

Computing noncollinear spins and spin torque in ATK from QuantumWise A/S

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Abstract

This document explains the formalism used for computing noncollinear spins and spin torque in the device structures by ATK.

NONCOLLINEAR SPINS

Systems with noncollinear spins are quite ubiquitous and refer to situations where the spin direction depends on position in such a way that there is no particular direction in which all the spins are (anti)parallel. This includes systems with spin spirals (e.g. chromium) and helicoids, canted spins (e.g. manganites), and most commonly domain walls in ferromagnetic materials. ATK allows you to study systems with noncollinear spins from first principles.

Unlike in a simple case of collinear spins (ferromagnetic (FM) or anti-ferromagnetic (AFM) ordering of moments in a crystal) the Kohn-Sham (KS) equations for different spin directions marked by Greek letters $\alpha, \beta = \uparrow, \downarrow$ do not decouple in a noncollinear system. The situation is simplified if one introduces the exchange-correlation field that plays a role of an internal magnetic field, \mathbf{B}_{xc} , given by the following variational derivative of the total exchange and correlation energy E^{xc} with respect to the magnetization density $\mathbf{m}(\mathbf{r})$:

$$\mathbf{B}_{xc}(\mathbf{r}) = \delta E^{xc}[n, \mathbf{m}] / \delta \mathbf{m}(\mathbf{r}),$$

where $\mathbf{m}(\mathbf{r}) = n_{\uparrow}(\mathbf{r}) - n_{\downarrow}(\mathbf{r})$ is the local spin density, $n_{\uparrow, \downarrow}(\mathbf{r})$ the electron density for spin up/down electrons with respect to a local quantization axis that coincides with the direction of \mathbf{B}_{xc} in the local spin density approximation (LSDA), where

$$\begin{aligned} \mathbf{B}_{xc}(\mathbf{r}) &= -\mathbf{e}(\mathbf{r}) n(\mathbf{r}) \partial[\epsilon^{xc}(n, m)] / \partial m \\ &\equiv \Delta \mathbf{e}(\mathbf{r}), \end{aligned} \tag{1}$$

where $\mathbf{e}(\mathbf{r}) = \mathbf{m}(\mathbf{r}) / m(\mathbf{r})$ is the unit vector in the direction of the local moment, $\epsilon^{xc}(n, m)$ the exchange-correlation energy *density*, and we have introduced the exchange splitting energy per unit moment Δ , frequently used in quantum theories of magnetic materials. This collinearity, $\mathbf{B}_{xc}(\mathbf{r}) \parallel \mathbf{m}(\mathbf{r})$, does not hold in the generalized gradient approximation (GGA) [1]. Then, the KS equations read [1]

$$\begin{aligned} \mathcal{H} \psi_i(\mathbf{r}) &= \varepsilon_i \psi_i(\mathbf{r}), \\ \mathcal{H} &= T + V^{ei}(\mathbf{r}) + V^H(\mathbf{r}) + V^{xc}(\mathbf{r}) - \mathbf{B}_{xc}(\mathbf{r}) \cdot \boldsymbol{\sigma} \end{aligned}$$

where \mathcal{H} is the standard Hamiltonian of a one-electron DFT problem, $V^{xc} = \delta E^{xc}[n, \mathbf{m}] / \delta n(\mathbf{r})$, which is simply $\partial[n\epsilon^{xc}(n, m)] / \partial n$ in the LSDA,

$$\psi_i(\mathbf{r}) = \begin{pmatrix} \alpha_i(\mathbf{r}) \\ \beta_i(\mathbf{r}) \end{pmatrix},$$

is the two-component spinor electron wavefunction. We will use the index s to denote the spin components of the wavefunction, index $i = \mathbf{R}L\lambda$ with $L = (l, m)$ denoting the orbital λ on site \mathbf{R} with angular momentum l and azimuthal quantum number m . Finally, $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ is the vector composed of three Pauli matrices.

One can define the noncollinear density matrix in a ‘‘spin space’’ given by

$$n(\mathbf{r}) = \sum_i^{\text{occ}} \psi_{i\alpha}^\dagger(\mathbf{r}) \psi_{i\beta}(\mathbf{r}) = \begin{pmatrix} n_{\alpha\alpha} & n_{\alpha\beta} \\ n_{\beta\alpha} & n_{\beta\beta} \end{pmatrix}$$

from which we can obtain the polarization vector

$$m^a(\mathbf{r}) = \sum_i^{\text{occ}} \psi_{i\alpha}^\dagger(\mathbf{r}) \sigma_{\alpha\beta}^a \psi_{i\beta}(\mathbf{r}),$$

with Roman letters marking Cartesian components, $a = x, y, z$, with summation over repeated indices, as

$$\begin{aligned} m^x &= 2 \operatorname{Re} n_{\alpha\beta}, \\ m^y &= -2 \operatorname{Im} n_{\alpha\beta}, \\ m^z &= n_{\alpha\alpha} - n_{\beta\beta}. \quad (\text{no summation}) \end{aligned} \quad (2)$$

The direction of the polarization vector \mathbf{m} defines a local spin quantization axis and the corresponding rotation matrix U which diagonalizes n through the unitary transformation

$$n^{diag} = U n U^\dagger,$$

which transforms the density matrix into the diagonal form

$$n^{diag} = \begin{pmatrix} n_\uparrow & 0 \\ 0 & n_\downarrow \end{pmatrix}.$$

The rotation matrix is defined in terms of standard spherical coordinates (θ, ϕ) of the polarization vector \mathbf{m} with (m^x, m^y, m^z) components in a laboratory frame [5, 6],

$$U = \begin{pmatrix} e^{i\frac{\phi}{2}} \cos \frac{\theta}{2} & e^{-i\frac{\phi}{2}} \sin \frac{\theta}{2} \\ -e^{i\frac{\phi}{2}} \sin \frac{\theta}{2} & e^{-i\frac{\phi}{2}} \cos \frac{\theta}{2} \end{pmatrix}.$$

To rotate from the diagonal back to the non-diagonal form, one applies the inverse operation

$$n = U^\dagger n^{diag} U.$$

SPIN TRANSFER TORQUE

Spin transfer torque (STT) refers to a situation when a current of spin-polarized carriers from one part of a system with a particular polarization given by the unit vector \mathbf{e}_{RL} (a ‘‘reference layer’’, RL] with the polarization enters e.g. a ‘‘free layer’’ (FL) with magnetization given by the vector \mathbf{e} , with $|\mathbf{e}_{RL} \cdot \mathbf{e}| < 1$, and exerts the torque on the magnetic moment in the FL [2, 3]; for a review, see Ref. [4, 5]. The polarized current with density J brings J/q electrons into the FL per second per unit area, each carrier on average bringing $\eta\hbar/2$ angular momentum with them, where q is the elementary charge, and $\eta = (J_\uparrow - J_\downarrow)/J$ is the average polarization. As a result, $g\eta(\hbar/2)J/q$ is the net flow of magnetization into a unit area of the FL, where g is the gyromagnetic ratio. Its ratio to the moment per unit area of the FL with saturated magnetization M_S and thickness t (that is, $M_S t$), gives the torque per unit area,

$$\mathbf{T}_{STT} = T_\parallel = -A \mathbf{e} \times \mathbf{e} \times \mathbf{e}_{RL}, \quad (3)$$

$$A = g\eta \frac{\hbar J}{2q} \frac{1}{M_S t}. \quad (4)$$

This is the so-called in-plane component of a total torque, \mathbf{T}_\parallel , while there is also a field-like perpendicular component $\mathbf{T}_\perp \propto \mathbf{e} \times \mathbf{e}_{RL}$.

One can use the definition of the torque as a rate of change of a spin moment under the effect of local exchange field at a general angle to a local spin moment direction (not at mutual angle $\sigma, \widehat{\mathbf{B}}_{xc} = 0, \pi$, i.e. at general *noncollinear* mutual orientation):

$$\hat{T}^a = -\frac{i}{\hbar} \left[\frac{\hbar}{2} \sigma^a, \mathcal{H} \right] = \frac{i}{2} B_{xc}^b [\sigma^a, \sigma^b] = \frac{i}{2} B_{xc}^b 2i \epsilon_{abc} \sigma^c = (\boldsymbol{\sigma} \times \mathbf{B}_{xc})^a, \quad (5)$$

where $a = x, y, z$, and ϵ_{abc} is the fully antisymmetric tensor. To get the expectation average of the torque, one needs to average the torque operator, Eq. (5), with the density matrix of the system ρ and sum it up over the all final states (in the right electrode; we presume for clarity sake that the electrons are flowing from the left electrode, which is the reference layer, into the right free layer electrode through the free layer):

$$\mathbf{T} = \operatorname{Tr}(\rho \boldsymbol{\sigma} \times \mathbf{B}_{xc}) = \operatorname{Tr}(\delta\rho \boldsymbol{\sigma} \times \mathbf{B}_{xc}). \quad (6)$$

It is worth noting that in the small current regime, the contribution to the torque is given only by the non-equilibrium part of the density matrix, $\delta\rho = \rho - \rho_{eq} \propto J$. Summation over both spins will add the polarization factor η , so in the linear regime the exact expression (6) yields the same functional form as the phenomenological (3). Since in the latter all parameters are pretty well defined or can be found from ab-initio simulations, it would be interesting to compare phenomenological and exact (DFT) values of the coefficient A . Technical details of the formalism are given in the Appendix.

In ATK, the torque can be calculated in the real space representation through the equilibrium effective internal field $\mathbf{B}_{R,xc}^{(eq)}$ and the non-equilibrium part of the local magnetization \mathbf{m}_R . The Cartesian components are found from

$$\begin{aligned} B_{eq}^x &= 2 \operatorname{Re} V_{\alpha\beta}^{xc} \\ B_{eq}^y &= -2 \operatorname{Im} V_{\alpha\beta}^{xc} \\ B_{eq}^z &= V_{\alpha\alpha}^{xc} - V_{\beta\beta}^{xc} \end{aligned}$$

If we assume that the current direction is along the z -axis, and the moment in the free layer $\mathbf{e}||x$, then the two components of the torque are

$$\begin{aligned} T_{||} &= \sqrt{T_x^2 + T_z^2}, \\ T_{\perp} &= T_y. \end{aligned}$$

In the linear response regime the non-equilibrium density is obtained through

$$\delta\rho = \rho^L(E_F)qU, \quad (7)$$

where ρ^L is the *left* (RL) local density of states and U the applied bias; see Eq. (15) below. From Eq. (2) we obtain \mathbf{m}_{neq} . This corresponds to an injected spin momentum that is absorbed in the free layer [7], see Fig. 1.

ATK provides an interface to calculate V^{xc} (`ExchangeCorrelationPotential`) and ρ^L (`LocalDeviceDensityOfStates`) in equilibrium, and from that ATK evaluates the torque Eq. (6). At finite bias ATK may calculate n_{neq} by evaluating ρ^L at a number of energies and integrating them over the window of energies available for transport, i.e. $(E_F - qU/2, E_F + qU/2)$.

A simple spin scattering picture of spin current and its ‘‘absorption’’ by the free layer is given in Ref. [5] along with a discussion of memory devices. A few general analytical results for spin torque in DFT have been presented in Ref. [9]. Recently, a spin torque stack like FeCoB/MgO/FeCoB became very popular because of a large resistance change as a result of spin moment change in the free layer, subject to a flowing polarized current, non-volatility, and a good potential for scaling of the normally used vertical stack, see Fig. 1. The corresponding physics and actual spin transfer torque magnetic random access memory (STT MRAM) technology is discussed on a basic physics level in various recent papers (see Ref. [10] and references therein). A more memory technology oriented review can be found in Ref. [11].

APPENDIX

The torque on a free layer is given by

$$\mathbf{T} = \operatorname{Tr} \left[\delta\rho \hat{\mathbf{T}} \right], \quad (8)$$

with $\hat{\mathbf{T}}$ from (5), where ρ is the actual density matrix calculated by ATK for a device system;

$$\delta\rho = \rho - \rho_{eq} = \rho + \frac{1}{\pi} \int_{-\infty}^{\infty} dE f_R(E) \operatorname{Im} G_0^r(E), \quad (9)$$

where

$$G_0^r(E) = [E - \mathcal{H} - \Sigma_L(E) - \Sigma_R(E)]^{-1}. \quad (10)$$

is the retarded Green function (GF) at zero bias voltage ($U = 0$) [12] with $\Sigma_{L(R)}$ denoting the left (right) self-energy operator [12]. In noncollinear LSDA

$$\operatorname{Tr} \left[\rho_{eq} \hat{\mathbf{T}} \right] \equiv 0, \quad (11)$$

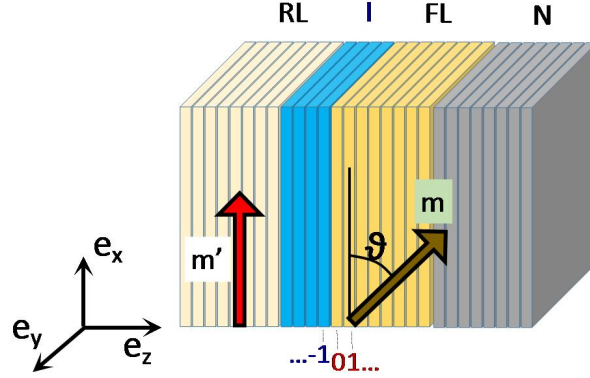


FIG. 1: Schematic of FM(RL)-I-FM(FL)-M device with FM(RL) the ferromagnetic reference layer with a fixed direction of magnetic moment m' , I the insulator, FL the ferromagnetic “free” layer with freely rotating magnetic moment m , and N the nonmagnetic metal electrode. The spin-polarized current runs in e_z -direction. When the general case of misaligned moments m and m' there is a torque exerted on the moment in the free layer by electron spins incident from the reference layer (RL). Quite naturally, the magnitude of the torque depends on the density of a spin-polarized electron states at the interface between the right-most atomic layer in the insulator (marked as -1) and the first atomic layer in the free layer (marked as 0).

so in that approximation $\mathbf{T} = \text{Tr} [\rho \hat{\mathbf{T}}]$. From (12) and (9) we obtain

$$\begin{aligned} \mathbf{T} = & \text{Tr} \left[-\frac{1}{\pi} \int dE f_R(E) \text{Im} G^r(E) \hat{\mathbf{T}} \right] \\ & + \text{Tr} \left[\frac{1}{2\pi} \int dE G^r(E) \Gamma_L(E) G^a(E) [f_L(E) - f_R(E)] \hat{\mathbf{T}} \right], \end{aligned} \quad (12)$$

where $f_{(L)R}(E) = f[E - (+)qU/2]$ is the Fermi functions for the left (right) electrode at bias U , $\Gamma_L(E - qU/2)$ is the coupling operator for the left electrode, and

$$G^r(E) = [E - \mathcal{H} - \Sigma_L(E - qU/2) - \Sigma_R(E + qU/2)]^{-1},$$

is the retarded GF at finite bias. The advanced GF is $G^a(E) = [G^r]^\dagger$. ATK has routines calculating both integrands in (12) and evaluating the integrals over energy.

The above general expression for a torque (which can be applied by analogy to evaluating an expectation value of *any* one-particle electron operator) is strongly simplified in a small bias regime $U \rightarrow 0$ (in practice, qU should be much less than the energy fine structure in the density of states or density matrix). In this case, the first term in (12) vanishes because of (11) and we get, to linear order in U ,

$$\mathbf{T} = \text{Tr} \left[\frac{qU}{2\pi} \int dE G_0^r(E) \Gamma_L(E) G_0^a(E) [-\partial f(E)/\partial E] \hat{\mathbf{T}} \right], \quad (13)$$

which at zero temperature reduces to quantities on the Fermi surface :

$$\mathbf{T} = \text{Tr} [qU \rho^L \hat{\mathbf{T}}], \quad (14)$$

$$\rho^L = G_0^r(E) \Gamma_L(E) G_0^a(E). \quad (15)$$

at $E = E_F$. This defines the quantities mentioned in the main text above.

We can use continuum-like theory to get an idea about *layer-resolved* spin torque:

$$\frac{\partial S_a}{\partial t} = \nabla_b J_{ab} + \frac{S_a - S_a^{\text{eq}}}{\tau_{sf}} + T_a,$$

where $J_{ab} = v_a S_b$ the tensor of spin flux, with v_α the Cartesian component of electron velocity at the Fermi surface, S_a the spin density, with S_a^{eq} its equilibrium value, and τ_{sf} the spin-flip time, and finally T_a the vector of spin torque, $a, b = x, y, z$ with summation implied over the repeating indices. In an atomistic model, all characteristics are the functions of the component of wave vector parallel to an interface, \mathbf{k}_\parallel . In a stationary case with $\partial/\partial t = 0$ and the spin flip length much larger than the thickness of the scattering free layer, $v_F \tau_{sf} \gg t$, the torque is simply the divergence of the spin flux tensor:

$$T_a = -\nabla_b J_{ab},$$

and we can define a torque on a particular (n-th) layer as

$$\mathbf{T}^n = -\nabla \cdot \mathbf{I} = \mathbf{I}^{n-1,n} - \mathbf{I}^{n,n+1}.$$

so the torque on a thick enough layer would be [7]

$$T = \sum_{n=0}^{\infty} \mathbf{I}^{n-1,n} - \mathbf{I}^{n,n+1} = \mathbf{I}^{-1,0} - \mathbf{I}^{\infty,\infty} = \mathbf{I}^{-1,0}. \quad (16)$$

Here, the superscripts -1 and 0 refer to the last monolayer of the I barrier and the first layer in the F barrier, respectively, Fig. 1. This layer representation would be helpful in atomistic studies of spin dynamics induced by a flow of spin-polarized current.

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