Current Induced Order Parameter Dynamics: Microscopic Theory Applied to Co/Cu/Co spin valves

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Transport currents can alter order parameter dynamics and change steady states in superconductors, in ferromagnets, and in hybrid systems. In this article we present a scheme for fully microscopic evaluation of order parameter dynamics that is intended for application to nanoscale systems. The approach relies on time-dependent mean-field-theory, on an adiabatic approximation, and on the use of non-equilibrium Greens function (NEGF) theory to calculate the influence of a bias voltage across a system on its steady-state density matrix. We apply this scheme to examine the spin-transfer torques which drive magnetization dynamics in Co/Cu/Co spin-valve structures. Our microscopic torques are peaked near Co/Cu interfaces, in agreement with most previous pictures, but surprisingly act mainly on Co transition metal d-orbitals rather than on s-orbitals as generally supposed.

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I. INTRODUCTION

Transport currents can be used to alter the order parameter dynamics of metals with broken symmetries, including ferromagnets, antiferromagnets, superconductors, and hybrid systems containing both magnetic and superconducting elements. A familiar and simple example of this type of phenomena is a circuit in which current flows between normal (N) metal elements though a superconductor (S). Because of Andreev reflection of the quasiparticle current at the N/S boundary, the Cooper pair amplitude in the superconductor is altered. In the presence of a normal metal transport current, the superconducting order parameter develops a spatial gradient in the steady state which allows the condensate to carry current through the superconducting element. A more recent example is quantum Hall bilayers which develop excitonic condensates\textsuperscript{5} under certain conditions and exhibit anomalies related\textsuperscript{2} to the influence of transport currents on interlayer phase coherence. An important class of related phenomena which has received a large amount of theoretical\textsuperscript{2,6} and experimental\textsuperscript{7} attention over the past decade is centered on the influence of transport currents on magnetization in magnetic metals, particularly ferromagnetic nanoparticles and ferromagnets containing domain walls. In this case the current-related torques exerted on the magnetization can usually be understood at least qualitatively by appealing to conservation of total spin: the magnetization torques are understood as the reaction counterpart to the action of the magnet’s collective exchange field on the quasiparticles, i.e. as spin-transfer torques (STTs). In STT physics, transport electrons can change the magnetic state of the device, by switching the orientation, or inducing microwave frequency oscillations in the orientation of magnetic layers. These phenomena hold out the promise of applications, for example for writing magnetically stored information.

Calculations of STTs generally proceed by computing the spatial dependence of spin currents in a circuit and invoking conservation of spin angular momentum to infer the torque which acts on the magnetization. This approach has so far had mixed levels of success in predicting important quantities like critical currents for magnetization switching. Most calculations to date have been based on free electron or on semi-empirical tight-binding models.

In this paper we discuss a practical scheme for estimating the influence of transport currents on order parameter dynamics in superconductors, magnetic metals, or hybrid systems. Our approach, which is explained in detail in Sec. III starts by assuming a time-dependent mean-field theory in which the electron dynamics is described by a single-particle Hamiltonian which is uniquely defined by the density-matrix of the system. In practice the most flexible and powerful choice for such a time-dependent mean-field theory will normally be spin-density functional theory, although any similar mean-field-like approximation is consistent with the procedures outlined below. Hartree-Fock theory, for example, has the same structure and has the advantage of being able to describe non-local exchange effects which might be important under some circumstances, for example when current is carried by a partially occupied bonding band. We then make an adiabatic approximation by assuming that the time-dependence of the single-particle Hamiltonian can be ignored, and use non-equilibrium Greens function (NEGF) theory to evaluate the influence of a bias voltage on the system density matrix. Our implementation of NEGF theory is explained in
The adiabatic approximation is normally appropriate since the driving terms are proportional to transport current and are typically weak compared to characteristic energy scales. Since our interest is in nanoscale systems, the neglect of inelastic scattering in the system implied by the use of steady state NEGF theory is normally justified. (Inelastic scattering lengths under ambient conditions are typically ~ 10nm. The approach could be extended to include inelastic scattering.) The influence of current on order parameter dynamics follows from the dependence of the density-matrix on bias voltage for any given single-particle Hamiltonian.

In the remaining sections of the paper, we apply our theory of current-induced order parameter dynamics to a Co/Cu/Co spin-valve system, an example of transition metal ferromagnet spintronics which is of great practical importance and has received considerable attention. In Sec. IV we describe this \textit{ab initio} calculation, for which we choose a geometry similar to that studied in Ref. 27 in detail. This calculation is intended to illustrate that \textit{ab initio} detail will play a key role in designing magnetic nanostructures whose non-linear magnetotransport properties are optimized for particular applications. In Sec. V we review the results, and discuss some of the surprising insights that this approach gives into the microscopic physics of spin transfer. Finally, in Sec. VI we review our results and outline some other interesting potential applications of this microscopic theory of order parameter dynamics in nanostructures.

## II. MICROSCOPIC THEORY OF CURRENT-INDUCED ORDER PARAMETER DYNAMICS

The practical scheme for microscopic calculation of order parameter dynamics outlined in this section is based on a previously described microscopic theory of spin-transfer torques in circuits containing ferromagnetic metal nanoparticles. This scheme views spin-transfer torques as a specific example of a more general class of phenomena in which collective dynamics is altered by a bias voltage because of the change it induces in the relationship between the single-particle density matrix and the effective single-particle Hamiltonian. This microscopic view of current-induced order parameter dynamics in magnetic metals has consequences that might be significant in some instances, for example in circuits containing antiferromagnetic metal elements. In this section we explain the approach, using a notation that is convenient for the NEGF calculations we apply Co/Cu/Co spin-valves in the body of the paper.

### A. Order Parameter Dynamics in an Isolated System

When an interacting electron system is described by a time-dependent mean-field theory the effective single-particle Hamiltonian can be constructed at each instant in time from the single-particle density matrix. Historically the first example of this type of theory is the Hartree-Fock approximation. In modern usage density-functional-theory is usually more accurate and easier to implement. For example, in the local spin-density-approximation, the Hamiltonian can be constructed from the density and the spin-density, \textit{i.e.} from elements of the single-particle density matrix \( \rho \) that are diagonal in a position representation. The exchange and correlation potentials in the Hamiltonian \( H \) are explicit non-linear functions of the density matrix: \( H = H(\rho) \).

We assume that a procedure for constructing the single particle Hamiltonian from the density matrix has been chosen. Then the dynamics of \( \rho \) is specified by its equation of motion:

\[
\frac{\partial}{\partial t}\rho = \frac{i}{\hbar} [H(\rho), \rho]. \tag{1}
\]

For systems with broken symmetries, for example ferromagnets, the order parameter is specified by a particular average of the density matrix so that Eq. (1) specifies its dynamics. In this purely electronic equation of motion we have ignored coupling between the electronic system and nuclear spins, phonons, or other environmental degrees of freedom which can play a role in some circumstances. Such couplings are accounted for by phenomenological additions to the right hand side of Eq. (1) or to appropriate averages of this equation.

This paper focuses on the influence of transport currents produced by a bias voltage on the collective magnetization dynamics of a small magnetic nanoparticle. It is helpful to consider first an isolated system in which transport currents are absent. We separate both the single-particle Hamiltonian and the density matrix into its spin-dependent and spin-independent contributions:

\[
\begin{align*}
\rho_{i'\delta}\, & = \frac{1}{2}[\rho_{i;\delta'} + \vec{m}_{i;\delta'} \cdot \vec{\sigma}_{\delta}], \\
H_{i'\delta} & = H^{(0)}_{i'\delta} + \frac{1}{2} \Delta_{i'\delta} \cdot \vec{\sigma}_{\delta}.
\end{align*}
\tag{2}
\]

where \( \vec{\sigma} \) is the vector of Pauli spin matrices, \( \delta' \) is orbital indices, and \( \delta \) is spin-indices. The notation for the spin-dependent part of the Hamiltonian is chosen to emphasize that it produces a spin-splitting \( \Delta \) when it is orbital independent, as often assumed in simple toy models of a ferromagnetic metal. In mean field approximations, the interaction contribution to \( \Delta \) and \( \vec{m} \) are locally related according to

\[
\Delta = \Delta_0 (n, m, \vec{m}/m) \tag{3}
\]

where \( n \) and \( \vec{m} \) are the local charge and spin densities, respectively, and \( \Delta_0 \) is some parameterization of the
exchange-correlation potential. Given this notation, it is possible to derive a useful expression for the time-dependence of the the \( \mathbf{S} \)-th component of the spin-density \( \mathbf{S} \) of a chosen subsystem (SS)

\[
\dot{S}^\alpha = \sum_{i \in SS} \left[ \frac{i}{2\hbar} \left( [H_{ij}^{(0)} m_{ij} - m_{ij} H_{ji}^{(0)}] + \Delta_{ij}^{\alpha} \rho_{ji}^{(0)} - \rho_{ij}^{(0)} \Delta_{ji}^{\alpha} \right) \right] + \sum_{i \in SS} \frac{1}{4} \varepsilon_{\alpha,\beta,\gamma} \left[ \Delta_{ij}^{\beta} m_{ij}^\gamma + m_{ij}^\gamma \Delta_{ji}^{\beta} \right].
\]

The first four terms on the right hand side of Eq. (4) represent the net spin-current into the subsystem which has contributions from both the spin-polarization of inter-orbital coherence and from the spin-dependence of the inter-orbital matrix elements in the Hamiltonian. In the final term, contributions in which \( j \notin SS \) represent an additional spin current from spin-dependent hopping. The contributions from \( j \in SS \) describes precessional time-evolution of spins in the subsystem under the influence of effective magnetic fields implied by the spin-dependent terms in the Hamiltonian. We make use of this expression below.

It follows from Eq. (4) that the total spin of an isolated magnetic nanoparticle satisfies

\[
\hbar \mathbf{S} = \frac{1}{2} \text{Tr}[\mathbf{\rho} \mathbf{\Delta}] = \frac{1}{2} \text{Tr}[\mathbf{\rho} \mathbf{\Delta}].
\]

If we assume that the magnetization in the nanomagnet is collinear (or at least nearly so), the interaction contribution to the spin-dependent part of the Hamiltonian, will be in the same direction as the magnetization, according to Eq. (3). It follows that electron-electron interactions, which always provide the dominant contribution to \( \Delta \), do not directly influence the total spin-dynamics. When the only other spin-dependent terms in the Hamiltonian are due to an external magnetic field which produces an orbital independent splitting field \( \Delta(\mathbf{S}) \), Eq. (5) reduces to

\[
\hbar \mathbf{S} = \mathbf{S} \times \Delta^{(z)}.
\]

More generally, additional spin-dependent terms in the Hamiltonian due to spin-orbit coupling and magnetic dipole-dipole interactions produce additional contributions to the effective field so that \( \Delta^{(z)} \) is replaced by an effective magnetic field \( \Delta^{(e\!\!f\!\!f)} \) that depends on the total spin orientation and includes magnetcocrystalline anisotropy, shape anisotropy, and the dissipative contribution due to the coupling between the total spin and incoherent particle hole excitations. These effects are normally described phenomenologically using the Landau-Lifshitz Gilbert equation:

\[
\hbar \mathbf{S} = \mathbf{S} \times \Delta^{(e\!\!f\!\!f)} + a \hbar \left[ \frac{\mathbf{S} \times \mathbf{S}}{|\mathbf{S}|} \right] \times \mathbf{S}.
\]

\section*{B. Influence of a Bias Voltage}

We now address corrections to the Landau-Lifshitz-Gilbert equations which apply when a bias voltage is applied to a metallic nanomagnet. We first describe our strategy for a first principles description of current-induced order parameter dynamics using a more general language with wider applicability and then specialize to the magnetic spin-transfer torque case. Our approach is based on the non-equilibrium Greens function description of non-interacting fermions under the influence of a bias voltage\(^{12} \) which we describe in more detail below. In this approach, the bias voltage is represented by placing the system in contact with particle reservoirs with chemical potentials \( \mu_S = \epsilon_F + eV_B/2 \) and \( \mu_D = \epsilon_F - eV_B/2 \) in source and drain respectively. When the system Hamiltonian and its coupling to source and drain electrodes is time-independent, electrons with energies inside of the transport window \( \mu_D < \epsilon < \mu_S \) solve a time-independent Schroedinger equation with incident-from-source scattering boundary conditions. The Schroedinger equation solution for the system plus reservoirs system is readily constructed using Greens function techniques. Electrons inside and outside the transport window behave very differently. Given a Hamiltonian, the density matrix may be separated into a contribution from electrons inside and outside the transport window:

\[
\rho_{\text{tot}}[\mathbf{H}] = \rho_{\text{cond}}[\mathbf{H}] + \rho_{\text{tr}}[\mathbf{H}].
\]

where we define \( \rho_{\text{cond}}[\mathbf{H}] \) as the contribution to the total density matrix from all states with energy below the transport window minimum \( \mu_D \) and \( \rho_{\text{tr}}[\mathbf{H}] \) as the contribution from states in the transport window. (The notation \( \rho_{\text{cond}} \) is intended to suggest a condensate density-matrix since we will ultimately take an average of the density matrix which highlights an observable associated with a broken symmetry.) To make progress we limit our attention to circumstances in which the order parameter and hence the effective Hamiltonian changes slowly in time and the relevant contributions to the density matrix are dominated by orbitals outside the transport window. Given these approximations, which are soundly based for magnetic systems at least,

\[
\dot{\rho}_{\text{tot}} = i[H, \rho_{\text{cond}}] + \frac{\partial \rho_{\text{tr}}}{\partial \rho_{\text{cond}}}.
\]

\[
\Rightarrow \dot{\rho}_{\text{tot}} \approx i[H, \rho_{\text{cond}}].
\]

Where we have noted that the second term of Eq. (9) is of order \( eV/\epsilon_F \), which is negligibly small for metallic systems. The current-induced contribution to the density-matrix equation of motion is due to the difference between \( H[\rho_{\text{tot}}] \) and \( H[\rho_{\text{cond}}] \):

\[
\dot{\rho}_{\text{CI}} = \frac{1}{\hbar}[H[\rho_{\text{tot}}] - H[\rho_{\text{cond}}, \rho_{\text{cond}}].
\]

Making the appropriate average for the total spin of a nanoparticle we obtain the version of Eq. (6) which describes the current-induced contribution to the dynamics.
of the total nanoparticle spin:
\[ \vec{h} \tilde{S}_{CI} = \frac{1}{2} \text{Tr}[\vec{m}_{\text{cond}} \times [\Delta_{\text{tot}} - \Delta_{\text{cond}}]] \]
\[ = \frac{1}{2} \text{Tr}[\vec{m}_{\text{cond}} \times \Delta_{\text{tr}}]. \tag{12} \]
where \( \Delta_{\text{tot}} \) and \( \Delta_{\text{cond}} \) are the spin-dependent Hamiltonians for the system arising from \( \rho_{\text{tot}} \) and \( \rho_{\text{cond}} \), respectively, and \( \Delta_{\text{tr}} \) is the difference between the two. As described above, we consider situations in which the states in the transport window have relatively little contribution to the order parameter \( (m_{\text{cond}} \gg m_{\text{tr}}) \), and focus on exchange contributions to \( \Delta \), which are dominant, so that, according to Eq. \( \ref{eq:exchange} \)
\[ \Delta_{\text{tot}} = \Delta_{0}(n, m) \frac{\vec{m}_{\text{cond}} + \vec{m}_{\text{tr}}}{m}. \]
\[ \Rightarrow \Delta_{\text{tr}} = \Delta_{0}(n, m) \frac{\vec{m}_{\text{tr}}}{m}. \tag{13} \]
To evaluate the current-induced magnetization dynamics, we need to evaluate the right hand side of Eq. \( \ref{eq:exchange} \).

We assume that we have a circuit containing a nanomagnet with approximately collinear magnetization. For electrons in the transport window we can apply Eq. \( \ref{eq:transport} \) to obtain for any orbital \( i \) in the system
\[ 0 = \frac{i}{2\hbar k} \sum_{\alpha} \left[ H^{(0)}_{ij} m_{\alpha}^{(0)} - m_{\alpha}^{(0)} H^{(0)}_{ji} + \Delta^{(0)}_{ij} \rho_{\alpha}^{(0)} - \rho_{\alpha}^{(0)} \Delta^{(0)}_{ji} \right] + \frac{1}{2} \left( \Delta_{\text{cond}} \times \vec{m}_{\text{tr}} \right). \tag{14} \]
In the above equation, \( \rho^{(0)} \) and \( \vec{m} \) refer to the transport contribution to the total density matrix. In writing the second term as a simple cross product, we have also made a simplifying assumption that spin-dependent hopping terms are negligible, which is valid for the systems studied here. As explained earlier, the first group of terms on the right-hand-side of Eq. \( \ref{eq:transport} \) represents the difference between the spin-current into and out of the nanoparticle (NP), while the last term represents the precession of transport electron spin in the presence of the exchange field from the condensate. In order to change their spin-polarization as they move from source to drain through the nanomagnet, transport electrons must align their spins at an angle to the exchange field. The exchange field produced by the condensate electrons produces a torque on the current carrying quasiparticles. Comparing with Eq. \( \ref{eq:spin_torque} \), we see that this torque is equal and opposite to the torque applied to the condensate by the transport electrons.

In summary, to find the current induced torque on the magnetization, we evaluate Eq. \( \ref{eq:spin_torque} \), or, equivalently, the 2nd term of Eq. \( \ref{eq:transport} \). Eq. \( \ref{eq:transport} \) implies that this torque is equal to the net spin current into or out of the nanoparticle, which is the standard picture of spin transfer torque, and which relies on conservation of total spin angular momentum arguments. As emphasized in Ref. \( \ref{ref:spin_torque} \) our more general approach is applicable to situations in which there is no conservation of spin, and is therefore imperative in systems with spin-orbit coupling, and in anti-ferromagnetic systems, for example.

Finally, to gain further insight into the physics of STT, we evaluate Eq. \( \ref{eq:spin_torque} \) locally by choosing the subsystem to be a single atom, or single atomic orbital, as opposed to the entire nanoparticle. To obtain the total STT on the nanoparticle, we sum over these individual contributions. Such a partition of STT is strictly speaking only valid in the case where hopping is spin-independent, which is approximately the case for our calculations. We have explicitly checked that the difference in STT on the nanoparticle found is this manner compared to evaluating Eq. \( \ref{eq:spin_torque} \) globally is negligible.

### III. NON-EQUILIBRIUM GREENS FUNCTION CALCULATIONS

To implement the ideas in Sec. \( \ref{sec:equilibrium} \) we use non-equilibrium Green’s functions (NEGF), within a density function theory framework. Briefly, the Hamiltonian of the device is calculated within standard parameterizations of LSDA \( \ref{ref:lda} \) generalized to include noncollinear magnetization. The electronic states are then populated according the the distribution functions of the left and right semi-infinite leads, determining a density matrix \( \rho^{(1)} \). The details of the calculation procedure have been given previously \( \ref{ref:텔시} \). Such formalism has been used to successfully calculate transport properties of similar systems \( \ref{ref:ʂ,ref:ʂ₂} \) and spin-dependent properties of molecular scale systems \( \ref{ref:ʂ₃} \).

Since the system under consideration here is in the metallic regime, we work within linear response approximation for the bias dependence \( V_B \). In this case, the expression for the current induced torque on atom \( i \) is given as
\[ \frac{\vec{S}_{CI}}{A} = \frac{e \mu_B}{\hbar (2\pi)^2} \int dk_{||} \sum_{\beta} (\Delta_{\text{cond}(i, \beta)} \times \vec{m}_{\text{tr}(i, \beta)}) V_B. \tag{15} \]
where the \( \beta \) is an orbital label for atom \( i \), and \( k_{||} \) refers to the transverse momentum of each propagating state. The transport contribution to the density matrix is
\[ \rho_{\text{tr}} = G^r \text{Im}(\Sigma_x^r) G^a. \tag{16} \]
Here \( \Sigma_x \) is the retarded self energy, which accounts for the presence of left semi-infinite lead, and \( G^r,a \) are the retarded (advanced) advanced Green’s function for the device. The above Green’s functions and self energy are evaluated at the fermi energy, and the \( \Sigma_L \) term indicates that non-equilibrium electrons emanate from the left lead. We have checked explicitly that the transport density matrix satisfies Eq. \( \ref{eq:transport} \).
Within the Landauer formalism (and staying within linear response), the current density for a bias $V_B$ is:

$$J = \frac{e^2}{h} \frac{1}{(2\pi)^2} \sum_\sigma \int dk_\parallel T_{k_\parallel,\sigma,\sigma}(\epsilon_F)V_B.$$ (17)

where the transmission coefficient is given by:

$$T_{k_\parallel,\sigma,\sigma'} = \text{Tr}[\text{Im}(\Sigma_L^\sigma G^\sigma \text{Im}(\Sigma_R^\sigma') G'^\sigma)\delta_{\sigma,\sigma'}].$$ (18)

The trace above refers to orbital and site. Since most experiments are done under fixed current bias, an experimentally relevant quantity is the total spin torque per current, given by the ratio of Eq. (15) (summed over all atoms) to Eq. (17). In linear response, this is:

$$\frac{\vec{S}}{I} = \frac{\mu_B}{e} \frac{\int dk_\parallel \sum_{i,\beta}(\Delta_{\text{cond}}(i,\beta) \times \vec{m}_{\text{tr}}(i,\beta))}{\sum_\sigma \int dk_\parallel T_{\parallel,\sigma,\sigma}(\epsilon_F)}.$$ (19)

**IV. CALCULATION DETAILS**

The system studied consists of a semi-infinite Co lead, a Cu spacer layer with 9 atomic planes, a Co free layer with 15 atomic planes, and a semi-infinite Cu lead. All layers have translational symmetry in the transverse direction, and therefore represent the bulk realistically. Both Co and Cu are assumed to be in the fcc phase, and we use a lattice constant of 3.54 ˚A throughout. We use norm-conserving pseudopotentials and an s, p, d single-zeta basis set. We have found excellent agreement with established band structure, density of states, and bulk conductivity for Co and Cu with this basis set. We have found that 800 $k$-points within the Brillouin zone is sufficient for convergence of the self-consistent density matrix. To calculate transmission coefficients and non-equilibrium spin densities, we have used 25,600 $k$-points. We have found that there is less than a 1 % difference in these quantities when using up to 32,400 $k$-points. In calculating the spin torque contribution for different channels in the Brillouin zone, we have found that some channels exhibit resonance states, in which the spin density contribution at the Fermi energy is extremely large (up to ~ 50 times larger than "typical" channels). In order to properly account for such states’ contributions to the spin density, we have isolated such points in the Brillouin zone (if their contribution to the spin torque/current is greater than 2 $\mu_B/e$ - such states constitute typically at most 1% of the Brillouin zone area), and integrated over energy from 0 to .8 mV (the potential required to reach typical critical current densities). This smooths out their contribution to the non-equilibrium spin density. We have verified that points in the Brillouin zone which do not exhibit such resonances at the Fermi energy contribute an essentially constant spin density over this energy range, and may be safely treated within linear response.

Once a self-consistent collinear calculation is completed, we initialized the various non-collinear systems by rotating the initial spin density of the free layer to the desired angle. We found that non-collinear configurations do converge to self-consistency, and ostensibly represent extrema of the total energy. This is perhaps surprising since the exchange coupling between the two magnetic layers implies that the energy is extremized in parallel or anti-parallel configurations only. We have calculated the difference in energy between parallel and anti-parallel alignments and have found the difference to be less that $10^{-5}$ Hartree/orbital, thus verifying that to within the tolerance we use for self-consistency (a maximum change of $10^{-5}$ Hartree in the Hamiltonian between iterations of the self-consistent cycle), a noncollinear configuration can be a self-consistent solution. Our value for the change in energy between parallel and anti-parallel (or the exchange energy) is consistent with previously found values.

**V. RESULTS**

Fig. 1 shows the calculated conductance per area versus angle. From the conductivity in the parallel and anti-parallel alignment, a GMR ratio of 48% is obtained. The absolute value of the conductance is consistent with previous calculations of similar systems. The conductance at $\theta = 90^\circ$ is not the mean between the conductance of the parallel and anti-parallel state, which indicates that the behavior can not be captured by a simple rotation of the collinear transmission coefficients in spin-space, but also includes higher order effects such as multiple spin-dependent scattering between the two layers.

Fig. 2 shows the spin torques as a function of the layers’ relative orientation. An important distinction is that between in-plane torques, which are non-energy conserving and present only in non-equilibrium cases, and out-

![Conductance vs. relative orientation](image_url)
of-plane torques, which are the result of itinerant electron exchange, and are responsible for RKKY-like interactions between layers. (In the following we refer to the out-of-plane torques as STT(θ).) According to Fig. 2, the ratio of these two torques varies with angle, but we find it to be consistently above 10%, which can have important implications for the behavior and stability of the magnetization dynamics. Interestingly, we also find that the out-of-plane torque undergoes a sign change near θ = 180°. Previous studies have found a difference in sign between these torques under certain conditions, but the relative sign is usually constant over all angles. The presence of an angle dependent relative sign of the torques may also have interesting consequences for the dynamics of the magnetization.

The angular dependence of the conductance is partially responsible for the departure from perfect sine behavior in STT(θ). This departure is encapsulated in g(θ), defined as STT(θ)/(1+sin(θ)), which has been calculated for simpler models and is an extremely important parameter in spin torque physics. It represents the amount of spin torque delivered per electron in the current flow, and is therefore a measure of the efficiency of spin transfer torque. Fig. 3 shows our calculated g(θ), and, for comparison, that found in the original calculation of Slonczewski. Note that the y-axis for the two curves are different by a factor of 2, so that at small angle, our calculated result is more than a factor of 2 smaller than that of Slonczewski. That is to be expected, as Slonczewski’s model calculation considered the limiting case of pure spin filters, where minority spins are completely reflected, and majority spin completely transmitted through the magnetic interfaces. In this sense the Slonczewski can be considered to give the most optimistic spin transfer efficiency. Interestingly our result shows a smaller difference in efficiency between θ = 0 and θ = π as compared to Slonczewski, which is more consistent with experimental data.

One can make further comparison to experiment in finding the amount of torque delivered per current. This quantity can be extracted from experimental data by finding the slope of the linear relation of critical current versus applied field. The experiment in Ref. 27 gives a slope of 29 mA/T. The resulting spin torque per current (or spin torque efficiency g(θ) at θ = 0) is given by α(EV/2M) = .35μB/e. Here α is the bulk magnetic damping of Co, assumed to be .007, Ms is the bulk magnetization of Co, and V is the volume of the free layer. The value obtained for the efficiency in this way is nearly identical to that determined in point contact experiments. This contrasts with our calculated g(θ) of .11. Our calculated efficiency is smaller than experimental by about a factor of 3. Remarkably, even Slonczewski’s efficiency is smaller than that seen in experiment by 50% (assuming polarization of Co to be .4). Some diffusive models of spin transfer typically predict much smaller efficiencies, with values for Co-Cu structures of about 1%. At first glance then, it is a puzzle as to why the efficiencies seen experimentally are so high. One potentially important consideration is that the deduced experimental efficiencies are not directly measured, but are rather model dependent on the mechanism for switching (usually simple coherent switching is assumed), and depend on parameters such as the magnetic damping, whose values and details are not well known.

Fig. 4 shows the layer resolved spin torques. As expected, the torques show a generally oscillatory decay, which is understood as the result of averaging over many transverse channels’ oscillatory contributions. The length of the free layer is 2.67 nm, thus our result that the transverse spin density is close to complete decay.
is consistent with other approaches, in which the decay length of transverse spin in Co is found to be 3nm.\textsuperscript{33}

We estimate the propensity (or lack thereof) for a spin wave or noncollinear structure in the free layer due to the non-uniform torques by comparing the magnitude of these torques (or effective fields) and the exchange field an atom experiences from its neighbors. The effective Heisenberg nearest neighbor coupling constant for bulk Co has been computed to be 1.085 mRy.\textsuperscript{36} The resulting exchange constant between planes (considering only nearest neighbor interactions) is then 4.34 mRy. This corresponds to a field of about $10^3\ T$. For a current of 1 mA, the figure shows that typical non-equilibrium exchange fields to be on the order of $0.0075\ T$. The resulting deflections of the spin are much less than $1^\circ$. This slight departure from collinearity indicates that the surface-effect aspect of spin transfer torques (more generally, non-uniform torques) are not manifest in thin layers.

![Relative orbital contribution to STT](image)

**FIG. 4**: Breakdown of relative orbital contributions to spin torque in the z-direction, for the $\theta = 90^\circ$ case.

Fig. 5 shows the relative contributions to the spin transfer from the $s$, $p$, and $d$ orbitals. Such a partition ignores hybridization between orbitals, but one can nevertheless extract meaningful results from such a division.\textsuperscript{34} We find the $d$-orbitals' contribution is dominant. This is due to the substantial amount of $d$-electron conduction in the system, and more importantly to the relatively larger spin-dependent exchange-correlation potential of the $d$-electrons. A commonly used model for spin torque calculations in multilayers or in domain walls is the $s$-$d$ model, in which the $d$-electrons are responsible for the exchange field, while the $s$-electrons are responsible for the current. Spin torque on the $d$-electrons’ magnetization is a result of the interaction of these two subsystems. However, in the ballistic limit for 3$d$ transition metals, our results show that it is largely the interaction between equilibrium and non-equilibrium $d$-electrons that is responsible for spin torque physics.

**VI. SUMMARY AND CONCLUSIONS**

In this work, we have formulated a general scheme for calculating the dynamics of an order parameter in the presence non-equilibrium, current carrying quasiparticles. This scheme is applied to find the current-induced torques that are present in magnetic spin valve structures under bias. For the specific system studied, we have found the STT to be localized in the surface planes of the free magnetic layer, and have found the out-of-plane torque to be a substantial fraction of the in-plane torque. The magnitude of the torque is appreciably smaller than that deduced from experiment, although we note that experimental measures of the absolute spin torque are model-dependent. In addition, we have found the STT to be due mostly to the interaction between non-equilibrium $d$-electrons with the exchange field, which is itself also due mostly to the spin splitting of the $d$-band electrons.

The formalism presented here is more general than that typically used in calculations of current induced torques in magnetic materials. In particular, since it does not rely on conservation of angular momentum, it may be applied to system with spin-orbit coupling, or to antiferromagnetic systems. And the calculation of current induced torques on an atomic, or even atomic orbital scale resolution allows for the study these effects in molecular scale systems. More generally, it may be applied to any mean-field system with an order parameter - for example superconductors, or ferromagnet-superconductor hybrids.

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27. The relation between partitioning STT by orbital and spin-dependent hopping can be understood in the following way: When summing over orbital spin fluxes, normally intra-orbital spin currents cancel, so that such spurious contributions do not contribute to the total spin flux into/out of the atom. If there is spin-dependent hopping, such contributions do not cancel. If spin-dependent hopping is weak, however, these spurious contributions are negligible.
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FIG. 5: Calculated layer resolved torque per current density and spin transfer induced change field per A. The (X,Y,Z) directions in the legend refer to the spin torques, while the direction of the effect...