Magnon spin-transfer torque from antiferromagnetic insulator to ferromagnetic metal: Time-dependent quantum transport combined with atomistic spin dynamics approach

Abhin Suresh,1 Marko D. Petrović,1 Hyunsoo Yang,2 and Branislav K. Nikolić1,3,*

1Department of Physics and Astronomy, University of Delaware, Newark DE 19716, USA
2Department of Electrical and Computer Engineering, National University of Singapore, 117576, Singapore
3Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106-4050

The recent experiment [Y. Wang et al., Science 366, 1125 (2019)] on magnon-mediated spin-transfer torque (MSTT) was interpreted in terms of a picture where magnons are excited within an antiferromagnetic insulator (AFI), by applying nonequilibrium electronic spin density at one of its surfaces, so that their propagation across AFI deprived of conduction electrons eventually leads to reversal of magnetization of a ferromagnetic metal (FM) attached to the opposite surface of AFI. However, microscopic understanding of how magnonic and electronic spin currents, both of which can exert torque on localized magnetic moments within FM, are generated and interconverted at multiple junction interfaces is lacking. We employ a recently developed time-dependent nonequilibrium Green functions combined with the Landau-Lifshitz-Gilbert equation (TDNEGF+LLG) formalism to evolve electrons quantum-mechanically while they interact via self-consistent back-action with localized magnetic moments described classically by atomistic spin dynamics solving a system of LLG equations. Upon injection of square current pulse as the initial condition, TDNEGF+LLG simulations of FM-polarizer/AFI/FM-analyzer junctions show that reversal of localized magnetic moments within FM-analyzer is less efficient, in the sense of requiring larger pulse height and its longer duration, than conventional electron-mediated STT (ESTT) driving magnetization switching in standard FM-polarizer/normal-metal/FM-analyzer spin valve. Since both electronic, generated by spin pumping from AFI, and magnonic, generated by direct transmission from AFI, spin currents are injected into the FM-analyzer, its localized magnetic moments will experience combined MSTT and ESTT. Nevertheless, we demonstrate, by artificially turning off ESTT, that MSTT plays a dominant role whose understanding paves the way for all-magnon-driven magnetization switching devices with no electronic parts.

I. INTRODUCTION

The magnon-mediated spin transfer torque (MSTT) [1–6] is a phenomenon where spin current carried by spin wave (SW) within an insulating or metallic magnetic material transfers spin angular momentum to its localized magnetic moments (LMMs). In the semiclassical picture [7, 8], SW is a disturbance in the local magnetic ordering of a magnetic material in which LMMs precess around the easy axis with the phase of precession of adjacent moments varying harmonically in space over the wavelength $\lambda$. The quanta of energy of SW behave as a quasiparticle, termed magnon, which carries energy $\hbar \omega$ and spin $\hbar$. The frequency $\omega$ of the precession is commonly in the GHz range of microwaves, but it can reach THz range in antiferromagnets [9–12].

The SWs are inevitably excited at finite temperature as incoherent thermal fluctuations. But they can also be induced in controllable fashion by using external fields [13], or by injecting spin-polarized or pure spin currents [14], thereby leading to coherent propagation of SWs as a dispersive signal. Since both electrons and magnons have intrinsic angular momentum, their translational flow is equivalent to a flux of spin angular momentum which is denoted as electronic and magnonic (or SW) spin current [1, 15, 16], respectively.

The MSTT provides an alternative to conventional electron-mediated spin-transfer torque (ESTT) where electronic spin current transfers spin angular momentum to LMMs, on the proviso that electronic spin polarization is noncollinear to the direction of LMMs [17–22]. Since SWs in magnetic insulators can transmit spin current over $\sim \mu$m distances in the absence of Joule heating, all-magnon-driven magnetization dynamics and switching, without any electronic motion, has been envisioned [15]. This requires, e.g., temperature gradients to excite SWs [2–5] and the corresponding magnonic spin current. Another proposal [6] is to insert a magnetic insulator barrier as a spacer between two ferromagnetic metals (FM) forming a magnetic tunnel junction where MSTT, driven by asymmetric heating of two FM layers, could enhance conventional ESTT. Besides fundamental interest, MSTT-based devices are envisioned as ultralow dissipation platform for magnon-based memory, logic and logic-in-memory [15].

Following theoretical predictions [1], a very recent experiment [23] has demonstrated MSTT-driven motion of magnetic domain wall in FM multilayer films based on Co/Ni. Another experiment [24] has shown how SW excited in an antiferromagnetic insulator (AFI) NiO by spin-orbit torque [25] from metallic surface of three-dimensional topological insulator (TI) Bi$_2$Se$_3$ was able to switch the magnetization of Py as FM-analyzer layer.

* bnikolic@udel.edu
FIG. 1. Schematic view of two-terminal junctions whose active region (modeled as 1D tight-binding chain) is attached via semi-infinite NM leads (modeled as 1D tight-binding chains without any spin-dependent interactions) to two macroscopic reservoirs of electrons. The active region hosts: (a) three fixed LMMs (blue arrows) pointing along the x-axis which comprise FM-polarizer layer, followed by two sites without LMMs, followed by Néel-ordered 20 LMMs (red arrows) comprising AFI layer, and three free LMMs (blue arrows labeled 1–3) comprising FM-analyzer which receives MSTT and/or ESTT; (b) same as (a) but without AFI layer. A square voltage pulse is applied (at \( t_1 = 1 \) ps) to inject unpolarized charge current \( I(t) \) from the left NM lead. Also denoted are local spin currents: \( I_{\text{NM} \rightarrow \text{API}}^{s} \) impinging on the first LMM of AFI in (a); \( I_{\text{API} \rightarrow \text{FM}}^{s} \) impinging on the first LMM of FM-analyzer in (a); and \( I_{\text{NM} \rightarrow \text{FM}}^{s} \) impinging on the first LMM of FM-analyzer in (b).

within Bi2Se3/NiO/Py heterostructure. Within AFI electrons do not move, hence SWs are the sole carrier of spin currents. Increasing the thickness of the AFI layer improves its antiferromagnetic ordering, so that MSTT acting on the FM-analyzer Py reaches an optimal magnitude at \( \approx 25 \) nm thick NiO layer in Ref. [24]. This was achieved without any external magnetic field and at room temperature as being highly relevant for applications. Furthermore, the absence of net magnetization in AFI forbids any stray magnetic fields which makes such materials largely insensitive to perturbations by externally applied magnetic fields or those from neighboring layers [9–12]. Since insertion of a normal metal (NM) layer, such as Cu of thickness \( \zeta \approx 6 \) nm, between NiO and Py layers did not substantially impede MSTT-driven magnetization switching of FM-analyzer, it was concluded [24] that direct exchange coupling between NiO and Py layers is not essential. Instead, one can conjecture that magnonic spin current is transmuted [16, 26] at the AFI/NM interface into electronic spin current which then exerts conventional ESTT on the magnetization of the FM-analyzer.

Motivated by the experiments of Ref. [24], we study MSTT in FM-polarizer/AFI/FM-analyzer setup illustrated in Fig. 1(a). We also compare its efficiency with conventional ESTT in standard FM-polarizer/NM/FM-analyzer spin valve setup in Fig. 1(b). For this purpose, we employ recently developed multiscale and numerically exact quantum-classical framework [27–30]. It combines time-dependent nonequilibrium Green functions (TDNEGF) [31, 32] description of electrons out of equilibrium in open quantum systems, such as those illustrated in Fig. 1 where the left (L) and right (R) macroscopic particle reservoirs make them open, with the Landau-Lifshitz-Gilbert (LLG) equation [7, 8, 33] describing classical time evolution of LMMs.

The classical treatment of LMMs, whose orientation is specified by unit vectors \( \mathbf{M}_i(t) \), is justified [34] in the limit of large localized spins \( S \rightarrow \infty \) and \( h \rightarrow 0 \) (while \( S \times h \rightarrow 1 \)), as well as in the absence of entanglement [35] between quantum states of individual LMMs. The latter condition is expected to be satisfied at room temperature (otherwise, since NiO is actually a strongly correlated insulator [36], we can expect its state to be highly entangled at low temperatures). We note that LLG description of the dynamics of local magnetization also appears in classical micromagnetics [7, 33]. But there \( \mathbf{M}_i \) describe magnetization of a small volume of space, typically (2–10 nm)\(^3\), rather than of individual atoms [8] that we have to assume in order to couple classical dynamics of \( \mathbf{M}_i(t) \) to TDNEGF calculations where electrons hop from atom to atom. Furthermore, despite the ubiquity of micromagnetic simulations, they cannot [8] properly
Our principal results for time evolution of LMMs and magnonic and electronic spin currents acting on them are summarized by Figs. 2–7, as well as their animations in embedded Videos 1–3. The paper is organized as follows. In Sec. II we introduce classical Hamiltonian for LMMs and quantum Hamiltonian for conduction electrons, where we also explain self-consistent coupling of LLG and nonequilibrium density matrix (DM) calculations for classical and quantum dynamics, respectively. We warm up by looking first in Sec. IIIA at ESTT in Fig. 1, which are allowed to evolve in time, is given by

$$H = J_{AFI} \sum_{(ij) \in AFI} M_i \cdot M_j - J_{FM} \sum_{(ij) \in FM} M_i \cdot M_j - J_{AFI-FM} M_{N,AFI} \cdot M_{1,FM} - J_{sd} \sum_i (\hat{s}_i)^{CD}(t) \cdot M_i - K \sum_i (M_i^z)^2. \quad (1)$$

Here $J_{AFI} = 0.1$ eV is the Heisenberg exchange coupling between the nearest-neighbor LMMs of AFI layer; $J_{FM} = 0.1$ eV is the exchange coupling between the nearest-neighbor LMMs of FM-analyzer; $J_{AFI-FM} = 0.1$ eV, or $J_{AFI-FM} = 0$ in some setups, is the exchange coupling between the last LMM $M_{N,AFI}$ of AFI layer and the first LMM $M_{1,FM}$ of FM-analyzer; and magnetic anisotropy is specified by $K = 0.0005$ eV which selects the $z$-axis as the easy axis. In the case of spin valve in Fig. 1(b) we use the same Hamiltonian in Eq. (1) but without AFI layer. The interaction of classical LMMs and current-driven (CD) part \cite{27, 38} of nonequilibrium

simulate antiferromagnets or ferrimagnets whose intrinsic magnetization direction varies strongly on the atomic scale.

FIG. 3. TDNEGF+LLG-computed time dependence of FL and DL components \cite{17} of ESTT vector $T_i(t)$ [Eq. (6)] on: (a) the first LMM of FM-analyzer; and (b) the last LMM of FM-analyzer within FM-polarizer/NM/FM-analyzer spin valve in Fig. 1(a). Panels (c) and (d) show steady-state-NEGF+LLG \cite{37, 38} computed time-dependence of the last LMM [compare with Fig. 2(b)] of FM-analyzer and FL and DL components of ESTT vector [compare with panel (b)] on the last LMM of FM-analyzer, respectively. The height $V_D = 0.25$ V and the duration $V_D = 0.6$ ps of bias voltage square pulse employed is the same as in Fig. 2(b).
ing parameter the gyromagnetic ratio; and the intrinsic Gilbert damp-
phonon interactions. We choose λ mechanism [40, 41] combining spin-orbit coupling and electron-
AFI layer and

electronic spin density \( \langle \hat{s}_i \rangle^{CD} \) (t) is described by s-d exchange coupling of strength \( J_{sd} = 0.1 \text{ eV} \), as measured experimentally [39]. The classical dynamics of \( \mathbf{M}_i(t) \) is obtained by solving a system of coupled LLG equations [7, 8, 33]

\[
\frac{\partial \mathbf{M}_i}{\partial t} = -\frac{g}{1 + \lambda^2} \left[ \mathbf{M}_i \times \mathbf{B}_i^{\text{eff}} + \lambda \mathbf{M}_i \times (\mathbf{M}_i \times \mathbf{B}_i^{\text{eff}}) \right],
\]

using the Heun numerical scheme with projection to the unit sphere [8]. Here \( \mathbf{B}_i^{\text{eff}} \) is the effective magnetic field \( (\mu_M \text{ is the magnitude of LMMs); } g \) is the gyromagnetic ratio; and the intrinsic Gilbert damping parameter \( \lambda \) arises due to the well-established mechanism [40, 41] combining spin-orbit coupling and electron-phonon interactions. We choose \( \lambda = 0.005 \) within the AFI layer and \( \lambda = 0.05 \) within the FM-analyzer.

The conduction electron subsystem is modeled by a quantum Hamiltonian

\[
\hat{H} = -\sum_{(ij)} \gamma_{ij} \hat{c}_i^\dagger \hat{c}_j - J_{sd} \sum_i \hat{c}_i^\dagger \mathbf{\hat{\sigma}} \cdot \mathbf{M}_i(t) \hat{c}_i,
\]

where the first term is a 1D TB model and the second term is the s-d exchange coupling between LMMs and conduction electron spins described by the vector of the Pauli matrices \( \mathbf{\hat{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \). Here \( \hat{c}_i^\dagger = (\hat{c}_{i\uparrow}^\dagger, \hat{c}_{i\downarrow}^\dagger) \) is a row vector containing operators \( \hat{c}_i^\dagger \) which create an electron of spin \( \sigma = \uparrow, \downarrow \) at the site \( i \), and \( \hat{c}_i \) is a column vector that contains the corresponding annihilation operators.

The semi-infinite NM leads attached to active region in Fig. 1 are modeled by the first term alone in Eq. (3). The nearest-neighbor hopping is \( \gamma_{ij} = 1 \text{ eV} \) in the NM leads, NM interlayer, FM-polarizer and FM-analyzer in Fig. 1, as well as between AFI layer and neighboring metallic layers. Within the AFI layer hopping is zero, \( \gamma_{ij} \equiv 0 \) as denoted by dotted lines between its sites in Fig. 1(a), so that no electron can propagate across it. The Fermi energy of macroscopic reservoirs in equilibrium for both junctions in Fig. 1 is chosen as \( E_F = -1.6 \text{ eV} \).

The quantum dynamics of the electrons is described by solving a matrix integro-differential equation for time dependence of the nonequilibrium DM [27, 42, 43]

\[
\frac{i\hbar}{\partial t} \frac{d\rho_{\text{neq}}}{dt} = [\mathbf{H}, \rho_{\text{neq}}] + i \sum_{p=L,R} \left[ \mathbf{\Pi}_p(t) + \mathbf{\Pi}_p^\dagger(t) \right].
\]

This can be viewed as the exact master equation for an open finite-size quantum system, described by \( \hat{H} \) and its matrix representation \( \mathbf{H} \), that is attached (via semi-infinite NM leads) to macroscopic reservoirs. The matrices \( \rho_{\text{neq}} \) and \( \mathbf{\Pi}_p \) are expressed in terms of TD-NEGF's [31] and/or integrals over them, as elaborated in Refs. [42, 43]. The CD part of nonequilibrium electronic spin density [27, 38]

\[
\langle \hat{s}_i \rangle^{CD}(t) = \text{Tr} \left[ (\rho_{\text{neq}}(t) - \rho_{\text{eq}}) |i\rangle \langle i| \otimes \tilde{\mathbf{\sigma}} \right],
\]

appears in the classical Hamiltonian [Eq. (1)]. Therefore, it introduces ESTT on each LMM

\[
\mathbf{T}_i(t) = J_{sd} \langle \hat{s}_i \rangle^{CD}(t) \times \mathbf{M}_i(t),
\]

into the LLG Eq. (2) via \( \mathbf{B}_i^{\text{eff}} \). Here \( \rho_{\text{eq}} \) is the grand canonical equilibrium DM [27] for instantaneous con-
FIG. 4. Time dependence of three components of bond electronic spin current [Eq. (8)] between: (a)–(c) the last site of AFI and the first site of FM-analyzer denoted by $I^{A_{\alpha}}_{\text{AFI}ightarrow FM}(t)$ in Fig. 1(a), where dotted lines show the same spin current components injected into FM-analyzer after direct exchange coupling $J_{\text{AFI}ightarrow FM} = 0$ between AFI and FM-analyzer is set to zero; (e)–(g) the last site of NM interlayer and the first site of FM-analyzer denoted by $I^{A_{\alpha}}_{\text{NM}ightarrow AFI}(t)$ in Fig. 1(b). Panel (d) shows time dependence of bond spin current $I^{S_{\alpha}}_{\text{NM}ightarrow AFI}(t)$ impinging onto AFI and reflecting from its first LMM in the setup of Fig. 1(a), while panel (h) shows time dependence of charge current pulse injected from left NM lead by applying bias voltage square pulse of height $V_{\text{H}} = 0.25$ V and duration $V_{\text{D}} = 0.6$ ps in the setup of Fig. 1(b). The height $V_{\text{H}} = 0.55$ V and the duration $V_{\text{D}} = 1.0$ ps of bias voltage square pulse employed in panels (a)–(c) is the same as in Fig. 2(a).

figuration of $M_{i}(t)$ at time $t$, so that ‘adiabatic electronic spin density’ [44, 45] determined by it assumes $\partial M_{i}/\partial t = 0$ [subscript $t$ signifies parametric dependence on time through $M_{i}(t)$].

The $\Pi_{p}$ matrices in Eq. (4) yield the charge, $I_{p}(t) = \frac{\delta}{i\hbar} \text{Tr} [\Pi_{p}(t)]$, and the spin, $I^{S}_{p}(t) = \frac{\delta}{i\hbar} \text{Tr} [\hat{s}_{p} \Pi_{p}(t)]$, currents flowing into the NM lead $p = \text{L, R}$. The local (bond) charge current [46] between sites $i$ and $j$ is computed as [32]

$$I_{i\rightarrow j}(t) = \frac{e}{i\hbar} \text{Tr}_{\text{spin}} \left[ \gamma_{ji} \rho_{\text{CD}}^{ij}(t) - \gamma_{ij} \rho_{\text{CD}}^{ji}(t) \right].$$

(7)

and the local spin currents are given by

$$I^{S}_{i\rightarrow j}(t) = \frac{e}{i\hbar} \text{Tr}_{\text{spin}} \left[ \hat{s}_{\alpha} \left\{ \gamma_{\alpha ji} \rho_{\text{CD}}^{ij}(t) - \gamma_{\alpha ij} \rho_{\text{CD}}^{ji}(t) \right\} \right].$$

(8)

Here the CD part of the nonequilibrium DM is obtained as $\rho_{\text{CD}}^{ij}(t) = \rho_{\text{eq}}^{ij}(t) - \rho_{\text{eq}}^{ji}(t)$, and the trace is performed only in the spin factor space of total electronic Hilbert space $\mathcal{H} = \mathcal{H}_{\text{orbital}} \otimes \mathcal{H}_{\text{spin}}$. In our convention, positive value of any lead or bond current defined above means that charge or spin is flowing along the +$x$-axis.

In the TDNEGF+LLG framework [27–29], we first solve for $(\hat{s}_{ij})_{\text{CD}}(t)$ using Eqs. (4) and (5), which is then fed into Eq. (2) to propagate LMMs $M_{i}(t)$ in the next time step. These updated $M_{i}(t)$ classical vectors are then fed back into the quantum Hamiltonian of the conduction electron subsystem in Eq. (3) and DM in Eq. (4) is updated. The active region in Fig. 1 is disconnected from the NM leads at $t = 0$; then we connect them through time evolution over a period of 1 ps during which $\rho_{\text{eq}}(t) \rightarrow \rho_{\text{eq}}^{0}$, so that all transient currents die out by $t_{0} = 1$ ps; finally at $t_{0} = 1$ ps, for all junctions in Figs. 2–7 and Videos 1–3, square voltage pulses of various durations $V_{D}$ and heights $V_{H}$ are applied to drive them out of equilibrium. The time step $\delta t = 0.1$ fs is used for numerical stability of TDNEGF calculations, as well as in LLG calculations, and recently developed TDNEGF algorithms scaling linearly [32, 43] in the number of time steps are employed to reach $\sim$ ps or $\sim$ ns time scales. Thus obtained time-dependences of $M_{i}(t)$, $(\hat{s}_{ij})_{\text{CD}}(t)$, $T_{i}(t)$, $I_{p}(t)$, $I^{S}_{\alpha}(t)$, $I_{i\rightarrow j}(t)$ and $I^{S}_{i\rightarrow j}(t)$ are numerically exact.

III. RESULTS AND DISCUSSION

A. Electronic spin currents and LMM dynamics in FM-polarizer/NM/FM-analyzer spin valve

As a warm-up, we first consider conventional ESTT in a standard FM-polarizer/NM/FM-analyzer spin valve setup employed in seminal spin torque experiments [19, 20], as well as in the early development [21, 22] of steady-state quantum transport theories of ESTT. Although we use 1D chain to model the spin valve in Fig. 1(b), this can be easily converted into a three-dimensional (3D) junction with macroscopic cross section by assuming that chain is periodically repeated in the $y$- and $z$-directions and $k$-point sampled [47]. This means that our TDNEGF calculations would have to be repeated at each $(k_{y}, k_{z})$ point [22]. When $(\hat{s}_{ij})_{\text{CD}}$ and $M_{i}$ of FM-analyzer...
are noncollinear, $\langle \hat{s}_i \rangle^{CD}$ due to propagating states and the corresponding ESTT $\propto \langle \hat{s}_i \rangle^{CD} \times \mathbf{M}_i$ oscillate [22] within the FM-analyzer of such 3D junction as a function of position and without decaying [21, 22]. Nevertheless, the transverse (with respect to $\mathbf{M}_i$) component of $\langle \hat{s}_i \rangle^{CD}$ is brought to zero (typically within $\sim 1$ nm in realistic materials like Co or Ni [22]) away from the normal-metal/FM-analyzer interface by averaging over all incoming propagating states with different transverse wavevectors $(k_y, k_z)$. This is due to the fact that frequency of spatial oscillations rapidly changes for different $(k_y, k_z)$ [21, 22]. The ESTT can also have smaller contribution from evanescent states, which decays exponentially in space when moving away from the NM/FM-analyzer interface [21, 22].

Even though we effectively use only the $\Gamma$-point $(k_y, k_z) = (0, 0)$ due to computational complexity of TDNEGF calculations, Fig. 2(b) showing $\mathbf{M}_i(t)$ and accompanying Video 1 animating complete time evolution of all $\mathbf{M}_i(t)$ demonstrate that ESTT is deposited within FM-analyzer in Fig. 1(b) to fully reverse all of its LMMs from positive to negative $z$-axis on the time scale comparable to voltage pulse duration $V_D$. In widely-used classical micromagnetics [33] ESTT has to be introduced as phenomenological term. More sophisticated steady-state-NEGF+LLG simulations [37, 38] compute ESTT microscopically from steady-state (i.e., time-independent) quantum transport calculations, but they consider time as parameter rather than dynamical variable so that noncommutativity of electronic Hamiltonian at different times is lost. In contrast to this plausible approach, we can extract rigorously time dependence of standard [17] field-like (FL) and damping-like (DL) components of ESTT

$$\mathbf{T}_i(t) = T_i^{FL}(t)\mathbf{M}_i(t) \times \hat{x} + T_i^{DL}(t)\mathbf{M}_i(t) \times [\mathbf{M}_i(t) \times \hat{x}],$$

from TDNEGF calculations. They are shown on the first and the last LMMs of FM-analyzer in Figs. 3(a) and 3(b), respectively.

It is also insightful to compare time-dependence of ESTT from TDNEGF+LLG calculations in Figs. 3(b) to ‘time-dependence’ from steady-state-NEGFL+LLG [37, 38] calculations in Fig. 3(d)—this reveals incorrect magnitude of torque and/or its sign in the latter case. Furthermore, there is a qualitative difference since steady-state-NEGF+LLG simulations predict incorrectly no reversal of LMMs of FM-analyzer in Fig. 3(c), in contrast to TDNEGF+LLG simulations in Fig. 2(b). The discrepancy stems from the fact that steady-state-NEGF+LLG approach assumes electrons responding instantaneously to time-dependent potential introduced by $\mathbf{M}_i(t)$. Technically, this means that only the lowest (adiabatic) term of the full nonadiabatic expansion of TDNEGF [28, 48, 49] is included in steady-state-NEGF+LLG approach. This discrepancy demonstrates the importance of taking into account back-action [28, 45, 50–53] of conduction electrons onto LMMs, as electrons are driven out of equilibrium both by the voltage pulse and the dynamics of $\mathbf{M}_i(t)$.

The time-dependence of injected unpolarized charge current pulse in the left NM lead $I_L(t)$ is shown in Fig. 4(h), while three components of bond spin current $I_{NM\rightarrow FM}^S(t)$ impinging on the FM-analyzer to generate ESTT [Fig. 3] on its LMMs are plotted in Fig. 4(e)–(g). Besides expected $I_{NM\rightarrow FM}^S(t) \neq 0$ [Fig. 4(e)] component due to FM-polarizer with all of its LMMs pointing along the $x$-axis, there are also an order of magnitude
smaller $I_{NM\rightarrow FM}^{S_y}(t) \neq 0$ [Fig. 4(f)] and $I_{NM\rightarrow FM}^{S_z}(t) \neq 0$ [Fig. 4(g)]. This is attributed to electronic spin reflection and rotation at the NM/FM-analyzer interface, so that bond spin current $I_{NM\rightarrow FM}^{S_y}(t)$ is superposition of incoming current whose spins are polarized by FM-polarizer along the $x$-axis and reflected spin currents polarized in the other two directions. This explanation is confirmed by noticing that $I_{NM\rightarrow FM}^{S_y}(t)$ [Fig. 4(f)] and $I_{NM\rightarrow FM}^{S_z}(t)$ [Fig. 4(g)] turning negative in the course of their time evolution means that those currents flow backward toward the left NM lead in our convention for the sign of bond current.

B. Magnonic and electronic spin currents and LMM dynamics in FM-polarizer/AFI/FM-analyzer junction

When unpolarized charge current pulse is injected from the left NM into FM-polarizer/AFI/FM-analyzer junction in Fig. 1(a), it gets spin-polarized along the $x$-axis and is subsequently fully reflected by AFI layer because of zero hopping ($\gamma_{ij} \equiv 0$) between its sites. In this process, the other two components of bond spin current, $I_{NM\rightarrow AFI}^{S_y}(t) \neq 0$ and $I_{NM\rightarrow AFI}^{S_z}(t) \neq 0$, emerge in Fig. 4(d). Due to back and forth reflection between AFI and FM-polarizer, they will change direction in oscillatory fashion which is the meaning of sign change of $I_{NM\rightarrow AFI}^{S_y}(t)$ shown in Fig. 4(d).

Note that in the experiment of Ref. [24], the unpolarized charge current pulse is injected parallel to the TI/AFI interface and polarized by the TI metallic surface [54] to have the largest component of nonequilibrium electronic spin density vector lying in the plane of the interface. Thus, features in Fig. 4(d), where charge current pulse is injected perpendicular to NM/AFI interface, would not be directly pertinent to the experiment. Nevertheless, in both cases nonequilibrium electronic spin density ($\delta(S_{AFI})_{CD}(t)$) [Eq. (5)] plotted in Fig. 5(a) is non-collinear to the first LMM of AFI, denoted by $\mathbf{M}_{1,AFI}(t)$, which then leads to ESTT on it. The time dependence of standard [17] FL and DL components of ESTT acting on the first LMM of AFI is shown in Fig. 5(b). The ESTT-driven dynamics of $\mathbf{M}_{1,AFI}(t)$ then generates SW within AFI because of the exchange coupling between its LMMs [encoded by the first term on the right-hand side of Eq. (1)]. This picture is also confirmed by Videos 2 and 3 which animate $\mathbf{M}_{1}(t)$ for all 20 LMMs of the AFI layer.

When SW reaches the last LMM of AFI layer, it will initiate its dynamics. Since TB site of this last LMM of AFI layer is connected directly by nonzero hopping to TB site of LMM 1 within the FM-analyzer, as well as via $J_{sd} \neq 0$ to electronic spins within the FM-analyzer, its dynamics will pump electronic spin current [18, 56–58] into the FM-analyzer (as well as charge current because the left-right symmetry of the device is broken [58–60]). The time-dependence of pumped bond spin current $I_{AFI\rightarrow FM}^{S_y}(t)$ between the last LMM of AFI layer and the first LMM of the FM-analyzer is plotted in Fig. 4(a)–(c) and animated in Videos 2 and 3. Additionally, Videos 2 and 3 show pumped spin current $I_{R}^{S_y}(t)$ outflowing into the right NM lead. Recall that all of $I_{AFI\rightarrow FM}^{S_y}(t)$ and $I_{R}^{S_y}(t)$ must be generated by spin pumping because none of the originally injected spin-polarized current pulse can pass through the AFI layer. In the absence of spin-flips, due to spin-orbit coupling in the band structure or spin-orbit and/or magnetic impurities [61], the sum of $\mathbf{T}_i$ [Eq. (6)] on each LMM is equal to absorbed spin current within the FM-analyzer [21, 22]

\[
\sum_i \mathbf{T}_i(t) = \frac{\hbar}{2e} \left[ I_{AFI\rightarrow FM}^{S_y}(t) - I_{R}^{S_y}(t) \right],
\]

at each instant of time $t$.

When direct exchange coupling between AFI and FM-analyzer is absent, $J_{AFI\rightarrow FM} = 0$, spin current $I_{AFI\rightarrow FM}^{S_y}(t)$ can also be viewed as the result of transmutation [16, 26] of magnonic spin-current into solely electronic spin current within the FM-analyzer layer via spin pumping by the last LMM of AFI layer. Such electronic spin current, plotted by dotted line in Fig. 4(a)–(c), turns out to be insufficient to reverse LMMs of FM-analyzer, as
visualized by Video 3. According to Eq. (10), this means that insufficient spin angular momentum is transferred to LMMs of the FM-analyzer.

The importance of \( J_{\text{AFI-FM}} \neq 0 \) in Fig. 2(a) and Video 2 for complete reversal of all LMMs within the FM-analyzer motivates us to further examine SW transmission into the FM-analyzer and thereby induce MSTT. The SW transmitted from AFI layer to FM-analyzer enhances injected electronic spin current \( I_{\text{AFI-FM}} (t) \) [solid lines in Fig. 4(a)–(c)] by SW-generated spin pumping [16]. This then leads to larger ESTT on LMMs of the FM-analyzer in Figs. 6(a) and 6(c) than for the case when \( J_{\text{AFI-FM}} = 0 \) in Figs. 6(b) and 6(d). Nonetheless, we see that ESTT in Fig. 6 due to pumped electronic spin current from AFI is an order of magnitude smaller than ESTT in spin valve in Fig. 3 where electronic spin current pulse is directly injected from FM-polarizer into FM-analyzer.

Since SW transmitted into FM-analyzer carries its own magnonic spin current, defined for continuous local magnetization \( \mathbf{M}(x,t) \) as [1]

\[
j^{\text{SW}} \propto \mathbf{M} \times \frac{\partial \mathbf{M}}{\partial x}, \quad (11)
\]

this means that both MSTT and ESTT act on LMMs of FM-analyzer in Fig. 2(a) and Video 2. In order to separate their individual contributions to total spin-transfer torque, we artificially turn off ESTT [Eq. (6)] by setting \( J_{sd} = 0 \) within the FM-analyzer in Fig. 2(c). This reveals that LMMs still reverse, on slightly longer time scale [Fig. 2(c)], thereby confirming that MSTT is the dominant mechanism of magnetization switching in FM-polarizer/AFI/FM-analyzer junction.

At first sight, this finding, together with Video 3 explicitly showing inability of ESTT alone to reverse LMMs of FM-analyzer via magnonic-to-electronic spin current conversion at AFI/FM-analyzer interface when \( J_{\text{AFI-FM}} = 0 \), differs from experimental conclusion [24]. In the experiment [24], torque from AFI layer to FM-analyzer is slightly impeded by inserting 6 nm of Cu in between them, which certainly suppresses direct exchange coupling \( J_{\text{AFI-FM}} = 0 \) that is operative on \( \sim 0.1 \) nm length scale. However, to obtain switching of the magnetization of FM-analyzer with Cu layer inserted, the current density of injected pulse also had to be increased in the experiment (see Fig. 4 in Ref. [24]), which is compatible with our finding.

The MSTT is driven by magnonic spin currents, which are visualized in Fig. 7 by plotting time dependence of bond magnonic spin current [62]

\[
(I^{\text{SW},S_x}_{ij}, I^{\text{SW},S_y}_{ij}, I^{\text{SW},S_z}_{ij}) = J_{ij} \mathbf{M}_i \times \mathbf{M}_j, \quad (12)
\]

that can also be viewed as the discretized version of Eq. (11). This is plotted between sites \( i \) and \( j \), which are either last two sites of the AFI layer [Figs. 7(a) and 7(c)] or first two sites of the FM-analyzer [Figs. 7(b) and 7(d)], so that \( J_{ij} \equiv J_{\text{AFI}} \) or \( J_{ij} \equiv J_{\text{FM}} \), respectively. When \( J_{sd} = 0 \) is turned off within the FM-analyzer, bond magnonic spin current within the FM-analyzer decays on longer time scale in Figs. 7(c) and 7(d) because of the elimination of a damping channel [18, 28, 50] via conduction electrons that are otherwise (i.e., when \( J_{sd} \neq 0 \)) driven out of equilibrium by SW dynamics of LMMs. Note that in Figs. 7(c) and 7(d) we keep \( J_{sd} \neq 0 \) between the last LMM of AFI and electrons on the right side of it. So, its dynamics pumps the same electronic spin current as in Figs. 7(a) and 7(b), but such current does not interact with LMMs of the FM-analyzer.

The MSTT alone in Fig. 2(c) or combined MSTT and ESTT in Fig. 2(a) show that they are less efficient, in the sense of requiring larger pulse height and its longer duration, than conventional ESTT-driven LMM switching [Fig. 2(b)] in standard FM-polarizer/normal-metal/FM-analyzer spin valves. This is not surprising in the sense that the same electronic current pulse injected from the left NM lead and spin-polarized by FM-polarizer layer in both setups in Fig. 1 will encounter more interfaces in Fig. 1(a) at which it is reflected and/or converted into magnonic current pulse. Both of these processes lead to reduced net spin angular momentum that can be deposited into the FM-analyzer via spin-transfer torque. Nevertheless, although FM-polarizer/AFI/FM-analyzer junction [Fig. 1(a)] is not efficient for applications (as is the case also of \( \text{Bi}_2\text{Se}_3/\text{NiO/Py} \) heterostructure in experiment of Ref. [24]), it offers a setting to controlably study properties of MSTT and how to optimize it toward all-magnon devices.

IV. CONCLUSIONS

In conclusion, using quantum-classical simulations based on recently developed TDNEGF+LLG framework [27–30], we evolve quantum orbital and spin degrees of freedom of electrons comprising injected unpolarized charge current square pulse and classical LMMs. This provides microscopic understanding of how MSTT and ESTT processes are initiated by magnonic and electronic spin currents, respectively, while these currents interconvert at different interfaces of FM-polarizer/AFI/FM-analyzer setup inspired by very recent experiment [24]. To assist such understanding, we provide Videos 2 and 3 revealing how electronic spin current, after spin-polarization by the FM-polarizer in Fig. 1(a), is reflected at the FM-polarizer/AFI interface to ignite magnonic spin current across the AFI layer since no electrons can move through it. Upon reaching the opposite edge of AFI layer, magnonic spin current initiates pumping of electronic spin current into the FM-analyzer by the dynamics of edge LMMs of AFI, while concurrently transmitting into the FM-analyzer if direct exchange coupling is present between the LMMs of AFI and FM-analyzer. This means that, in general, FM-analyzer receives combined MSTT and ESTT which can completely reverse the direction of all of its LMMs. Akin to exper-
ments (see Fig. 3C in Ref. [24]), switching by ESTT alone in FM-polarizer/NM/FM-analyzer setup with AFM layer removed is still more efficient, by requiring shorter voltage pulses of lower height [Fig. 2], than combined MSTT and ESTT in FM-polarizer/AFI/FM-analyzer setup. By artificially turning off ESTT [Fig. 2(c)], we demonstrate that MSTT, due to magnonic spin current flowing directly from AFM to FM-analyzer, is actually the dominant mechanism of LMMs reversal within the FM-analyzer. Despite smaller efficiency, MSTT in FM-polarizer/AFI/FM-analyzer junction offers a playground for detailed theoretical understanding of necessary vs. unnecessary phenomena for the development of all-magnon-driven magnetization switching without involving any electronic parts. Finally, we also use conventional spin valve setup to demonstrate that popular steady-state-NEGF+LLG approach [37, 38], which neglects noncommutativity of electronic Hamiltonians at different times and it can be viewed as the lowest (i.e., adiabatic) approximation to full TDNEGF+LLG approach, gives wrong magnitude of ESTT while not being able to reproduce magnetization switching of FM-analyzer found in TDNEGF+LLG approach.

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