sites m and n and between sites p and q, as shown in Fig. 1(d). Because of the conservation law of charge current, the charge current through the m-n interface $\langle J_m^C\rangle$ is the same with that through the p-q interface. On the other hand, the spin current through the m-n interface $\langle \boldsymbol{J}_m^S\rangle$ is different from that through the p-q interface $\langle \boldsymbol{J}_p^S\rangle$, and the difference between these currents gives the STT exerted on the FI.

The general expressions of the charge and spin currents through m-n interface are

$$\langle J_m^C\rangle = \frac{e}{\hbar}\mathrm{Tr}\int \frac{1}{2\pi}d\omega(\boldsymbol{G}_{mn}^{+}\boldsymbol{t}_{nm} - \boldsymbol{t}_{mn}\boldsymbol{G}_{nm}^{+})\mathbf{1} \tag{1}$$

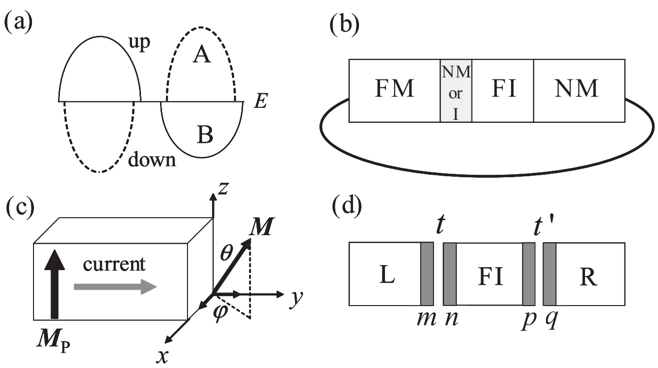

FIG. 1. (a) Schematic of the DOS of an ferromagnetic insulator (FI) composed of two types of magnetic atoms A and B, (b) a typical structure of the unctions, (c) magnetization alignment of the junctions, and (d) site indices of the junctions with hopping integrals t and t' at the m-n and p-q interfaces, respectively.

and

$$\langle \boldsymbol{J}_m^S \rangle = \frac{1}{2}\mathrm{Tr}\int \frac{1}{2\pi} d\omega (\boldsymbol{G}_{mn}^{+} \boldsymbol{t}_{nm} - \boldsymbol{t}_{mn} \boldsymbol{G}_{nm}^{+}) \boldsymbol{\sigma}, \tag{2}$$

respectively. Here, $\boldsymbol{G}^+$ is the nonequilibrium (Keldysh) Green's function for the whole junction, and is defined as $G_{ij}^+(t,t') = i\langle c_j^+(t')c_i(t)\rangle/\hbar$, where $c_i^+(t)$ $[c_i(t)]$ represents the creation (annihilation) operator of an electron at site i, t represents the time in the Heisenberg representation, and $\boldsymbol{\sigma}$ represents the Pauli matrix. A trace is taken over the spin, orbitals, and momentum $k_\parallel$ parallel to the layer planes. We omit $k_\parallel$ in the equations for simplicity because we are dealing with the ballistic transport.

In order to obtain the spin current responsible for STT, the equilibrium spin current $\langle \boldsymbol{J}_m^S \rangle_{\mathrm{eq}}$ (exchange coupling between ferromagnetic layers) should be subtracted as

$$\langle \boldsymbol{J}_m^S \rangle_{n-\mathrm{eq}} = \langle \boldsymbol{J}_m^S \rangle - \langle \boldsymbol{J}_m^S \rangle_{\mathrm{eq}}, \tag{3}$$

and the STT is given by the change in the nonequilibrium spin current between the m-n and p-q layers

$$\boldsymbol{N} = \langle \boldsymbol{J}_p^S \rangle_{n-\mathrm{eq}} - \langle \boldsymbol{J}_m^S \rangle_{n-\mathrm{eq}}, \tag{4}$$

where the spin current through the p-q interface is given by $m \to p$ and $n \to q$ in Eq. (2). In FM/I/FM junctions, only interface scattering at I/FM is crucial since the thickness of the left FM is assumed to be infinity.[7] The equilibrium spin current is calculated by using the relation $\boldsymbol{G}^+ = (\boldsymbol{G}^A - \boldsymbol{G}^R) f_{\mathrm{eq}}$,[29] where f_{eq} is the Fermi distribution function in the equilibrium state, and A and R indicate that the Green's functions are advanced and retarded ones, respectively. Hereafter, we omit the vector representation of Green's functions for simplicity.

The flow of the calculation is as follows.[28] First, the Green's function G_{mn}^+ is expressed in terms of G in the insulator as

$$G_{mn}^+ = g_{mm}^+ t_{mn} G_{nn}^A + g_{mm}^R t_{mn} G_{nn}^+, \tag{5}$$
$$G_{nm}^+ = G_{nn}^+ t_{nm} g_{mm}^A + G_{nn}^R t_{nm} g_{mm}^+, \tag{6}$$

where g is the Green's function in the equilibrium state. Substituting them into Eqs. (1) and (2), we obtain

$$\langle J_m^C \rangle = \frac{e}{h}\mathrm{Tr}\int d\omega \big[g_{mm}^+ t_{mn} G_{nn}^A t_{nm} + g_{mm}^R t_{mn} G_{nn}^+ t_{nm} - t_{mn} G_{nn}^+ t_{nm} g_{mm}^A - t_{mn} G_{nn}^R t_{nm} g_{mm}^+ \big] \mathbf{1}, \tag{7}$$

$$\langle \boldsymbol{J}_m^S \rangle = \frac{1}{4\pi}\mathrm{Tr}\int d\omega \big[g_{mm}^+ t_{mn} G_{nn}^A t_{nm} + g_{mm}^R t_{mn} G_{nn}^+ t_{nm} - t_{mn} G_{nn}^+ t_{nm} g_{mm}^A - t_{mn} G_{nn}^R t_{nm} g_{mm}^+ \big] \boldsymbol{\sigma}. \tag{8}$$

Next, the Green's functions $G_{nn}^\pm$ is expanded as

$$G_{nn}^\pm = G_{nn}^R t_{nm} g_{mm}^\pm t_{mn} G_{nn}^A + G_{np}^R t'_{pq} g_{qq}^\pm t'_{qp} G_{np}^A, \tag{9}$$

with respect to t_{mn} and t'_{pq}, which are hopping integrals at the m-n and p-q interfaces, respectively, and are dealt as perturbations. This is an approximation for G_{nn}^+ where the site n is included in the insulator. In the above expression, only the second term contributes to tunneling when there is no additional interaction in the FI layer. The first term corresponds to the reflection of electrons. We further replace the intersite Green's functions G_{np}^R with an unperturbed one that is, g_{np}^R. This replacement may be justified when we note that the FI is an insulator and that the tunneling electrons would not go back and forth many times in the junction. Then

$$G_{nn}^\pm \sim g_{np}^R t'_{pq} g_{qq}^\pm t'_{qp} g_{np}^A. \tag{10}$$

Similar approximations are used for advanced and retarded Green's functions as

$$G_{nn}^{A(R)} \sim g_{np}^{A(R)} t'_{pq} g_{qq}^{A(R)} t'_{qp} g_{np}^{A(R)}. \tag{11}$$

By using these approximations, the charge and spin currents are given as

$$\langle J_m^C \rangle = \frac{e}{h}\mathrm{Tr}\int d\omega \big[-g_{mm}^+ t_{mn} g_{np} t'_{pq} g_{qq}^- t'_{qp} g_{pn} t_{nm} + g_{mm}^- t_{mn} g_{np} t'_{pq} g_{qq}^+ t'_{qp} g_{np} t_{nm} \big] \mathbf{1}, \tag{12}$$

$$\langle \boldsymbol{J}_m^S \rangle = \frac{1}{4\pi}\mathrm{Tr}\int d\omega \big[g_{mm}^+ t_{mn} g_{np} t'_{pq} g_{qq}^A t'_{qp} g_{pn} t_{nm} + g_{mm}^R t_{mn} g_{np} t'_{pq} g_{qq}^+ t'_{qp} g_{np} t_{nm} - t_{mn} g_{np} t'_{pq} g_{qq}^+ t'_{qp} g_{np} t_{nm} g_{mm}^A - t_{mn} g_{np} t'_{pq} g_{qq}^R t'_{qp} g_{pn} t_{nm} g_{mm}^+ \big] \boldsymbol{\sigma}, \tag{13}$$

where superscripts R and A in g have been omitted since g is real in the FI. It should be noted that a more general expression of the charge current is obtained by using the property of the trace in Eq. (7) and a relation $G^A - G^R = G^+ - G^-$. However, it cannot be used for the spin current because of the Pauli spin matrix in Eq. (8). Therefore, we have used simpler approximations for both currents to make them consistent. The conservation of charge current is easily verified for both general and approximate expressions.

Now the Green's functions $g_{mm(qq)}^\pm$ are expressed in terms of the local density of states $D_{m(q)}$ at site $m(q)$ with Fermi distribution functions $f_{L(R)}$, as $g_{mm}^+ = 2\pi i D_m f_L$ and $g_{mm}^- = 2\pi i D_m (f_L - 1)$. Note that in general $D_{m(q)}$ is dependent on $k_\parallel$, however, we focus our attention on a state $k_\parallel = (0,0)$ ($\bar{\Gamma}$ point), which contributes mostly to tunnel currents in junctions with an I or FI. In the equilibrium state, $f_L = f_R = f_{\mathrm{eq}}$. In the nonequilibrium state, in general, $f_{\rm eq} \neq f_R \neq f_L$, however, we assume $f_{\rm eq} = f_L \neq f_R$ and calculate the spin current in the nonequilibrium state by using Eq. (3). Then the first and fourth terms, which include a factor of f_L in $[\cdots]$ of Eq. (13), are canceled by the corresponding terms in the equilibrium state. The second and third terms result in terms proportional to $2\pi i D_q(f_R - f_L)$. The resultant expression is

$$\langle \boldsymbol{J}^S_m \rangle_{n-\rm eq} = \frac{i}{2}{\rm Tr}\int d\omega\big[g^R_{mm} t_{mn} g_{np} t'_{pq} D_q t'_{qp} g_{np} t_{nm} - t_{mn} g_{np} t'_{pq} D_q t'_{qp} g_{np} t_{nm} g^A_{mm}\big](f_R - f_L)\boldsymbol{\sigma}. \quad (14)$$

Spin current through the p-q interface $\langle \boldsymbol{J}^S_p \rangle_{n-\rm eq}$ may be calculated in a similar manner, and the STT is given by Eq. (4). Up to now, the expressions of both charge and spin currents are applicable to realistic junctions using a full-orbital TB model.

Finally, adopting the single-orbital model with $t_{mn} = t_{nm} = t$ and $t'_{pq} = t'_{qp} = t'$ and transforming the spin axis into the global spin axis, we get $\boldsymbol{N} = N_\parallel \bar{\boldsymbol{M}} \times (\bar{\boldsymbol{M}}_P \times \bar{\boldsymbol{M}}) + N_\perp(\bar{\boldsymbol{M}}_P \times \bar{\boldsymbol{M}})$ using the unit vectors of the magnetization with

$$N_\parallel = -\int d\omega C(\omega) P_m (g^\uparrow_{np} - g^\downarrow_{np})^2, \quad (15)$$

$$N_\perp = \int d\omega C(\omega) \frac{1}{2\pi D^0_m}\{(g^\uparrow_{np})^2 - (g^\downarrow_{np})^2\}(R^\uparrow_m - R^\downarrow_m), \quad (16)$$

and

$$C(\omega) = \pi (tt')^2 (f_R - f_L) D^0_q D^0_m. \quad (17)$$

Here, P_m is the spin polarization of the DOS $D^{\uparrow(\downarrow)}_m = D^0_m(1 + (-)P_m)$ and $R^\sigma_m = {\rm Re}(g^\sigma_m)$. Because the right electrode is a NM, $D_q \equiv D^0_q$.

There are several interesting points to be noted: Both $N_\parallel$ and $N_\perp$ are linear in the bias voltage V, which is caused by the asymmetric structure of the junctions, and the sign of $N_\perp$ may change depending on the magnitude of R^σ_m. Owing to our simple approximations in Eqs. (13) and (14), in which multiple scattering at interfaces has been neglected, the STT is proportional to a product of the DOS at the left and right electrodes and to the spin polarization P_m at the left electrode, similar to the results obtained by Slonczewski.[13] When the multiple scattering, that is, band mixing between the left electrode and the FI is included, higher orders of the angle dependence may appear in the STT. Although the term $f_R - f_L$ in Eq. (17) includes an arbitrary value of V, the expressions of $\boldsymbol{N}$ may be applicable to low-bias voltages because a change in the electronic structure by V is disregarded in the present formalism.

The charge current is given as

$$\langle J^C_m \rangle = c\int d\omega\, D^0_q D^0_m \sum_\sigma \left(g^{\sigma 2}_{np} + \sigma P_m g^{\sigma 2}_{np}\cos\theta\right)(f_R - f_L), \quad (18)$$

with $c = 2\pi e(tt')^2/\hbar$. The MR defined as ${\rm MR} = (J_P - J_{AP})/J_P$, where $J_{P(AP)}$ is the charge current in parallel ($\theta = 0$) and antiparallel ($\theta = \pi$) alignment, is easily evaluated. For example, when $g_{np\uparrow} \gg g_{np\downarrow}$, ${\rm MR} = 2P_m/(1 + P_m)$, and an inverse MR is obtained in the opposite limit.

Because the charge current J and the STT N are proportional to $(|e|/\hbar)(tt')^2 D^2 V(g^{\uparrow 2}_{np} + g^{\downarrow 2}_{np})$ and $(tt')^2 D^2 V(g^{\uparrow 2}_{np} - g^{\downarrow 2}_{np})$ or to $(tt')^2 D^2 V(g^\uparrow_{np} - g^\downarrow_{np})^2$, respectively, we find that $N \sim (\hbar/|e|)J\eta$, where η is a product of the spin polarization P_m and ratio of the spin dependence of the nonlocal Green's function g^σ_{np}. When $g_{np\uparrow} \gg g_{np\downarrow}$, $\eta \sim P_m$, which should be compared with the TMR ratio. These results are consistent with those of previous studies.[2,4,13]

It was reported that impurities within MgO in magnetic tunnel junctions strongly affect the exchange coupling between the ferromagnetic layers and TMR ratio.[30,31] When impurities with spin-dependent potential υ^σ_i are included within the FI, the nonlocal Green's functions vary as $\tilde{g}^\sigma_{np} \sim g^\sigma_{np} + g^\sigma_{ni}\tilde{\upsilon}^\sigma_i g^\sigma_{ip}$ with $\tilde{\upsilon}^\sigma_i = \upsilon^\sigma_i(1 - g^\sigma_{ii}\upsilon^\sigma_i)^{-1}$. Therefore, STT may also be affected by the impurities.

Here, we show qualitative features of the nonlocal Green's function g_{np} calculated by using a single-orbital TB model for a FI and adopting a layered structure with six atomic layers ($n,p = 1,6$ in this case), in which four layers have positive magnetization and two layers have negative magnetization. Occupied and unoccupied bands of each layer are characterized by negative and positive hopping integrals, respectively, to approximately reproduce the electronic states near the Γ point calculated for Co and Ni spinels. We assume that the interlayer hopping integral is the same as that in layers with positive magnetization. Figure 2 shows the energy dependence of ${\rm Re}[g^\sigma_{16}(E)]$ at $k_\parallel = (0,0)$ near the energy gap. The local DOS of an interface layer with positive magnetization is shown in the inset. The local DOS is similar to the DOS depicted by the solid curves in Fig. 1(a). We find that the real part of $g^\sigma_{16}(E)$ exhibits a peak at the band edge where the DOS vanishes and decays quickly with decreasing energy. Therefore, once the chemical potential is located near either an up- or down-spin band edge, we may have a strong spin asymmetry in the nonlocal Green's function, and we expect a large TMR and STT.

Finally, let us summarize the difference between the features of the STT in FM/I/FM junctions studied previously and those obtained in the present Rapid Communication.

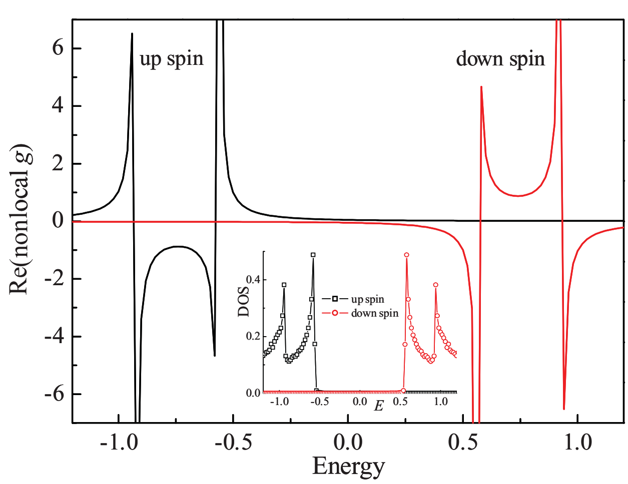

FIG. 2. (Color online) Energy dependence of up- and down-spin nonlocal Green's functions ${\rm Re}(g_{16})$ with $k_\parallel = (0,0)$ near the energy band gap calculated by using a simple model of an ferromagnetic insulator with six atomic planes. The inset shows the local DOS at an interface layer of the FI, in units of $1/|t|$/atom/spin, where t is a hopping integral within the insulator.

It is worthwhile to note first that the STT is formulated for junctions with a thin FI layer, in contrast to junction structures FM/I/FM studied previously.[14,17–19] A main difference between the feature resides in the role of electronic states on STT. Detailed studies of the STT in FM/I/FM junctions[14,18,19] have clarified that the electronic structure near the Fermi energy of FM is crucial for the bias dependence of the STT. Band symmetry has also been pointed out to be important for Fe/MgO/Fe junctions.[15] On the other hand, the STT in junctions with FI is governed by the real part (not the imaginary part) of the spin-dependent nonlocal Green's function within the energy gap of FI, as explicitly shown in Eqs. (15) and (16).

In conclusion, analytical expressions of the spin-transfer torque (STT) have been formulated as the change in the spin angular momentum produced by tunneling of spin-polarized electrons through a ferromagnetic insulator (FI) by using the Keldysh formalism. Adopting simple approximations, both parallel and perpendicular torques are expressed in terms of spin-dependent intersite Green's functions of the FI. It is found that they depend linearly on the bias voltage, due to the asymmetry of the junctions. The relationship between STT and tunnel magnetoresistance, and the effects of electronic structures of the FI and of impurities are presented. More studies on interactions between magnetic excitation in FI and tunneling spins would be desirable to clarify how the magnetization dynamics of FI is affected by the STT.

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