Wide ferromagnetic domain walls can host both adiabatic reflectionless spin transport and finite nonadiabatic spin torque: A time-dependent quantum transport picture

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The key concept in spintronics of current-driven noncollinear magnetic textures, such as magnetic domain walls (DWs), is adiabaticity, i.e., how closely electronic spins track classical localized magnetic moments (LMMs) of the texture. When mistracking occurs nonadiabatic effects arise, the salient of which is nonadiabatic spin transfer torque (STT) where spin angular momentum is exchanged between electrons and LMMs to cause their dynamics and enable DW motion without any current threshold. The microscopic mechanisms behind nonadiabatic STT have been debated theoretically for nearly two decades, but with unanimous conclusion that they should be significant only in narrow DWs. However, this contradicts sharply experiments [O. Boulle et al., Phys. Rev. Lett. \textbf{101}, 216601 (2008); C. Burrows et al., Nat. Phys. \textbf{6}, 17 (2010)] observing nonadiabatic STT in DWs much wider than putatively relevant $\sim 1$ nm scale, as well as largely insensitive to further increasing the DW width $w$. Here we employ time-dependent quantum transport for electrons, combined self-consistently with the Landau-Lifshitz-Gilbert (LLG) equation for LMMs, to obtain both nonadiabatic and adiabatic STT from the exact nonequilibrium density matrix and its lowest order as adiabatic density matrix defined by assuming that LMMs are infinitely slow. This allows us to demonstrate that our microscopically, and without any simplifications of prior derivations like effectively static DW, extracted nonadiabatic STT: (i) does not decay, but instead saturates at a finite value, with increasing $w$ of a moving DW ensuring entry into the adiabatic limit, which we characterize by showing that electronic spins do not reflect from the static DW in this limit; and (ii) it has both out-of-DW-plane, as is the case of phenomenological expression widely used in the LLG equation, and in-plane components, where the former remains finite with increasing $w$.

Introduction.—One of the key concept in electronic spin transport through noncollinear static or dynamic (i.e., time-dependent) magnetic textures—such as magnetic domain walls (DWs) [1–4], skyrmions [5] and vortex cores [6, 7]—is that of adiabaticity [2, 8–14]. For example, within a ferromagnetic nanostructure, DW is a transition region that separates two different but uniformly magnetized regions, as illustrated in Fig. 1. Moving DWs with charge currents [15], instead of external magnetic fields, is a topic of both great fundamental interest [1, 2] for nonequilibrium quantum many-body physics and applications of DWs for digital memory [16] and logic [17] or neuromorphic computing [18].

The DWs in nanowires of conventional 3d metallic ferromagnets (Fe, Ni, Co) can be thick (i.e., of width $w \sim 100$ nm) and $sd$ exchange interaction $J_{sd}$ between the spin of conduction electrons and localized spins is strong [19], so that intuitive picture [2, 8, 11] is the one in which electronic spin tracks spatially noncollinear magnetic textures while traversing DW. In clean magnetic wires, the condition [2, 10, 20] for such adiabatic limit is

$$J_{sd}wS/\hbar v_F \gg 1. \quad (1)$$

This “adiabaticity parameter” is defined as the ratio of two time scales—$w/v_F$, needed for electron to traverse the DW of width $w$ with Fermi velocity $v_F$, and $h/J_{sd}S$ governing electron spin rotation within the DW (composed of localized spins $S$) by $sd$ exchange interaction. This criterion can be generalized [21] to $J_{sd}w^2/hD \gg 1$ for diffusive electronic transport ($D$ is the diffusion constant). Since $J_{sd}$ (typically measured as $\sim 0.1$ eV [19]), $v_F$ and $D$ are fixed by materials properties, increasing $w$ can satisfy either of these two conditions to explain how wide DW allows electron to pass through it without reflection [2] and, therefore, with vanishing electrical resistance of DW.

In spintronic experiments and applications, any deviation from adiabaticity of electron spin dynamics leads to fundamental effects, such as finite DW resistance [2, 8, 22–27] and particularly important nonadiabatic [9, 28] spin-transfer torque (STT) in electronic transport through DWs [3, 4, skyrmions [5] and vortex cores [6, 7]. The STT is a phenomenon [29] in which flowing electrons transfer spin angular momentum to local magnetization $\mathbf{M}(\mathbf{r})$ viewed as classical vector, as long as nonequilibrium spin expectation value of an electron and $\mathbf{M}(\mathbf{r})$ are noncollinear, as illustrated in Fig. 1. Spintronic experiments on current-driven dynamics of noncollinear textures are standardly interpreted [3, 4, 6, 7] using the Landau-Lifshitz-Gilbert (LLG) equation

$$\partial_t \mathbf{M} = -g_0 \mathbf{M} \times \mathbf{B}_{\text{eff}} + \frac{\lambda}{g_0} \mathbf{M} \times \left(\nabla \times \frac{\partial_t \mathbf{M}}{g_0} \right) - \left(\mathbf{u} \cdot \nabla\right)\mathbf{M} + \beta \mathbf{M} \times \left(\mathbf{u} \cdot \nabla\right)\mathbf{M}, \quad (2)$$

extended to include adiabatic [30–32] and nonadiabatic [9, 28, 33] STT terms. Here we use shorthand notation $\partial_t = \partial/\partial t$; $g_0$ is gyromagnetic factor [34]; $\mathbf{B}_{\text{eff}}$ is the effective magnetic field; $\lambda$ is dimensionless Gilbert damp-
being of the order of $\sim$ wavelength, Larmor precession or the mean free path, transport scale $\ell$ for relevant transport scale $\ell$.

The DW width $w$ is discussed in terms of its own gradient in Eq. (34) in Ref. [14], unlike the one in Eq. (2) which has only $[2, 9, 36]$ out-of-DW-plane (assuming Néel DW) component. Nevertheless, both standard nonadiabatic STT and modified form of Ref. [14] decay (such as, $\propto w^{-1}e^{-cw/t}$ in Ref. [14] or $\propto 1/w$ in Ref. [20]) as the DW width $w$ increases due to diminishing magnetization gradient in $(\mathbf{u} \cdot \nabla)\mathbf{M}$. Thus, unless $w$ is comparable to relevant transport scale $\ell$ as set by the Fermi wavelength, Larmor precession or the mean free path, being of the order of $\sim 1$ nm in transition ferromagnetic metals (FM)—nonadiabatic STT is negligible. In sharp contrast, variety of experimental techniques developed to directly measure $\beta$ have observed large nonadiabatic STT in DW of much larger width $w \sim 10$ nm [3, 4, 6]. This suggests that widely used nonadiabatic STT term in Eq. (2) does not fully capture all relevant nonadiabatic effects in electronic spin transport through noncollinear magnetic textures.

In this Letter, we employ numerically exact and fully microscopic (i.e., requiring only quantum Hamiltonian of electrons and classical Hamiltonian of LMMs) time-dependent quantum transport (QT) formalism [43–48] to resolve this issue. This is achieved by splitting the exact nonequilibrium density matrix [45, 47, 48] of time-dependent QT into two terms to rigorously define adiabatic and nonadiabatic STT, whose properties are then studied as a function of DW width $w$. Our principal results in Figs. 3 and 4 show that thus defined nonadiabatic STT becomes insensitive to increasing $w$, once putative adiabatic limit is reached as signified [2] by electronic spins ceasing to reflect from DW [Fig. 2(b)]. Thus, our predictions are in full accord with apparently highly accurate quantum-mechanical calculations [33, 35, 38, 39], going beyond early phenomenological analysis [9, 28], have focused on computing the dimensionless $\beta$-term [40, 41]. The understanding of conditions for nonzero $\beta$-term is crucial for anticipated DW motion-based technologies because nonadiabatic STT makes possible current-driven DW motion at any finite current and in the absence of externally applied magnetic field.

In particular, microscopic quantum-mechanical calculations [33, 35, 38, 39], going beyond early phenomenological analysis [9, 28], have focused on computing the dimensionless $\beta$-term while not questioning the form of nonadiabatic STT in Eq. (2). An exception is Ref. [14] where different form has been proposed, with both in-plane and out-of-plane components of nonadiabatic STT (see Eq. (34) in Ref. [14]), unlike the one in Eq. (2) which has only $[2, 9, 36]$ out-of-DW-plane (assuming Néel DW) component. Nevertheless, both standard nonadiabatic STT and modified form of Ref. [14] decay (such as, $\propto w^{-1}e^{-cw/t}$ in Ref. [14] or $\propto 1/w$ in Ref. [20]) as the DW width $w$ increases due to diminishing magnetization gradient in $(\mathbf{u} \cdot \nabla)\mathbf{M}$. Thus, unless $w$ is comparable to relevant transport scale $\ell$ as set by the Fermi wavelength, Larmor precession or the mean free path, being of the order of $\sim 1$ nm in transition ferromagnetic metals (FM)—nonadiabatic STT is negligible. In sharp contrast, variety of experimental techniques developed to directly measure $\beta$ have observed large nonadiabatic STT in DW of much larger width $w \sim 10$ nm [3, 4, 6]. This suggests that widely used nonadiabatic STT term in Eq. (2) does not fully capture all relevant nonadiabatic effects in electronic spin transport through noncollinear magnetic textures.

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FIG. 1. Schematic view of FM nanowire of $N = 40$ sites hosting a DW and sandwiched between two semi-infinite NM leads. Bias voltage $V_b(t)$ is turned on at $t = 0$ to inject unpolarized charge current from the left NM lead. Light red arrows illustrate orientation of unit vectors $\mathbf{M}_i$ of classical LMMs comprising two domains and DW in between; gray and cyan arrows illustrate adiabatic ($\langle \hat{s}_i \rangle_{t=0}^{\text{ad}}$ [Eq. (4)]) and nonequilibrium ($\langle \hat{s}_i \rangle_{t=\alpha}^{\text{neq}}$ [Eq. (5)]) expectation values of electron spin, respectively. These three vectors are in general noncollinear, so that cross products of spin expectation values with $\langle \mathbf{P} \rangle_{t=\alpha}^{\text{neq}}$ in Ref. [14] or $\langle \mathbf{P} \rangle_{t=\alpha}^{\text{ad}}$ (see Eq. (34) in Ref. [14]), unlike the one in Eq. (2) which has only $[2, 9, 36]$ out-of-DW-plane (assuming Néel DW) component. Nevertheless, both standard nonadiabatic STT and modified form of Ref. [14] decay (such as, $\propto w^{-1}e^{-cw/t}$ in Ref. [14] or $\propto 1/w$ in Ref. [20]) as the DW width $w$ increases due to diminishing magnetization gradient in $(\mathbf{u} \cdot \nabla)\mathbf{M}$. Thus, unless $w$ is comparable to relevant transport scale $\ell$ as set by the Fermi wavelength, Larmor precession or the mean free path, being of the order of $\sim 1$ nm in transition ferromagnetic metals (FM)—nonadiabatic STT is negligible. In sharp contrast, variety of experimental techniques developed to directly measure $\beta$ have observed large nonadiabatic STT in DW of much larger width $w \sim 10$ nm [3, 4, 6]. This suggests that widely used nonadiabatic STT term in Eq. (2) does not fully capture all relevant nonadiabatic effects in electronic spin transport through noncollinear magnetic textures.

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can be computed as the expectation value
\[ \langle s_i \rangle_t = \langle \Psi_0(t) | s_i \rangle_{\Psi_0(t)} \]

in the instantaneous ground state \[ \Psi_0 \] of the Hamiltonian \[ \hat{H} \] for
configuration of LMMs at time \[ t \], \[ \Psi(t) = \Psi_0 \hat{M}_i(t) \]. Here
we switch the notation from \[ \hat{M}_i \] to unit vectors \[ M_i \] describing
LMMs on the sites of a discrete lattice in Fig. 1, hosting both them and localized electronic orbitals \[ |i\rangle \]. In an open quantum system, such as the one in Fig. 1, we need adiabatic \[ [45, 51, 52] \] density matrix \[ \rho_{ad} \] to express

surprising experimental observations \cite{3, 4, 6, 7}. Prior
to delving into these results, we first introduce rigorous
definitions of adiabatic and nonadiabatic electronic spin
expectation values—also visualized in Figs. 1, 2(c) and
2(d)—and the corresponding STTs, as well as our models
and time-dependent QT methodology.

**Defining adiabatic and nonadiabatic STT rigorously from time-dependent QT.**—The intuitive picture
(see, e.g., Figs. 14 and 19 in Ref. \cite{2} or Fig. 4 in Ref. \cite{11})
of how spin of injected conduction electron propagates
through a magnetic DW is commonly built around the
idea that in the adiabatic limit expectation value of
electron spin will be parallel to local magnetization. This
is also a usual starting point of phenomenological calcu-
lations of nonadiabatic STT where one assumes that
nonequilibrium electronic spin density can be split as
\[ \langle s(r) \rangle_{\text{neq}}(t) = \langle s(r) \rangle_{\text{ad}}(t) + \delta \langle s(r) \rangle(t) \]

(see, e.g., Eq. (5) in Ref. \cite{9}). Here \[ \langle s(r) \rangle_{\text{ad}}(t) \parallel \hat{M}(r) \] is assumed \cite{9} to
point along \[ \hat{M}(r) \] and represents adiabatic spin density
due to electronic spin relaxing to its *equilibrium* value at
an instantaneous time \[ t \]; and \[ \delta \langle s(r) \rangle(t) \] is nonadiabatic
correction.

However, in spintronics \cite{12}, Berry phase \cite{13, 49}
and noncollinear density functional theory \cite{50} li-
terature it has been already noticed that electronic
spin *never* \cite{2(c) and 2(d)} simply aligns with
\[ \hat{M}(r) \]. Instead, \[ \langle s(r) \rangle_{\text{ad}}(t) \] tends to align perfectly
with another effective \cite{13} local magnetization
\[ \hat{M}_{\text{eff}}(x) = \hat{M}(x) + Q(x) \hat{M}(x)/dx \times \hat{M}(x) \]
where \[ Q \] is a function of electron velocity \cite{14} and we assume
sufficiently slowly varying \[ \hat{M}(x) \] along the \[ x \]-axis (as perti-
ent to Fig. 1). This also means that the natural basis for
an electron spin moving through a noncollinear magnetic
texture is not along the local magnetization \[ \hat{M}(x) \], as of-
ten assumed \cite{2, 8, 9}, but rather along \[ \hat{M}_{\text{eff}}(x) \]. Thus,
even in equilibrium \cite{50}, or in nonequilibrium but per in-
fectly adiabatic \cite{45, 49} limit, there is nonzero \cite{45, 49, 50}
local torque \[ \langle s(r) \rangle_{\text{ad}}(t) \times \hat{M}(r, t) \neq 0 \].

Since “adiabatic” means that electron spin remains
in the the lowest energy state at each time, in
closed quantum systems \cite{49} adiabatic spin density
at time \[ t \] can be computed as the expectation value
\[ \langle s_i \rangle_{\text{ad}} = \langle \Psi_0(t) | s_i \rangle_{\Psi_0(t)} \]

in the instantaneous ground state \[ \Psi_0 \] of the Hamiltonian \[ \hat{H} \] for
configuration of LMMs at time \[ t \], \[ \Psi(t) = \Psi_0 \hat{M}_i(t) \]. Here
we switch the notation from \[ \hat{M}_i \] to unit vectors \[ M_i \] describing
LMMs on the sites of a discrete lattice in Fig. 1,
\begin{align}
\langle \hat{s}_{t}\rangle_{t}^{\text{ad}} &= -\frac{1}{\pi} \int dE \text{Im} G_{f}(E), \tag{3} \\
\langle \hat{s}_{t}\rangle_{t}^{\text{ad}} &= \text{Tr} \left[ \rho_{t}^{\text{ad}} |i\rangle \langle i| \otimes \hat{\sigma} \right]. \tag{4}
\end{align}

Here $G_{f} = \left[ E - \hat{H} |M_{i}(t)\rangle - \Sigma_{L} - \Sigma_{R} \right]^{-1}$ is the retarded Green’s function (GF); $\Sigma_{L,R}$ are self-energies due to the left ($L$) and right ($R$) NM leads; and $\text{Im} G_{f} = \left( G_{f} - G_{f}^{\dagger} \right)/2i$. Such $\rho_{t}^{\text{ad}}$ is grand canonical equilibrium density matrix, but depending parametrically \cite{51–53} (or implicitly, so we put $t$ in the subscript) on time via instantaneous configuration of $M_{i}(t)$, thereby effectively assuming $\partial_{t}M_{i}(t) = 0$.

The nonadiabatic corrections take into account $\partial_{t}M_{i}(t) \neq 0$, so that $\rho_{t}^{\text{ad}}$ can be viewed as the lowest order term \cite{45, 51, 52} of nonequilibrium density matrix $\rho_{t}^{\text{neq}}(t)$ expanded \cite{53} in powers of small $\partial_{t}M_{i}(t)$. We compute $\rho_{t}^{\text{neq}}(t) = \hbar G^{<}(t,t)/i$ exactly in terms of the lesser Green’s function of time-dependent nonequilibrium GF (TDNEGF) formalism \cite{47, 54}, which makes it possible to obtain nonadiabatic spin density $\delta\langle \hat{s}_{i}\rangle(t)$ and the corresponding nonadiabatic STT as

\begin{align}
\delta\langle \hat{s}_{i}\rangle(t) &= \langle \hat{s}_{i}\rangle_{t}^{\text{neq}}(t) - \langle \hat{s}_{i}\rangle_{t}^{\text{ad}} \\
&= \text{Tr} \left[ \left( \rho_{t}^{\text{neq}}(t) - \rho_{t}^{\text{ad}}(t) \right) |i\rangle \langle i| \otimes \hat{\sigma} \right]. \tag{5}
\end{align}

The total STT acting on DW is then given by

\begin{align}
T_{i}^{\text{ad}}(t) &= J_{sd} \langle \hat{s}_{i}\rangle_{t}^{\text{ad}} \times M_{i}(t). \tag{7}
\end{align}

The Models and methods.—The LMMs hosted by FM nanowire in Fig. 1 are described by a classical Hamiltonian

$$\mathcal{H} = -J \sum_{ij} M_{i} \cdot M_{j} - K \sum_{i} (M_{i}^{z})^{2} + D \sum_{i} (M_{i}^{y})^{2},$$

where $J = 0.1 \text{ eV}$ is the Heisenberg exchange coupling between the nearest-neighbor (NN) LMMs; $K = a^{2}J/w^{2}$ is magnetic anisotropy along the $z$-axis; and $D = 0.03 \text{ meV}$ is demagnetization field. The spatial profile of a Néel DW in equilibrium, or in the presence of injected current but kept static as in Figs. 2, 4(c) and 4(d), is given by $M_{i} = \left( \text{sech}[(X_{DW} - i)/w], 0, \tanh[(X_{DW} - i)/w] \right)$, where $X_{DW}$ is the center of the DW.

The same sites also host conduction electrons described by a quantum tight-binding Hamiltonian

$$\hat{H}(t) = -\gamma \sum_{(ij)} \epsilon_{j}^{\dagger} \hat{c}_{j} - J_{sd} \sum_{(ij)} \epsilon_{j}^{\dagger} \hat{\sigma} \cdot M_{i}(t) \hat{c}_{i},$$

where $\epsilon_{j}^{\dagger} = (\epsilon_{j}^{\uparrow}, \epsilon_{j}^{\downarrow})$ is a row vector containing operators $\hat{c}_{i}^{\dagger}$ which create an electron of spin $\sigma = \uparrow, \downarrow$ at the site $i$; $\hat{c}_{i}$ is a column vector that contains the corresponding annihilation operators; $\gamma = 1 \text{ eV}$ is the NN hopping; and $J_{sd} = 0.1 \text{ eV}$ \cite{19}. The FM nanowire is attached to semi-infinite NM leads, modeled by the first term alone in $\hat{H}(t)$ \cite{Eq. (10)], which terminate into macroscopic reservoirs at infinity. The Fermi energy of the reservoirs is set at $E_{F} = 0 \text{ eV}$ in Fig. 2 or $E_{F} = -1.95 \text{ eV}$ in Figs. 3 and 4.

The time dependence of $M_{i}(t)$ entering into $\hat{H}(t)$ is obtained by solving a system of LLG equations \cite{34}

$$\partial_{t}M_{i} = -g_{0} \frac{\partial \mathcal{H}}{\partial M_{i}} + \lambda M_{i} \times \partial_{t}M_{i}$$

$$+ \frac{g_{0}}{\mu_{M}} (T_{i}^{\text{sd}} + T_{i}^{\text{ad}}),$$

where $B_{i}^{\text{eff}} = -\frac{1}{\mu_{M}} \partial \mathcal{H}/\partial M_{i}$ is obtained from $\mathcal{H}$ in Eq. (9); $\mu_{M}$ is the magnitude of LMMs \cite{34}; and Gilbert damping is chosen as $\lambda = 0.01$ as typically measured \cite{55} in metallic ferromagnets. In the case of current-driven motion of DW analyzed in Figs. 3, 4(a) and 4(b), we self-consistently couple Eq. (11) to calculations of $T_{i}^{\text{ad}}$ and $T_{i}^{\text{sd}}$ via Eqs. (6) and (7), respectively, in terms of nonequilibrium density matrices obtained from TDNEGF formalism, as explained in Refs. \cite{43, 44}. Such quantum-classical TDNEGF+LLG approach uses time step $\delta t = 0.1 \text{ fs}$ in both quantum [i.e., TDNEGF] computation of $\rho^{\text{neq}}(t) = \hbar G^{<}(t,t)/i$ and classical [i.e., LLG Eq. (2)] parts of the self-consistent loop \cite{43, 44}. We underscore that $\delta\langle \hat{s}(r)\rangle$ was originally obtained \cite{9} from semiclassical transport theory, leading to phenomenological expression for nonadiabatic STT in Eq. (2), while assuming \cite{2, 9} that “$\delta$” denotes deviation from $M(r)$ rather than from $\langle \hat{s}(r)\rangle_{t}^{\text{ad}}$. This result was also re-derived microscopically in Ref. \cite{33} to reveal some of the limiting assumptions behind the phenomenological expression, such as that local equilibrium can be defined and $M_{i}(t)$ has to be nearly constant in time during time scale set by $\hbar/J_{sd}$.
by either changing $J_{sd}$ at fixed $w$ (circles) or by changing $w$ at fixed $J_{sd}$ (triangles), so that overlap of these two sets of data confirms that $J_{sd}w/\gamma a$ is indeed relevant parameter for adiabaticity. For this purpose, we analyze in Fig. 2 how unpolarized charge current becomes spin polarized, and how its polarization then adjusts to DW profile by computing local (or bond) spin currents [42] (instead of previously used Landauer spin-resolved transmission functions [24, 27]) $I_{i+1}^{S_{x}}(t)$ from site $i$ to site $i + 1$ before $(i = 2)$ and after $(i = 38)$ static (i.e., not allowed to move) DW in Fig. 1. The unpolarized charge current is injected by time-dependent bias voltage $V_{b}(t) = \max \left[\tanh((t - t_{0})/\tau) + 1\right]$, where $V_{\max} = 0.05$ eV, $t_{0} = 25$ fs, and $\tau = 10$ fs.

Negative $I_{2\rightarrow 3}^{S_{x}}(t)$ for small $J_{sd}$ [Figs. 2(c) and 2(d)] means that most of spins are reflected (our convention is that positive $I_{i+1}\rightarrow i(t)$ spin-up moves along the $\alpha$-axis from site $i$ to site $i + 1$, with $I_{i+1}\rightarrow i(t) \rightarrow 0$ around $J_{sd}w/\gamma a \geq 1$. Such reflection is nonadiabatic effect, where previous studies has explored thereby generated force [2] on DW and its electrical resistance [2, 8, 22–27]. Our time-dependent QT approach also reveals [Fig. 2(a)] that $I_{38\rightarrow 39}^{S_{x}}(t)$ is not immediately negative, as expected for spin-down (along the $z$-axis) moving in the direction of the positive $x$-axis in Fig. 1, but it takes about $\approx 50$ fs for that to happen [dashed red curve in Fig. 2(a)]. Figure 2(b) shows that adiabatic limit, in which $I_{38\rightarrow 39}^{S_{x}}(t)/I_{2\rightarrow 3}^{S_{x}}(t) \rightarrow -1$ due to electronic spin alignment, smoothly changes orientation from up to down to surrender to surrender [2, 20] a quantum $h$ of angular momentum on the DW, is established for $J_{sd}w/\gamma a \gtrsim 1.5$. In this limit, $\langle s_{z} \rangle^{\text{med}}(t)$ tracks [Fig. 2(d)] adiabatic spin density $\langle s_{z} \rangle_{\text{ad}}^{t}$, but $\langle s_{z} \rangle_{\text{ad}}^{t}$ must continue to mistrack $\mathbf{M}_{i}$ [Fig. 2(c)] so that $\dot{\mathbf{M}}_{i} = h$ (assuming single-electron current pulse injection [56, 57]).

The magnitude of nonadiabatic and adiabatic STT across FM nanowire hosting current-driven moving DW is show in Fig. 3(d), with their maximum values [14] analyzed in Fig. 3(a)–(c). Figure 3(a) demonstrates that nonadiabatic STT does not decay to zero in adiabatic limit (as deciphered from Fig. 2) of wide DW walls, but instead saturates at an asymptotic value. This result is in full accord with experiments [3, 4, 6] where relative insensitivity of nonadiabatic STT to DW width was observed. In addition, phenomenological nonadiabatic STT is out-of-DW-plane [9] (see also Fig. 19 in Ref. [2]), which has already been questioned by Ref. [14] which finds additional in-plane component that is reproduced by our Fig. 4(a). However, our out-of-plane (i.e., along the $y$-axis) component in Fig. 4(b) remains finite with increasing DW width, while that of Ref. [14] decays exponentially with $w$.

We note, however, that STT in Ref. [14] was computed for static DW using time-independent QT. So, in Fig. 4(c) we also employ static DW to demonstrate that out-of-plane nonadiabatic STT does decay in Figs. 4(d), in contrast to STT on dynamic DW in Fig. 4(a). Interestingly, in the case of static DW nonadiabatic STT in Fig. 4(c) is nonzero outside of DW region, which was pointed out in Ref. [14] to be the signature of nonlocality of nonadiabatic STT. But such effect is an artifact of using static DW in calculations, and it disappears in full TDNEGF+LLG self-consistent calculations of Fig. 4(a).

Conclusions and outlook.—Using numerically exact time-dependent QT [43, 44, 47], we demonstrate that wide DWs harbor adiabatic spin transport, in which no spin reflection from static DW takes place [Fig. 2(b)] as analyzed previously [2, 24, 27], as well as nonadiabaticity [Figs. 3 and 4] of microscopically extracted nonequilibrium spin density [Eq. (5)] and thereby generated STT [Eq. (6)] on moving DW. These findings are in full accord with experiments [3, 4, 6]. The origin of discrepancy between them and prior analysis [2, 9, 33], providing widely used [3, 4, 6, 58] in micromagnetics phenomenological expression [Eq. (2)] for nonadiabatic STT that is exponentially suppressed in wide DWs [14], can be traced [Fig. 4] to the usage of static [14] or effectively static [33] [i.e., $\mathbf{M}_{i}(t)$ is assumed to be nearly constant in time on the time scale $h/J_{sd}$] DWs, as well as general expectation that electrons can be completely “integrated out” [9, 59, 60] to arrive at an effective formula. Such formula, plugged into the LLG Eq. (2), then makes possible describing current-driven DW motion using solely classical micromagnetics [28, 58].

However, it has been demonstrated recently [44, 61] that such strategy can work only when $J_{sd}$ is weak and can be treated perturbatively [59, 60]. In other regimes, self-consistent [43, 44, 61, 62] coupling of quantum dynamics of electrons to LLG equation for LMMs can lead to a plethora of new effects in the classical dynamics of LMMs comprising DW—such as nonlocal-in-time response kernel which generates both additional damping [44, 46, 60] and inertia (even in clean system) [44, 60, 62]—whose intricacy can hardly be captured by a simple expression as in Eq. (2).

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