

Anomalous Bias Dependence of Spin Torque in Magnetic Tunnel Junctions

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We predict an anomalous bias dependence of the spin transfer torque parallel to the interface, T_{\parallel} , in magnetic tunnel junctions, which can be selectively tuned by the exchange splitting. It may exhibit a sign reversal *without* a corresponding sign reversal of the bias or even a quadratic bias dependence. We demonstrate that the underlying mechanism is the interplay of spin currents for the ferromagnetic (antiferromagnetic) configurations, which vary linearly (quadratically) with bias, respectively, due to the symmetric (asymmetric) nature of the barrier. The spin transfer torque perpendicular to interface exhibits a quadratic bias dependence.

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Theoretical calculations predict that when a spin-polarized current passes through a magnetic multilayer structure, whether spin valve [1] or magnetic tunnel junction, (MTJ) [2,3], it can transfer spin angular momentum from one ferromagnetic electrode to another, and hence exert a torque on the magnetic moments of the electrodes. At sufficiently high current densities, this spin transfer can stimulate spin-wave excitations [4,5] and even reverse the magnetization of an individual domain [6]. Current-induced magnetic switching (CIMS) has now been confirmed in numerous experiments both in spin valves [6,7] and more recently, in MTJs [8,9]. Thus, CIMS provides a powerful new tool for the study of spin transport in magnetic nanostructures. In addition, it offers the intriguing possibility of manipulating high-density nonvolatile magnetic-device elements, such as magnetoresistive random access memory (MRAM), without applying cumbersome magnetic fields [10].

While the fundamental physics underlying the spin transfer torque (STT) in spin valves has been extensively studied theoretically [1,11–13], its role in MTJs remains an unexplored area thus far, except for the pioneering work of Slonczewski [2,3], who employed the free-electron model in the low bias regime. One of the most pressing needs is a comprehensive understanding of the bias dependence of the STT in MTJs, which will be important for the development of MRAM that uses CIMS for writing the magnetic memory cell.

In this Letter, we present for the first time a comprehensive study of the effect of bias on the spin torques, parallel (T_{\parallel}) and perpendicular (T_{\perp}) to the interface, in MTJs, using tight-binding (TB) calculations and the nonequilibrium Keldysh formalism. We predict an anomalous bias dependence of the spin torque, contrary to the general consensus. We demonstrate first that depending on the exchange splitting, T_{\parallel} may exhibit an unusual nonmonotonic bias dependence: it may change sign *without* a sign reversal in bias or current, and it may even have a quadratic

bias dependence. Second, by generalizing the equivalent circuit in Ref. [3] using angular-dependent resistances, we show that T_{\parallel} satisfies an expression involving the *difference* in spin currents between the ferromagnetic (FM) and antiferromagnetic (AF) configurations. This expression is general and *independent* of the details of the electronic structure. Our numerical results both for the TB model and the free-electron model (not presented here) confirm the validity of this relation for any parameter set and bias. Third, the spin current for the FM (AF) alignment is shown to have a linear (quadratic) bias dependence, whose origin lies in the symmetric (asymmetric) nature of the barrier. The interplay of the spin currents for the FM and AF configurations is the key underlying mechanism that can lead to a rich behavior of the STT on bias. Finally, we find that the bias dependence of T_{\perp} is quadratic.

The MTJ under consideration depicted in Fig. 1 consists of a left and right semi-infinite noncollinear FM leads, separated by a nonmagnetic insulating (I) spacer contain-

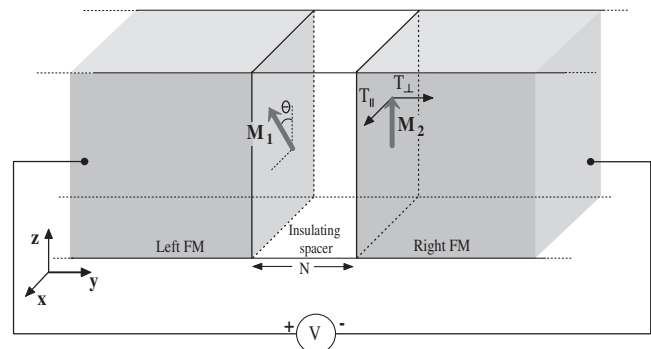


FIG. 1. Schematic structure of the MTJ, consisting of left and right semi-infinite FM leads separated by a thin nonmagnetic insulating system containing N atomic layers. The magnetization \mathbf{M}_2 of the right FM lead is along the z axis, whereas the magnetization \mathbf{M}_1 of the left lead is rotated by angle θ around the y axis with respect to \mathbf{M}_2 .

ing N atomic layers. The right FM lead is magnetized along the z axis (\mathbf{M}_2) of the coordinate system, shown in the inset of Fig. 1. The magnetization of the left FM lead (\mathbf{M}_1) lies in the $x - z$ interfacial plane, i.e., it is rotated by angle θ around the axis y (normal to the FM/I interfaces) with respect to \mathbf{M}_2 . The chemical potentials of the right and left leads are shifted by the external bias, $eV = \mu_L - \mu_R$, where the charge current is positive when it flows along the y axis from left to right. The Hamiltonian for each region is described by a single orbital simple-cubic TB model with a nearest-neighbor (NN) spin-independent hopping term, t_α , and a spin-dependent on-site energy term, $\varepsilon_\alpha^\sigma$, where $\alpha = L, R$, and I refer to the left, right, and insulating regions, respectively. In the present calculations the left and right FM leads are identical with an exchange splitting, $\Delta_{L(R)} = \varepsilon_{L(R)}^\uparrow - \varepsilon_{L(R)}^\downarrow$. We use $\Delta_I = 0$, $\varepsilon_{L(R)}^\uparrow - E_F = 1.2$ eV, $\varepsilon_I - E_F = 5.4$ eV, $N = 5$, and $t_{R(L)} = t_I = t_{R(L),I} = t = 0.4$ eV, where the Fermi energy $E_F = 0$ eV, and the $t_{L,I}$ and $t_{R,I}$ are the NN hopping matrix elements at the two FM/I interfaces [14]. Note that $\Delta_{L(R)}$, refers to the *local effective s-d* exchange interaction, with values between 0.2 eV to 2 eV [15] depending on the material. Under applied bias, $\varepsilon_R^\sigma - \varepsilon_L^\sigma = eV$, the potential inside the insulator, $\varepsilon_{I,n} = \varepsilon_I - eV \frac{n-1}{N-1}$, varies linearly with layer number n .

The one-electron Schrödinger equation in spin space for each uncoupled region α is [16]

$$\sum_{p,q,p_1 \in \alpha} \left\{ [(E - \varepsilon_{\mathbf{k}_\parallel})\delta_{pp_1} - \bar{H}_{pp_1}] \hat{I} - \delta H_{pp_1} \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \right\} \begin{pmatrix} g_{p_1,q}^\uparrow & g_{p_1,q}^\downarrow \\ g_{p_1,q}^\downarrow & g_{p_1,q}^\uparrow \end{pmatrix} = \delta_{pq} \hat{I}, \quad (1)$$

where p and q are atomic sites indices in region α , $\varepsilon_{\mathbf{k}_\parallel}$ is the energy of the in-plane wave vector, \mathbf{k}_\parallel , of the Bloch state, $g_{pq}^{\sigma\sigma'}$ is the spin-dependent retarded Green's function for each region, and \hat{I} is the 2×2 unit matrix. The quantities $\bar{H}_{pq} = \frac{1}{2}[(\varepsilon_\alpha^\uparrow + \varepsilon_\alpha^\downarrow)\delta_{pq} + t_\alpha(\delta_{p,q+1} + \delta_{p,q-1})]$ and $\delta H_{pq} = \frac{1}{2}\Delta_\alpha$ describe the spin-average and the spin-split part of the Hamiltonian, respectively.

Having determined the $g_{pq}^{\sigma\sigma'}$ for each uncoupled subsystem from Eq. (1), one can calculate the retarded Green's function for the entire coupled system by solving a system of Dyson equations which couples the $g_{pq}^{\sigma\sigma'}$ through the hopping matrix elements $t_{L,I}$ and $t_{I,R}$ at the two interfaces. In order to calculate the nonequilibrium Keldysh Green's function, $\hat{G}_{i,i+1}^{<\sigma,\sigma'}$, we have extended the approach of Caroli *et al.* [17] in spin space using 2×2 Green's function matrices.

The charge current density is [13]

$$I = I^\uparrow + I^\downarrow = \frac{et}{2\pi\hbar} \int \text{Tr}_\sigma [\hat{G}_{i,i+1}^{<\sigma,\sigma'} - \hat{G}_{i+1,i}^{<\sigma,\sigma'}] dE d\mathbf{k}_\parallel, \quad (2)$$

and the spin-current density between sites i and $i + 1$ is

$$\mathbf{I}_{i,i+1}^{(s)} = \frac{t}{4\pi} \int \text{Tr}_\sigma [(\hat{G}_{i,i+1}^{<\sigma,\sigma'} - \hat{G}_{i+1,i}^{<\sigma,\sigma'}) \boldsymbol{\sigma}] dE d\mathbf{k}_\parallel, \quad (3)$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a vector of the Pauli matrices. Both I^\uparrow and I^\downarrow are conserved across the MTJ, while the spin current is not conserved ($\nabla \cdot \mathbf{I}^{(s)} \neq 0$), due to spin-dependent scattering caused by the local exchange field inside the FM leads [12]. Conservation of the total angular momentum implies that the spin current lost at an atomic site is transferred to its local magnetic moment, thereby exerting a local STT [12,13] \mathbf{T}_i on site i in the right FM lead per unit area defined by

$$\mathbf{T}_i \equiv -\nabla \cdot \mathbf{I}^{(s)} = \mathbf{I}_{i-1,i}^{(s)} - \mathbf{I}_{i,i+1}^{(s)}, \quad (4)$$

where the second equality represents the discrete form of the divergence of the spin current. The local spin torque, \mathbf{T}_i , shown in Fig. 1, has components parallel ($T_{i,\parallel}$) and perpendicular ($T_{i,\perp}$) to the interfacial plane. The z component of \mathbf{T}_i vanishes because $I_{(i,i+1),z}^{(s)} = I_{(i-1,i),z}^{(s)} = \frac{\hbar}{2e}(I^\uparrow - I^\downarrow)$. Both $T_{i,\parallel}$ and $T_{i,\perp}$ oscillate with different phase and decay with distance from the I/FM interface, as in the case of spin valves [11,12,16].

The *net* STT transverse to the magnetization on the right FM lead, a quantity which presumably experiment measures, is the sum of local torques, \mathbf{T} ,

$$\mathbf{T} = \sum_{i=0}^{\infty} (\mathbf{I}_{i-1,i}^{(s)} - \mathbf{I}_{i,i+1}^{(s)}) = \mathbf{I}_{-1,0}^{(s)} - \mathbf{I}_{\infty,\infty}^{(s)} = \mathbf{I}_{-1,0}^{(s)}, \quad (5)$$

where the subscripts -1 and 0 refer to the last site inside the barrier and the first site in the right FM lead, respectively. In the above equation, $\mathbf{I}_{\infty,\infty}^{(s)} = 0$ because the components of $\mathbf{I}_{i,i+1}^{(s)}$ transverse to \mathbf{M}_2 decay to zero as $i \rightarrow \infty$ [11]. Thus, the *net* spin torque exerted on the right FM lead is simply the spin current calculated at the I/FM interface [12].

In Fig. 2 we show the bias dependence of the current-induced perpendicular component, $T_\perp(V) - T_\perp(V=0)$, of the *net* spin torque for $\theta = \pi/2$, and various values of ε^\downarrow . The inset displays the bias dependence of $T_\perp(V)$. We find that $T_\perp(V)$ varies quadratically with bias, as originally suggested, but not calculated, by Slonczewski [3]. The equilibrium ($V=0$) value of $T_\perp(V)$, related to the interlayer exchange coupling energy [1], decreases in absolute value as the exchange splitting Δ is reduced.

In Fig. 3 we display the bias dependence of the parallel component of the *net* spin torque, T_\parallel (curves associated with the left ordinate), for $\theta = \pi/2$ and for the same values of ε^\downarrow as in Fig. 2. The most striking and surprising feature of T_\parallel is its nonmonotonic bias dependence, which can vary from almost linear to purely quadratic behavior, depending on the exchange splitting Δ . The quadratic bias dependence of T_\parallel for $\varepsilon^\downarrow = 1.5$ eV persists even for small bias. Interestingly, for $\varepsilon^\downarrow = 2$ eV and 2.2 eV, T_\parallel reverses its sign

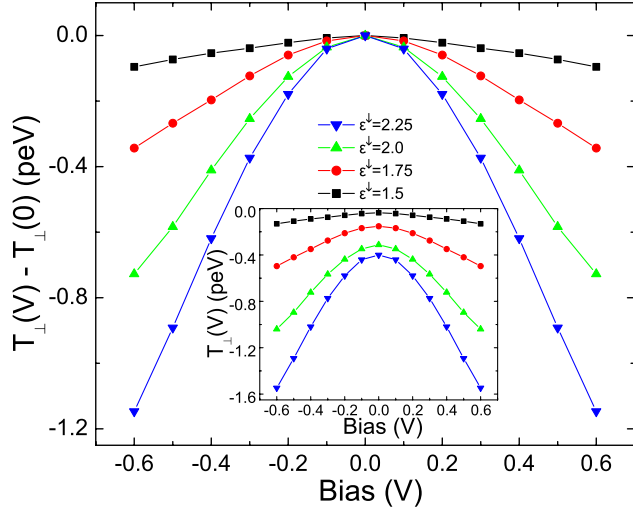


FIG. 2 (color online). Bias dependence of the current-induced perpendicular component of the *net* spin torque per unit area, $T_{\perp}(V) - T_{\perp}(0)$, for $\theta = \pi/2$, and various values of ε^l . $T_{\perp}(0)$ is related to the exchange coupling energy between left and right FM leads. Inset: bias dependence of $T_{\perp}(V)$.

without a sign reversal in bias or current. This anomalous bias behavior may have important practical implications, since it suggests that the CIMS in MTJ may not require reversal of the current. Note that T_{\perp} and T_{\parallel} are comparable in size in MTJ, in contrast to metallic spin valves, where $T_{\perp} \ll T_{\parallel}$ [11].

In order to understand the underlying mechanism responsible for the bias dependence of T_{\parallel} , we have generalized the equivalent circuit for MTJ [3], using angular-dependent resistances, $R^{\sigma,\sigma'}(\theta) = R^{\sigma}(0)\cos^{-2}(\theta/2)$ and $R^{\sigma,\bar{\sigma}}(\theta) = R^{\sigma}(\pi)\sin^{-2}(\theta/2)$, as displayed in Fig. 4. The angular dependence of $R^{\sigma,\sigma'}(\theta)$ is equal to the inverse probability $[P^{\sigma,\sigma'}(\theta)]^{-1}$ for an electron with spin state $|\sigma\rangle$ quantized along \mathbf{M}_1 to tunnel to a spin state $|\sigma'\rangle$ quantized along \mathbf{M}_2 , where multiple reflections within the barrier are neglected [18]. Substituting the currents $I_{L(R)}^{\sigma}$ in Fig. 4 into Eq. (5) of Ref. [3], we obtain

$$T_{\parallel}(\theta) = \frac{I_z^{(s)}(\pi) - I_z^{(s)}(0)}{2} \mathbf{M}_2 \times (\mathbf{M}_1 \times \mathbf{M}_2), \quad (6)$$

where $I_z^{(s)}(\pi) = \frac{\hbar}{2e} [I^{\uparrow}(\pi) - I^{\downarrow}(\pi)]$ and $I_z^{(s)}(0) = \frac{\hbar}{2e} [I^{\uparrow}(0) - I^{\downarrow}(0)]$ are the spin-current densities for the AF and FM configurations, respectively. This important result is quite general, *independent* of the details of the electronic structure, and reduces the calculation of $T_{\parallel}(\theta)$ simply to the evaluation of the spin-current densities for the FM and AF configurations [3]. The angular dependence of both T_{\perp} and T_{\parallel} is proportional to $\sin\theta$ [2], in contrast to metallic spin valves [1,11].

Defining the dynamic current polarization [19], $P(\theta) = [I^{\uparrow}(\theta) - I^{\downarrow}(\theta)]/I(\theta)$, where $I(\theta) = I^{\uparrow}(\theta) + I^{\downarrow}(\theta)$ is the total current, Eq. (5) reduces to

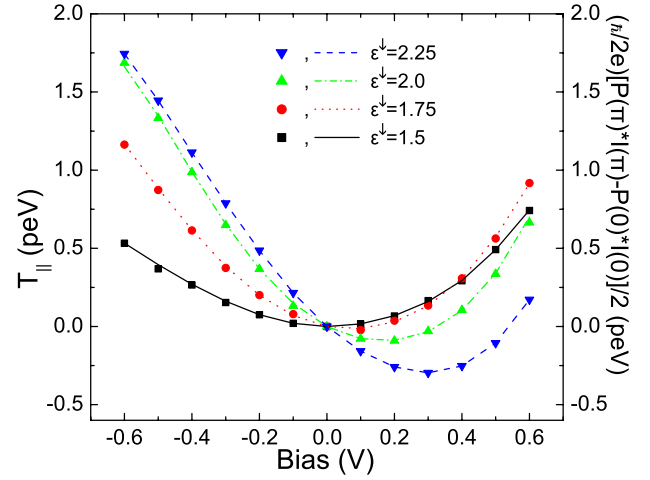


FIG. 3 (color online). Bias dependence of the parallel component of the *net* spin transfer torque per unit area, T_{\parallel} , for $\theta = \pi/2$, and various values of ε^l . The curves (symbols) refer to the left- (right-) hand ordinate, respectively.

$$T_{\parallel}(\theta) = \frac{\hbar}{2e} \frac{P(\pi)I(\pi) - P(0)I(0)}{2} \mathbf{M}_2 \times (\mathbf{M}_1 \times \mathbf{M}_2). \quad (7)$$

In order to confirm Eq. (6) and (7) we display also in Fig. 3 the bias dependence of $\frac{\hbar}{2e} [P(\pi)I(\pi) - P(0)I(0)]/2$ (symbols associated with the right ordinate) for the same values of ε^l , where the agreement is excellent.

In order to elucidate the atomistic origin of the bias dependence of T_{\parallel} in Eq. (6), we plot in Fig. 5 the spin-current densities, $I_z^{(s)}(\pi)$ and $I_z^{(s)}(0)$, versus bias for the AF and FM orientations, respectively, for $\varepsilon^l = 2.0$ eV. One can clearly see that $I_z^{(s)}(0)$ [$I_z^{(s)}(\pi)$] varies linearly (quadratic) with bias for $V < 0.5$ eV. For the FM and AF configurations the tunneling can be considered as the superposition of two independent spin channels. This different bias behavior can be understood on the basis of the Brinkman tunnel model [20] for asymmetric barriers, generalized so as to take into account both spin channels. The bias dependence of I^{σ} can be written as [20]: $I^{\sigma}(V) = f_1(\bar{\Phi}^{\sigma})V - f_2(\bar{\Phi}^{\sigma})\Delta\Phi^{\sigma}V^2 + O(V^3)$, where f_1 and f_2 are

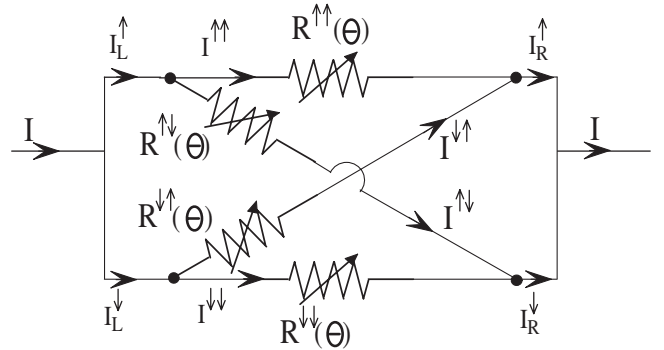


FIG. 4. Equivalent circuit for spin-channel currents, with angular-dependent resistances.

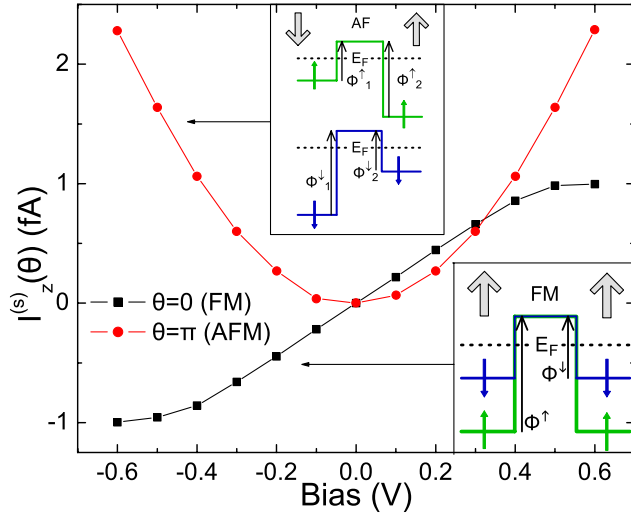


FIG. 5 (color online). Bias dependence of the spin-current density, $I_z^{(s)}(\theta) \equiv I^{\uparrow}(\theta) - I^{\downarrow}(\theta)$, for the FM and AFM orientations, respectively. In the FM case the majority and minority electrons tunnel through a symmetric barrier (lower inset) with different barrier heights, Φ^σ , from the bottom of the band. In the AFM case (upper inset), the two spin channels tunnel through asymmetric barriers with the same average barrier height, $\bar{\Phi}^\sigma$, but with a barrier asymmetry, $\Delta\Phi^\sigma$, of opposite sign.

functions of the average barrier height, $\bar{\Phi}^\sigma = [\Phi_1^\sigma + \Phi_2^\sigma]/2$, and $\Delta\Phi^\sigma = \Phi_1^\sigma - \Phi_2^\sigma$ is the barrier asymmetry. Here, $\Phi_{1(2)}^\sigma$ is the spin-dependent barrier height at the left (right) interface from the bottom of the band.

In the FM configuration, the majority and minority electrons tunnel through a *symmetric* barrier (lower inset in Fig. 5) but with different barrier heights, Φ^σ , for each spin channel. In this case, $\bar{\Phi}^\uparrow \neq \bar{\Phi}^\downarrow$ and $\Delta\Phi^\uparrow = \Delta\Phi^\downarrow = 0$. Thus, both $I^{\uparrow}(0)$ and $I^{\downarrow}(0)$ vary linearly with V , and hence also $I_z^{(s)}(0)$. On the other hand, in the AFM configuration (upper inset in Fig. 5), both spin channels tunnel through asymmetric barriers with the same average barrier height, $\bar{\Phi}^\uparrow = \bar{\Phi}^\downarrow$, but with barrier asymmetry of opposite sign, $\Delta\Phi^\uparrow = -\Delta\Phi^\downarrow$. Hence, the linear bias dependence of $I^{\uparrow}(\pi) - I^{\downarrow}(\pi)$ vanishes identically, and $I_z^{(s)}(\pi)$ exhibits a quadratic bias dependence.

Thus, the *interplay* between the linear and quadratic bias dependence of $I_z^{(s)}(0)$ and $I_z^{(s)}(\pi)$, respectively, in Eq. (5) is responsible for the nonmonotonic bias dependence of T_{\parallel} in Fig. 3. This competition can be selectively tuned by varying Δ , giving rise to a wide range of rich bias behavior. For example, the purely quadratic bias behavior for $\varepsilon^\downarrow = 1.5$ eV arises from the fact that $I^{\uparrow}(0) = I^{\downarrow}(0)$. Contrary to the free-electron model [2], this behavior is possible within the TB model due to the bell-like form of the density of states at the interfaces [18].

In summary, we predict an anomalous bias behavior of T_{\parallel} in MTJ, which varies with the exchange splitting in the FM leads. T_{\parallel} may exhibit a sign reversal *without* a corresponding sign reversal of the bias, or even an unexpected

quadratic bias dependence. The underlying mechanism for the unusual bias dependence is the interplay between the bias dependence of the spin currents for the FM and AFM configurations. The origin for the linear (quadratic) bias dependence of the spin currents is the symmetric (asymmetric) nature of the tunnel barrier for the FM (AFM) orientations. We should emphasize that the nonmonotonic bias behavior is not associated with the simple TB model; other systems with more complex electronic structures can also show this behavior, provided that the condition $I_z^{(s)}(0) < I_z^{(s)}(\pi)$ is satisfied. On the other hand, T_{\perp} exhibits a quadratic bias dependence.

An experimental test of our prediction can be achieved by relating the (observable) critical voltage for switching measured as a function of external magnetic field to the spin torque. This can be done for a magnetic element that has been characterized as to damping factor, anisotropy, and magnetic moment. Future work will be aimed to include the results of these calculations as an input into the Landau-Lifshitz-Gilbert equation, to calculate the critical current for the CIMS.

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