Quantum spin torque driven transmutation of antiferromagnetic Mott insulator

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The standard model of spin-transfer torque (STT) in antiferromagnetic spintronics considers exchange of angular momentum between quantum spins of flowing electrons and noncollinear-to-them localized spins treated as classical vectors. These vectors are assumed to realize Néel order in equilibrium, ↑↑...↑↓, and their STT-driven dynamics is described by the Landau-Lifshitz-Gilbert (LLG) equation. However, many experimentally employed materials (such as archetypical NiO) are strongly electron-correlated antiferromagnetic Mott insulators (AFIs) where localized spins form a ground state quite different from the unentangled Néel state |↑↓...↑↓⟩. The true ground state is entangled by quantum spin fluctuations, leading to expectation value of all localized spins being zero, so that LLG dynamics of classical vectors of fixed length rotating due to STT cannot even be initiated. Instead, a fully quantum treatment of both conduction electrons and localized spins is necessary to capture exchange of spin angular momentum between them, denoted as quantum STT. We use a recently developed time-dependent density matrix renormalization group approach to quantum STT to predict how injection of a spin-polarized current pulse into a normal metal layer coupled to AFMI overlayer via exchange interaction and possibly small interlayer hopping—which mimics, e.g., topological-insulator/NiO bilayer employed experimentally—will induce nonzero expectation value of AFMI localized spins. This new nonequilibrium phase is a spatially inhomogeneous ferromagnet with zigzag profile of localized spins. The total spin absorbed by AFMI increases with electron-electron repulsion in AFMI, as well as when the two layers do not exchange any charge.

Introduction.—The emergence of antiferromagnetic spintronics [1–4] has elevated antiferromagnetic (AF) insulators (AFIs) and metals into active elements of spintronic devices. They exhibit dynamics of their localized spins at a much higher frequencies, reaching THz [4], when compared to ferromagnetic spintronics. Furthermore, the absence of net magnetization forbids any stray magnetic fields, making them largely insensitive to perturbations by external fields. They also exhibit magneto-resistance effects [5, 6] enabling electric readout of changes in the orientations of their localized spins.

Basic spintronic phenomena like spin-transfer torque (STT) [7–10]—where spin angular momentum is exchanged between flowing conduction electrons and noncollinear-to-them [11] localized AF—and spin pumping [12]—where precessing localized AF spins pump pure spin current in the absence of any bias voltage—have been demonstrated recently using different AF materials. The theoretical description [13–22] of these phenomena invariably assumes that localized magnetic moments on two sublattices of the AF material, \( \mathbf{M}^A \) and \( \mathbf{M}^B \), are classical vectors with net zero total magnetization in equilibrium due to assumed Néel classical ground state (GS), ↑↑...↑↓. Out of equilibrium, the dynamics of such classical vectors of fixed length is described by the Landau-Lifshitz-Gilbert (LLG) equation [23]. The STT is typically introduced into the LLG equation either as a phenomenological term [17–20], or it is calculated microscopically by using steady-state single-particle quantum transport formalism applied to model [13, 14, 21] or first-principles [15, 16, 22] Hamiltonians of AF materials. Recently STT [24] from time-dependent single-particle quantum transport formalism [25] has been coupled [26] to the LLG equation, capturing additional quantum effects like electronic spin pumping by moving \( \mathbf{M}^A(t) \) and \( \mathbf{M}^B(t) \) and the corresponding enhanced damping on them, but this remains conventional [11] quantum-for-electrons—classical-for-localized-spins theory of STT.

However, AFIs employed in spintronics experiments are typically strongly electron-correlated transition metal oxides due to narrow \( d \) bands. For example, widely used [6–10] NiO shares features of both Mott and charge-transfer insulators [27, 28]. Due to quantum (or zero-point) spin fluctuations [29–31], the AF GS is highly entangled [30, 32–34], which results in zero expectation value of all localized spins, \( \mathbf{S}_i = 0 \) \( \mathbf{M}_i \propto \mathbf{S}_i = 0 \). Thus, conventional [11] STT \( \mathbf{M}_i \propto \mathbf{s}_i \times \mathbf{S}_i = 0 \) due to injected nonequilibrium electronic spin density \( \mathbf{s}_i \) cannot be initiated because \( \mathbf{S}_i(t = 0) \equiv 0 \). Even if \( \mathbf{S}_i(t = 0) \neq 0 \) is provoked by spin-rotation-symmetry-breaking anisotropies [35] or impurities (see Supplemental Material [36] for illustrations), the LLG equation is inapplicable [38, 39] because the length \( |\mathbf{S}_i(t)| < |\mathbf{S}_i^{\text{Néel}}| \) will be changing in time, with smaller value signifying higher entanglement (unobserved quantum systems exhibit unitary evolution toward states of higher entanglement [40]). Thus, both situations necessitate to describe localized spins fully quantum mechanically where \( \mathbf{S}_i(t) \) is calculated at the end.

The entanglement in the AF GS leading to \( \mathbf{S}_i = 0 \) can be illustrated using an example [41, 42] of a one-dimensional (1D) AF quantum spin-\( \frac{1}{2} \) Heisenberg chain

\[
\hat{H}_\text{AFI} = J \sum_{i=1}^{N_{\text{AFI}}-1} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1},
\]

energy of the unentangled (i.e., direct-product) \( N \) \( \rightarrow \) AFI on \( N_{\text{AFMI}} \) sites. Here \( \hat{S}_i^\alpha = \hat{I}_i \otimes \ldots \otimes \frac{1}{2} \hat{\sigma}^\alpha \otimes \ldots \otimes \hat{I}_{N_{\text{AFMI}}/2} \) acts nontrivially, as the Pauli matrix \( \hat{\sigma}^\alpha \), only on the Hilbert space of site \( i \); \( \hat{I}_i \) is the unit operator; and \( J > 0 \) is AF exchange interaction. The true GS is easy to write explicitly for small \( N_{\text{AFMI}} \), such as for \( N_{\text{AFMI}} = 4 \) we find

\[
|\text{GS} \rangle = \frac{1}{\sqrt{12}} (2|\uparrow \downarrow \uparrow \downarrow \rangle + 2|\downarrow \uparrow \downarrow \uparrow \rangle - |\uparrow \uparrow \downarrow \downarrow \rangle - |\downarrow \downarrow \uparrow \uparrow \rangle).
\]

Its energy, \( \langle \text{GS} | H_{\text{AFI}} | \text{GS} \rangle = -2J \), is lower than the energy of the unentangled (i.e., direct-product) Néel state, \( \langle \uparrow \downarrow | H_{\text{AFI}} | \uparrow \downarrow \rangle = -J \). This is in sharp contrast to ferromagnets where quantum spin fluctuations are absent, and both classical \( \uparrow \uparrow \ldots \uparrow \uparrow \) and its unentangled quantum counterpart \( |\uparrow \uparrow \ldots \uparrow \uparrow \rangle \) are GS of the respective classical and quantum Hamiltonian [such as Eq. (1) with \( J < 0 \)]—it justifies [38, 39] the picture of interacting classical \( M_i \) in spintronics [11] and micromagnetics [23], even as the size of the localized spin is reduced to that of a single electron spin. Conversely, in the case of many-body entangled [30, 32–34] AF GS, the quantum state of each localized spin subsystem \( \text{must} \) be described by the reduced density matrix, \( \hat{\rho}_i = \text{Tr}_{\text{other}} (|\text{GS} \rangle \langle \text{GS}|) \), where partial trace is performed in the Hilbert subspace of all other localized spins \( j \neq i \). The expectation value

\[
S_i = \text{Tr} [\hat{\rho}_i \hat{S}_i],
\]

is then identically zero vector, \( S_i = 0 \), on all sites (see the SM [36]). The GS in the limit \( N_{\text{AFI}} = \infty \) is computable by Bethe ansatz [42], and its entanglement ensures \( S_i = 0 \). The entanglement in the GS of crystalline realization of a two-dimensional (2D) quantum Heisenberg antiferromagnet or antiferromagnetic Mott insulator (AFMI) realized with cold atoms on a square lattice has been detected by neutron scattering [34] or optically [43], respectively, at ultralow temperatures.

In this Letter, we employ the emerging concept of quantum STT [44–47] where both conduction electrons and localized spins are treated fully quantum-mechanically to describe the exchange of spin angular momentum between them. This allows us to predict nonequilibrium phase transition of AFMI driven by absorption of spin angular momentum from spin-polarized current pulse injected into an adjacent normal metal (NM). To model such genuine quantum many-body problem, we evolve in time a nonequilibrium quantum state of NM/AFMI system via very recently developed [46] time-dependent density matrix renormalization group (tDMRG) approach [48–51] to quantum STT.

Our system geometry in Fig. 1 consists of a NM modeled as 1D tight-binding (TB) chain, which is split into the left (L) and the right (R) leads sandwiching a central region. The conduction electron spins in the central region are exchange coupled to an AFMI chain modeled by Hubbard model with the on-site Coulomb repulsion \( U \). The current pulse, carrying electrons initially spin-polarized in the direction perpendicular to the interface (i.e., along the \( z \)-axis in Fig. 1), is injected from the L lead into the central region of NM in order to initiate the AFMI dynamics via quantum STT. Our geometry mimics recent experiment [10] on injection of current pulses into metallic surface of topological insulator \( \text{Bi}_2\text{Se}_3 \), which then exert spin torque on the surface of NiO overlayer covering \( \text{Bi}_2\text{Se}_3 \), except that in the experiment spin-orbit coupling polarizes injected electrons in the plane of the interface (i.e., along the \( y \)-axis in Fig. 1). Nevertheless, since singlet with \( s'_0 (t = 0) \equiv 0 \) on all sites of AFMI is rotationally invariant, the final spin state of
AFMI driven by quantum STT will be the same for arbitrary spin-polarization of injected electrons.

Our main results in Figs. 3–5 demonstrate how quantum STT deposits spin angular momentum [Figs. 4 and 5] into the AFMI by driving its on-site electronic spin expectation value from $s_i(z) = 0$ to $s_i(z) = 1$ at site $i$ of AFMI. The on-site Coulomb repulsion, such as $U = 0–10\, \hbar$ in Fig. 3(b), is expressed in the units of hopping $\gamma$ (typically $\gamma = 1\, eV$) which we use as a unit of energy. The operators for the total number of electrons, $N_{\text{AFMI}} = \sum_i n_i$, and total electronic spin along the $\sigma$-axis, $s^\sigma = \sum_i s^\sigma_i$, are given by sums of local (per-site) charge and spin operators, $n_i = \sum_{\sigma = \uparrow, \downarrow} \hat{\sigma}^\dagger_i \sigma \sigma \hat{\sigma}^i$, and $s^\sigma_i = \sum_{\sigma = \uparrow, \downarrow} \hat{\sigma}^\dagger_i \sigma \sigma \hat{\sigma}^i$, respectively. The interchain exchange interaction $J_v$ between electronic spins within NM and AFMI is described by

$$
\hat{H}_{\text{NM–AFMI}} = -J_v \sum_{i=1}^{N_{\text{AFMI}}} \hat{\sigma}^i_{i+N_L}\hat{\sigma}^i_i - \gamma_v \sum_{i=1}^{N_{\text{AFMI}}} \left( \hat{\sigma}^{\dagger}_{i+N_L} \hat{\sigma}^i_i + \hat{\sigma}^{\dagger}_i \hat{\sigma}^i_{i+N_L} + \text{h.c.} \right),
$$

where $\hat{\sigma}^i_i$ and $\hat{\sigma}^i_i$ are local electron spin operators in NM and AFMI chains, respectively. Here we also add a term with possible $\gamma_v \neq 0$ hopping between $N_{\text{AFMI}}$ sites of the central region of the NM chain and $N_{\text{AFMI}}$ sites of AFMI in Fig. 1(a), which can arise in realistic devices used in spintronics [7–10] due to evanescent wavefunctions penetrating [22] from the NM surface into the region of AFMI.
FIG. 4. Time dependence of the total number of electrons within (a) AFMI and (b) NM chains in the setup of Fig. 1(b) for two different interchain hoppings $\gamma_v = 0$ (blue lines) and $\gamma_v = 0.1\gamma$ (red lines). Panels (c) and (d) show the corresponding time dependence of the sum of the $z$-component of electronic spin expectation values, $\sum_i s_i^z$ and $\sum_i s_i^z$, respectively. The on-site Coulomb repulsion is $U = 8\gamma$ [Eq. (5)] within the AFMI and interchain exchange interaction is $J_v = 0.5\gamma$.

near the interface, thereby leading to charge transfer in equilibrium or current leakage [22] between the two materials. Such normal-metal proximity effect on finite-size Mott insulators can also create exotic many-body states in equilibrium [52]. To prepare the initial state of the conduction electrons in the NM chain, we confine them within $N_{\text{conf}}$ sites of the L lead in Fig. 1(a) and polarize their spins along the $+z$-axis by means of an additional term $\hat{H}_{V,B}(t < 0) = -V \sum_{i=1}^{N_{\text{conf}}} \left( \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} + \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \right) - \sum_{i=1}^{N_{\text{conf}}} g_H V B_z^2$. Here $V = 2\gamma$ is the confining potential; $B_z$ is the external magnetic field; and $g_H V B_z^2 = 10\gamma$, where $g$ is the electron gyromagnetic ratio and $g_H$ is the Bohr magneton. After the initial state is prepared for $t < 0$, $\hat{H}_{V,B}(t \geq 0)$ is set to zero, so that spin-polarized electrons from the L lead propagate toward the R lead, as illustrated in Fig. 1(b) and computed in Fig. 2.

In the limit $U \gg \gamma$, the half-filled ($n_i = 1$) 1D Hubbard model describes electrons localized one per site, so it can be mapped [41, 42] to isotropic AF quantum spin-$\frac{1}{2}$ Heisenberg chain with the effective Hamiltonian given in Eq. (1). Therefore, for comparison we also analyze the NM/AFI setup in Fig. 1(c) where AFI sites hosts localized spin-$\frac{1}{2}$ operators $\hat{S}_i$, as described by the Hamiltonian $\hat{H} = \hat{H}_{\text{NM}} + \hat{H}_{\text{AFI}} + \hat{H}_{\text{NM-AFI}} + \hat{H}_{V,B}(t < 0)$. Here $\hat{H}_{\text{NM}}$ is the same as in Eq. (4); $\hat{H}_{\text{AFI}}$ is the same as in Eq. (1) where we use $J = 4\gamma^2/U$ as the exchange interaction in the limit $U \gg \gamma$ [41, 42]; the interchain interaction is described by $\hat{H}_{\text{NM-AFI}} = -J_v \sum_{i=1}^{N_{\text{AFI}}} \hat{S}_{i+N_L} \cdot \hat{S}_i$ where $J_v = 0.5\gamma$; and $\hat{H}_{V,B}(t < 0)$ is the same as in Eq. (4).

The tDMRG simulations [48–51] evolve the nonequilibrium state of the whole system in Fig. 1, $|\Psi(t + \delta t)\rangle = e^{-i\hat{H}\delta t/\hbar} |\Psi(t)\rangle$, using time step $\delta t = 0.1\hbar/\gamma$. We start the propagation with $m = 100$ states and limit the truncation error to $10^{-7}$, while the maximal number of states allowed during the evolution is set to $m_{\text{max}} = 400$. Any single-particle expectation value at site $i$ can be obtained from $\hat{\rho}_i(t) = \text{Tr}_{\text{other}} |\Psi(t)\rangle \langle \Psi(t)|$, as exemplified by Eq. (3).

Since fermionic leads are not semi-infinite as in usual quantum transport calculations [26], the system in Fig. 1 can be evolved only for a limited time [53–56] before electrons are backscattered by the right boundary which breaks L→R current flow. For example, in Fig. 2 such backscattering occurs at $t \simeq 40\hbar/\gamma$. Nevertheless, the quantum dynamics of the conduction electrons in the NM chain and charge and spin confined within the AFMI chain can be safely assumed to be effectively equivalent to that in an infinite open quantum system before the boundary reflection takes place.

Results and discussion.—The Hubbard 1D chain modeling the AFMI possesses a sizable energy gap $\Delta$, for charge excitations at $U \gtrsim 2\gamma$, whose value is exactly known [42] in the limit $N_{\text{AFMI}} \to \infty$ ($\Delta_c = 0.173\gamma$ at $U = 2\gamma$; or $\Delta_c = 0.631\gamma$ at $U = 3\gamma$). In chains of finite length, such as ours with $N_{\text{AFMI}} = 12$ sites, DMRG predicts slightly larger $\Delta_c$ values [57]. However, the spin sector of the half-filled Hubbard chain is gapless in the thermodynamic limit. This means that injecting a charge in the AFI is energetically costly, but creating a spin excitation is not. Figures 2(a) and 3 demonstrate that AFMI with $U \gtrsim 4\gamma$ will be driven out of its GS with $s_i^z = 0$ on all sites toward a nonequilibrium phase with
quantum materials, as well as a benchmark for any pivotal test case that provides intuition about quantum only a very few sites. Therefore, this study represents a or its nonperturbative implementation can handle [60]

Even after the current pulse in the NM chain has ended, the spin angular momentum remains deposited within AFMI, with its total value increasing with $U$ [Fig. 5(a)]. Such Mott insulator transmuted into a phase with nonzero total magnetization remains magnetized also when intrachain hopping is switched on, $\gamma_v = 0.1\gamma$, in Fig. 4(c). However, $\gamma_v = 0.1\gamma$ allows electrons to leak from AFMI [Fig. 4(a)] to NM [Fig. 4(b)] chain, so that total spin deposited into AFMI is reduced in Fig. 4(c) when compared to isolated AFMI.

Figure 5 explains, pedagogically and at the microscopic level, quantum STT [44–47] as the transfer of total spin angular momentum from NM conduction electrons (dashed lines in Fig. 5) to confined electrons within the AFMI [solid lines in Fig. 5(a)] or to localized spins within the AFI [solid lines in Fig. 5(b)]. The NM/AFMI case with $U = 10\gamma$ shows that $\sum_i s_i^z(t)$ within AFMI is nearly identical to $\sum_i S_i^z(t)$ within AFI with $J = 4\gamma^2/U$, as anticipated from mapping [41, 42] of AFMI to AFI in the limit $U \gg \gamma$. However, this correspondence fails for $U < 10\gamma$. The absorbed spin by AFMI or AFI can be viewed as multiple excitations of any two-spinon or higher-order spinon states [58], as long as they are compatible with total angular momentum conservation [46].

Conclusions.— In conclusion, we demonstrate how the very recently developed tDMRG [46] approach to quantum STT [44–47] makes it possible to study spin torque on strongly electron-correlated antiferromagnets. In contrast, quantum-classical theory of conventional STT [11, 13–22] would conclude that entangled AF true GS does not undergo any current-driven dynamics when its localized spins have zero expectation value at $t = 0$ as the initial state used in this study. Although tDMRG has been previously applied to study charge current through AFMI [53–55] or spin-charge separation [56] in geometries where electrons are injected into AFMI by finite bias voltage, spin-dependent transport phenomena in geometries like Fig. 1 of relevance to spintronics [7–10] remain unexplored. Realistic spintronic devices would require to consider two- or three-dimensional geometries. But Keldysh Green functions [25, 59], as the only available nonequilibrium quantum many-body formalism for higher dimensions and longer times, cannot at present access large $U$ with perturbative self-energies [57, 59], or its nonperturbative implementation can handle [60] only a very few sites. Therefore, this study represents a pivotal test case that provides intuition about quantum STT phenomena in strongly correlated and/or entangled quantum materials, as well as a benchmark [59] for any future developments via the Keldysh Green functions.

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[17] K. M. D. Hals, Y. Tserkovnyak, and A. Brataas, Phenomenology of current-driven dynamics in antiferro-
[36] See Supplemental Material at https://wiki.physics.udel.edu/qttg/Publications, which includes Ref. [37], for spatial profiles of the expectation value of spin $\mathbf{S}$ in Eq. (3) in 1D and 2D spin-1/2 quantum Heisenberg antiferromagnets in Eq. (1) which posses global spin rotation invariance or they contains a single symmetry-breaking impurity generating magnetic field on one site.
This Supplemental Material provides one additional Figures showing expectation value $S_z^i$ of spin-$\frac{1}{2}$ operators, as defined in Eq. (3) of the main text, in the ground state (GS), $|\text{GS}\rangle$, at each site $i$ of either antiferromagnetic one-dimensional (1D) quantum Heisenberg chain composed of $N_{\text{AFI}} = 12$ sites [Figs. S1(a) and S1(b)] or two-dimensional (2D) quantum Heisenberg antiferromagnet on $6\times4$ square lattice [Figs. S1(c) and S1(d)]. Periodic boundary conditions are employed in both cases. Both models are described by the quantum Heisenberg Hamiltonian

$$
\hat{H}_{\text{AFI}} = J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j - h \hat{S}_m^z,
$$

where the exchange interaction $J = 1$ eV is nonzero between the nearest-neighbor sites, as denoted by $\langle i,j \rangle$. Here

$$
\hat{S}_i^\alpha = I_1 \otimes \ldots \otimes \frac{1}{2} \hat{\sigma}^\alpha \otimes \ldots \otimes I_{N_{\text{AFI}}},
$$

acts nontrivially, as the Pauli matrix $\hat{\sigma}^\alpha$, only on the Hilbert space of site $i$; and $I_i$ is the unit operator. We consider systems with the global spin rotation symmetry, as described by the first term only in Eq. (1); or we introduce an additional local magnetic field $h = 0.2J$ at site $m$ of 1D or 2D lattice, due to, e.g., impurity whose spin is large and

![Figure S1](image.png)

FIG. S1. Spatial profile of the $z$-component $S_z^i$ [Eq. (3) in the main text] of spin operator in Eq. (2) within: (a) 1D chain of 12 sites described by the first term in Eq. (1); (b) 1D chain of 12 sites with the local magnetic field $h = 0.2J$ in the second term in Eq. (1) at site $m = 2$; (c) 2D square lattice described by the first term in Eq. (1); (d) 2D square lattice with the local magnetic field $h = 0.2J$ in the second term in Eq. (1) at site $m = (3,2)$.

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can be considered as a classical vector. The nonzero second term in Eq. (1) breaks the global spin rotation symmetry. The GS is found by exact diagonalization in 1D or in 2D by using QUIMB package [1].

One of the standard tools to quantify entanglement in many-body quantum systems is entanglement entropy of its subsystem [2], such as half of 1D chain or 2D lattice. We compute

\[ \hat{\rho}_{\text{half}} = \text{Tr}_{\text{other-half}} |\text{GS}\rangle \langle \text{GS}|, \]

and from it obtain the von Neumann entanglement entropy

\[ S_{\text{half}} = -\text{Tr} \hat{\rho}_{\text{half}} \log_2 \hat{\rho}_{\text{half}}. \]

This entropy for systems in Fig. S1(a)–(d) is: (a) \( S_{\text{half}} = 1.71 \); (b) \( S_{\text{half}} = 1.67 \); (c) \( S_{\text{half}} = 2.96 \); and (d) \( S_{\text{half}} = 2.91 \), respectively. Thus, even though systems in Fig. S1(b) or Fig. S1(d) exhibit staggered pattern of expectation values \( S_z \), akin to Néel classical ground state \( \uparrow \downarrow \ldots \uparrow \downarrow \), their |GS⟩ remains highly entangled. This is also signified by \( |S_i| \ll |S_i^{\text{Néel}}| \), where \( |S_i^{\text{Néel}}| = 1/2 \) is for unentangled (i.e., direct-product) Néel quantum state \( |\uparrow \downarrow \ldots \uparrow \rangle \).
