Spin-mixing conductance of ferromagnet/topological-insulator and ferromagnet/heavy-metal heterostructure: A first-principles Floquet-nonequilibrium Green function approach

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The magnitude of experimentally observed spin pumping in ferromagnet/topological-insulator and ferromagnet/heavy-metal heterostructures is routinely interpreted in terms of standard spin-mixing conductance (SMC). However, this quantity is not well-defined when strong spin-orbit coupling (SOC) is present directly at the interface. Nevertheless, an effective SMC can be extracted as the pre-factor in pumped spin current $I^{\uparrow\downarrow}$ vs. precession cone angle $\theta$ dependence, as long as such dependence remains $I^{\uparrow\downarrow} \propto \sin^2 \theta$. Here we compute directly the pumped spin current, using noncollinear density functional theory Hamiltonian combined with charge conserving Floquet-nonequilibrium Green function formalism, flowing into semi-infinite Cu electrodes of two-terminal multilayers Cu/X/Co/Cu, where X = Bi$_2$Se$_3$, Pt and W and Cu. We show that pumped spin current gets reduced in the presence of interfacial SOC. However, stacking sequence and materials selection for constituting the heterostructure can eventually modulate the effective SMC.

I. INTRODUCTION

The spin pumping is a ubiquitous phenomenon in spintronic devices where magnetization dynamics generates pure spin current even in the absence of any applied bias voltage [1]. In ferromagnetic-metal/normal-metal (FM/NM) heterostructures, with precessing magnetization driven by the absorption of microwaves under the ferromagnetic resonance condition, the spin pumping from FM to NM layer has been detected as an electric signal into which pumped spin current is injected to the NM at the interface to the FM.

In scattering theory [1], the pumped spin current that is injected to the NM is given as

$$I_{\text{pump}} = \frac{\hbar}{4\pi} \left[ \text{Re}(g_{\uparrow\downarrow}) \mathbf{m} \times \frac{d\mathbf{m}}{dt} - \text{Im}(g_{\uparrow\downarrow}) \frac{d\mathbf{m}}{dt} \right],$$

(1)

where $\mathbf{m}$ is a unit vector for representing the orientation of magnetization in FM and $g_{\uparrow\downarrow}$ is the so-called spin-mixing conductance of the FM/NM interface given by,

$$g_{\uparrow\downarrow} = \sum_{nn'} \delta_{nn'} - \langle r_{nm}^\dagger \rangle^* \langle r_{nm} \rangle$$

where $r_{nm}$ is the reflection amplitude between transverse modes $m$ and $n$ with spin $\sigma = \uparrow, \downarrow$ in the NM at the interface to the FM. When the FM/NM interface is Ohmic, Im($g_{\uparrow\downarrow}$) becomes insignificant due to the random phase of electrons in reciprocal space [4]. In the presence of interfacial SOC, the phenomenological parameter $g_{\uparrow\downarrow}$ is ill-defined within the scattering formalism. Moreover, the evaluation of $g_{\uparrow\downarrow}$ becomes computationally cumbersome as one has to compute the scattering matrix at all times within a pumping cycle to find the time-averaged pumped spin currents. However, an effective spin-mixing conductance can be extracted as the pre-factor of DC spin current vs. precessing cone angle ($\theta$) dependence, where the spin current is expressed as

$$I^{\uparrow\downarrow}(\theta) = \frac{\hbar \omega}{4\pi} \text{Re}(g_{\uparrow\downarrow}) \sin^2 \theta,$$

(2)

where $\omega$ is the frequency of precession of magnetization.

The efficiency of the spin pumping can be modulated largely by replacing the NM with a heavy metal (HM) [5] or Dirac materials [7,9,11], in which SOC plays a crucial role.
II. THEORY

Within the non-collinear DFT (ncDFT) framework, the single-particle spin-dependent Kohn-Sham (KS) Hamiltonian describing our system takes the form

$$H_{KS} = T_{KS} + V_H + V_{XC} + V_{\text{ext}} + V_{\text{SOC}} + \sigma \cdot B_{XC},$$

where $T_{KS}$, $V_H(r)$, $V_{\text{ext}}(r)$, and $V_{XC}(r) = \delta E_{XC}[n(r), m(r)]/\delta n(r)$ are the kinetic energy, Hartree potential, external potential and exchange-correlation (XC) potentials, respectively. $\sigma = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ is the vector for the Pauli Matrices and $V_{\text{SOC}}$ represents the potential arising due to SOC. The XC-magnetic field can be expressed as $B_{XC}(r) = \delta E_{XC}[n(r), m(r)]/\delta m(r)$ and one can extract the $B_{XC}$ matrices from $H_{KS}$ as

$$B_{XC}^x = 2 \cdot \text{Re}(B_{XC}^+)$$

$$\begin{align*}
B_{XC}^y &= -2 \cdot \text{Im}(B_{XC}^+) \\
B_{XC}^z &= (B_{XC}^{++} - B_{XC}^{++})
\end{align*}$$

where $\mathcal{H} = H_{KS} - V_{\text{SOC}}$.

If the magnetization in a FM is steadily precessing with a frequency \( \omega \) about an axis with a precession cone angle \( \theta \), the time-dependent Hamiltonian of the system is given by

$$H(t) = H_0(\theta) + V(\theta)e^{i\omega t} + V^+(\theta)e^{-i\omega t}.$$

In principle, for a realistic device setup one can extract the matrices $H_0$ and $V$ from time-independent ncDFT calculations, given as

$$H_0(\theta) = H_{KS}(\theta) - V(\theta) - V^+(\theta),$$

and

$$V(\theta) = \frac{1}{4} B_{XC}^\sigma(\theta) \otimes \{ \hat{\sigma}_x - i\hat{\sigma}_y \}. $$

A time-dependent nonequilibrium Green function formalism has previously been introduced to describe spin pumping in magnetic and semimagnetic tunnel junctions [18]. When a system is periodically driven in time, one can compute time-averaged spin and charge currents injected into leads by constructing the so-called Floquet Hamiltonian of the system, described as

$$\mathbf{\hat{H}}_F = \begin{pmatrix}
\mathbf{H}_0 & \mathbf{V} \\
\mathbf{V}^\dagger & \mathbf{H}_0
\end{pmatrix},$$

and simultaneously, we define the matrix

$$\mathbf{\hat{\Omega}} = \begin{pmatrix}
\mathbf{1} & \mathbf{0} & \mathbf{0} \\
\mathbf{0} & -\omega \mathbf{1} & \mathbf{0} \\
\mathbf{0} & \mathbf{0} & -\omega \mathbf{1}
\end{pmatrix}.$$

Now Floquet retarded Green function of the system can be calculated as

$$[(E + \mathbf{\hat{\Omega}})\mathbf{\hat{S}} - \mathbf{\hat{H}}_F - \mathbf{\hat{\Sigma}}'(E)]\mathbf{\hat{G}}^r(E) = \mathbf{1},$$

FIG. 2. Convergence of DC spin current injected in the left Cu lead denoted by $I_{Cu}^{\uparrow \uparrow}$ in the presence of SOC: (a) with respect to number of $k_y$ points calculated for fixed precession cone angle $\theta = 90^\circ$ and photon number, $N_{ph} = 1$; (b) with respect to number of photons $N_{ph}$ calculated for fixed precession cone angle $\theta = 90^\circ$ and $k_y = 25$. Both panels show the results for TI/FM and HM/FM vertical heterostructure, in which TI = 1QL of Bi$_2$Se$_3$ (red curve), HM = Pt (green curve) and W (magenta curve) calculated for $\hbar \omega = 1$ meV.
are carried out for heterostructure, the curve is multiplied with factor of $10^3$ included in the calculations, respectively. Red, blue, black, green, and magenta curves denote the angular dependence for as illustrated in Fig. 1. Upper panels (a), (b), (e), (f) and lower panels (c), (d), (g), (h) indicate that SOC is either excluded or heterostructure in which the magnetization of FM, $m$, is precessing with a precession cone angle $\theta$ with respect to $z$-axis as illustrated in Fig. 1. Upper panels (a), (b), (e), (f) and lower panels (c), (d), (g), (h) indicate that SOC is either excluded or included in the calculations, respectively. Red, blue, black, green, and magenta curves denote the angular dependence for 1QL-Bi$_2$Se$_3$/Co, 6QL-Bi$_2$Se$_3$/Co, Cu/Co, Pt/Co, and W/Co heterostructure, respectively. Note that for 6QL-Bi$_2$Se$_3$/Co heterostructure, the curve is multiplied with factor of $10^3$ and with $10^2$ in panel (a) and (c), respectively. All the calculations are carried out for $k_y = 25$, $N_{ph} = 2$ and $\hbar \omega = 10^{-3}$ eV.

FIG. 3. The angular dependence of the DC spin current injected into left and right Cu leads for TI/FM and HM/FM vertical heterostructure in which the magnetization of FM, $m$, is precessing with a precession cone angle $\theta$ with respect to $z$-axis as illustrated in Fig. 1. Upper panels (a), (b), (e), (f) and lower panels (c), (d), (g), (h) indicate that SOC is either excluded or included in the calculations, respectively. Red, blue, black, green, and magenta curves denote the angular dependence for 1QL-Bi$_2$Se$_3$/Co, 6QL-Bi$_2$Se$_3$/Co, Cu/Co, Pt/Co, and W/Co heterostructure, respectively. Note that for 6QL-Bi$_2$Se$_3$/Co heterostructure, the curve is multiplied with factor of $10^3$ and with $10^2$ in panel (a) and (c), respectively. All the calculations are carried out for $k_y = 25$, $N_{ph} = 2$ and $\hbar \omega = 10^{-3}$ eV.

where $\Sigma^r(E)$ is the Floquet self-energy matrix given as

$$\Sigma^r(E) = \begin{pmatrix} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \Sigma^r(E - \hbar \omega) & 0 & 0 & \cdots \\ \cdots & 0 & \Sigma^r(E) & 0 & \cdots \\ \cdots & 0 & 0 & \Sigma^r(E + \hbar \omega) & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}.$$ (13)

Here, $\Sigma^r(E) = \sum_{p=L,R} \Sigma^r_p(E)$ is self-energy of the Cu leads obtained using conventional steady-state-NEGF. Furthermore, the Floquet overlap matrix $S$ is given by

$$S = \begin{pmatrix} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & S & 0 & 0 & \cdots \\ \cdots & 0 & S & 0 & \cdots \\ \cdots & 0 & 0 & S & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}.$$ (14)

Here $S$ is the overlap matrix whose elements are given by $S_{ab} = \langle \phi_a | \phi_b \rangle$, where $| \phi_a \rangle$ or $| \phi_b \rangle$ denote the states that belong to the nonorthogonal basis set used to solve the Kohn-Sham equations. In principle, the matrices in Eq. (10)-(14) reside in a Hilbert space given by $\mathcal{H} = \mathcal{H}_{ph} \otimes \mathcal{H}_e$, where $\mathcal{H}_{ph}$ is the Hilbert space of active photon modes and is ideally infinite dimensional. However, in practice we truncate it to a finite number of photon modes indicated by $N_{ph}$ seeking for convergence of the observables. If the operators in electronic Hilbert space $\mathcal{H}_e$ are represented by matrices of dimension $N_e \times N_e$, any operator in Hilbert space $\mathcal{H}$ is represented by matrices of dimension $(2N_{ph} + 1)N_e \times (2N_{ph} + 1)N_e$. Finally, the time-averaged pumped spin and charge currents in the adiabatic limit $| \hbar \omega << E_F \rangle$ injected in lead $p = L, R$ (left or right) are given by

$$I_p = \frac{e}{2N_{ph} A_{cell}} \int_{\mathbf{BZ}} d\mathbf{k} \text{Tr} [ \hat{\Gamma}_p \hat{\Omega} \hat{G}^\dagger \hat{G}^a - \hat{\Gamma}_p \hat{G} \hat{G}^\dagger \hat{\Omega} \hat{G}^a ],$$ (15)

where $A_{cell}$ is the area of the unit cell. We also have

$$I_p^{S^a} = \frac{\hbar}{4N_{ph} A_{cell}} \int_{\mathbf{BZ}} d\mathbf{k} \text{Tr} [ \hat{\sigma}^a \hat{\Gamma}_p \hat{\Omega} \hat{G}^\dagger \hat{G}^a - \hat{\sigma}^a \hat{\Gamma}_p \hat{G} \hat{G}^\dagger \hat{\Omega} \hat{G}^a ],$$ (16)

where $\hat{\sigma}^a = \mathbf{1}_{ph} \otimes \hat{\sigma}^a$, is the Pauli operator residing in $\mathcal{H}_e$. Here, $\mathbf{1}_{ph}$ is the identity matrix in $\mathcal{H}_{ph}$, $\hat{\Gamma}_p(E) = i[\Sigma^r_p(E) - (\Sigma^r_p(E))^\dagger]$, $\hat{\Gamma}(E) = \sum_{p=L,R} \hat{\Gamma}_p(E)$ and the Floquet advanced Green function is given by $\hat{G}^a(E) = [\hat{G}(E)]^\dagger$. 

We note that here

\[ \text{rents is not more than 6\% of the value obtained with} \]

\[ \text{for which the relative error introduced in the spin current} \]

\[ \text{computational complexity due to the large dimension of} \]

\[ \text{H} \]

\[ \text{mixing conductance given by} \]

\[ g_{\downarrow\uparrow}^p \equiv \frac{4\pi}{\hbar\omega} I_p^{S_z}\left|_{\theta=90^\circ}\right. \]  

(17)

We note that \( g_{\downarrow\uparrow}^p \) can have different values depending upon \( p = L, R \). In other words, \( g_{\downarrow\uparrow}^L \) and \( g_{\downarrow\uparrow}^R \) render an effective SMC of the hetero-junctions residing to the left side (LHJ) and to the right side (RHJ) of the ferromagnet Co, respectively. In Table I (see appendix A), we list the SMC of LHJ and RHJ for various Co/X/Co/Cu multilayer heterostructure in the presence as well as the absence of SOC. We find that \( g_{\downarrow\uparrow}^L \approx g_{\downarrow\uparrow}^R \) for Cu/Co/Cu setup [black curve in Fig. 3(a) and (b)] due to the preservation of left-right symmetry in the heterostructure. Once 1QL of Bi$_2$Se$_3$ is sandwiched between left Cu/Co interface, the left-right symmetry is broken which results not only in suppression of both \( g_{\downarrow\uparrow}^L \) and \( g_{\downarrow\uparrow}^R \) but also in decrease of \( g_{\downarrow\uparrow}^L \) < \( g_{\downarrow\uparrow}^R \). This result suggests that insertion of Bi$_2$Se$_3$ layers which induce a backflow of spin currents, can not only modify the SMC of its own constituted LHJ but also modulate the SMC of the RHJ. Such a backflow may disappear if the ferromagnet is thicker than its spin-diffusion length. When number of QL is increased from 1 to 6 [blue curve in Fig. 3(a) and (b)], \( g_{\downarrow\uparrow}^L \) further gets suppressed while \( g_{\downarrow\uparrow}^R \) remains approximately the same. This trend of \( g_{\downarrow\uparrow}^L \) < \( g_{\downarrow\uparrow}^R \) is also observed in Pt/Co and W/Co heterostructure as shown in Fig. 3(c) and (f). Interestingly, \( g_{\downarrow\uparrow}^L \) and \( g_{\downarrow\uparrow}^R \) are suppressed for all heterostructure in comparison to respective SMC of Cu/Co/Cu heterostructure, with an exception of W/Co heterostructure, where \( g_{\downarrow\uparrow}^R \) is enhanced instead [see Fig. 3(f)].

In Fig. 3(c),(d),(e) and (h) we show the effect of SOC on spin currents in all the heterostructure discussed

FIG. 4. The \( k_z \)-resolved DC spin current injected in either; (a),(c) left Cu lead or; (b),(d) right Cu lead for TI/FM vertical heterostructure. The thickness of TI is either 1QL (upper panels) or 6QL (lower panels). The units for \( k_x \) and \( k_z \) are \( \pi/b \) and \( \pi/c \) where \( b \) and \( c \) are the lattice constants along the \( y \) and the \( z \) axis, respectively.
above. In general we observe that presence of SOC leads to a suppression $I_L^{z\parallel}$ and $I_R^{z\parallel}$ and hence causes a reduction of both left and right SMC of the heterostructure. We note that inclusion of SOC does not affect the spin current in the Cu/Co/Cu heterostructure due to the fact that the presence of inversion symmetry prohibits to generate the spin-texture which would cause a back flow of spin current. On the contrary, we observe an enhancement ($\sim 50$ times) of $g_{k}$ for 6QL-Bi$_2$Se$_3$ in the presence of SOC. Such an enhancement is attributed to the emergence of topologically protected Dirac cone inside the bulk gap of 6QL-Bi$_2$Se$_3$ in the presence of SOC [23], which provides a transport channel for conduction of spin current. On the other hand, 1QL of pristine Bi$_2$Se$_3$ remains insulating even in the presence of SOC [23].

Finally, fig. 4 shows the $k_{\parallel}$-resolved contributions to the spin-current $I_{p}^{z\parallel}$ for 1QL- and 6QL-Bi$_2$Se$_3$ heterostructure at a fixed precession cone angle $\theta = 90^\circ$ in the presence of SOC. For 1QL-Bi$_2$Se$_3$ case, the contribution spreads over the whole BZ, because the electronic states of 1QL-Bi$_2$Se$_3$ are largely hybridized with that of metallic Co and Cu layers, underpinning the flow of spin current from ferromagnet to the left lead. Note that these evanescent metallic states can only penetrate up to 2-3 QL-Bi$_2$Se$_3$ [24]. Therefore, spin-current is carried predominately by the surface states associated to the Dirac cone of 6QL-Bi$_2$Se$_3$, exhibited as hotspots, i.e., area of large spin current in the BZ as shown in Fig. 4(c). On the other hand, the $k_{\parallel}$-resolved contribution to $I_R^{z\parallel}$ is also scattered over the BZ due the presence of Co/Cu metallic states.

V. CONCLUSIONS

In conclusion, we have developed a Floquet-NEGF formalism combined with DFT Hamiltonian which makes possible first-principles quantum transport calculation of DC component of pumped spin and charge currents in realistic FM/TI and FM/HM heterostructure hosting strong interfacial SOC effects. Interfacial SOC diminishes the SMC of a certain interface, however, such a presence of SOC can eventually modulate the SMC by constructing a multilayer heterostructure, which shows that not only interfacial SOC but also material’s intrinsic properties such as conductivity play a crucial role in spin-pumping. Our study show a pathway for materials design in order to tune the SMC for spintronics applications.

We note that rigorous application of the Floquet theorem to first-principles Hamiltonian driven by time-periodic field would require to start from time-dependent density functional theory (TDDFT) where time-independent external field would generate real-time evolution of the self-consistent electronic density [25, 26]. Such Floquet-TDDFT approach also includes dynamical screening and intra-atomic dipole transitions in a self consistent way [26]. However, due to small frequency of microwave radiation when compared to the Fermi energy of heterostructures in Fig. 1, $\hbar \omega \ll E_F$, we expect very small perturbation by such field of electronic density of in the static noncollinear DFT. In other words, our much less expensive calculation is in the spirit of linear-response theory and first-principles scattering matrix calculation [1, 13, 14, 16] of SMC where one also uses static DFT Hamiltonian as an input.

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Appendix A: Supplementary Information

FIG. 5. The $k_y$-resolved DC spin current injected in either; (a),(c) left Cu lead or; (b),(d) right Cu lead for HM/FM vertical heterostructure. HM is either Pt (upper panels) or W (lower panels). The units for $k_y$ and $k_z$ are $\pi/b$ and $\pi/c$ where $b$ and $c$ are the lattice constants along the $y$ and the $z$ axis, respectively.

| Heterostructure          | $g_{l1}^L$ (w/o SOC) | $g_{l1}^R$ (w/o SOC) | $g_{l1}^L$ (SOC) | $g_{l1}^R$ (SOC) |
|--------------------------|----------------------|----------------------|------------------|------------------|
| Cu/Co/Cu                 | 4.5874               | 4.8513               | 4.4742           | 4.7088           |
| Cu/1QL-Bi_2Se_3/Co/Cu    | 1.2554               | 1.8720               | 0.4565           | 1.8084           |
| Cu/6QL-Bi_2Se_3/Co/Cu    | 0.0004               | 1.7547               | 0.0197           | 1.5812           |
| Cu/Pt/Co/Cu              | 2.9419               | 3.6373               | 1.4329           | 3.0809           |
| Cu/W/Co/Cu               | 2.4619               | 6.3767               | 1.0784           | 6.0060           |

TABLE I. Spin-mixing conductance, $g_{l1}^{L,R}$ for various heterostructure (in units of $10^{20}\Omega^{-1}m^{-2}$) in the presence or absence of SOC.