Doppler shift picture of the Dzyaloshinskii–Moriya interaction

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We present a physical picture for the emergence of the Dzyaloshinskii–Moriya (DM) interaction based on the idea of the Doppler shift by an intrinsic spin current induced by spin–orbit interaction under broken inversion symmetry. The picture is confirmed by a rigorous effective Hamiltonian theory, which reveals that the DM coefficient is given by the magnitude of the intrinsic spin current. The expression is directly applicable to first principles calculations and clarifies the relation between the interaction and the electronic band structures. Quantitative agreement with experimental results is obtained for the skyrmion compounds Mn$_{1-x}$Fe$_x$Ge and Fe$_{1-x}$Co$_x$Ge.

Magnets with broken inversion symmetry such as chiral magnets and those in multilayers have been studied intensively in recent years owing to their potential application in nanomagnetic devices. Their attractive properties originate from the Dzyaloshinskii–Moriya (DM) interaction\cite{1, 2}, whose Hamiltonian takes the following form in the continuum limit:

$$H_{\text{DM}} \equiv \int d^3 r \sum_{ia} D_i^a (\nabla_i \mathbf{n} \times \mathbf{n})^a,$$

with $\mathbf{n}$ a unit vector denoting the direction of magnetization and $D_i^a$ the DM coefficient. While the exchange interaction tends to align the local magnetizations (anti)parallel, the DM interaction makes them twist, which yields numerous magnetization structures at the nanoscale such as helices\cite{3} and skyrmions\cite{4, 5} and gives high mobility to domain walls\cite{6, 7}. The DM interaction is also a key ingredient in multiferroics since it connects magnetizations to electric polarization\cite{8, 9}.

In 1960, Moriya\cite{2} clarified microscopically that the DM interaction arises at the first order of the spin–orbit coupling of electrons. Since recent investigations involving the DM interaction have become very diverse and precise, its quantitative estimation scheme applicable both to metals and insulators has been strongly demanded. However, the relation between the strength or sign of the DM interaction and the electronic band structure is not clearly seen in those formalisms based on the twist energy.

Recently, Berry’s phase formalism for the DM interaction was presented\cite{17} where the relation between the DM interaction and the electronic band structure became clear. In this formulation, however, twist torque operators need to be evaluated, which is not always easy. It was recently proposed that the DM coefficient is given by a derivative of a spin correlation function with respect to the wave vector\cite{21}. This spin correlation function representation has the advantage of having a direct relation between the DM coefficient and the spin correlation function $\chi_{nk}$ for band $n$ and wave vector $\mathbf{k}$. However, this approach turned out to be insufficient to reproduce the value $x_c \approx 0.8$ for Mn$_{1-x}$Fe$_x$Ge at which the DM coefficient changes its sign\cite{20}.

The aim of this paper is to present a new picture for the emergence of the DM interaction as well as to develop a calculation scheme for its coefficient with accuracy and predictability. We show that the DM interaction is a consequence of the “Doppler shift” due to an intrinsic spin current induced by the spin–orbit interaction under broken inversion symmetry. This fact leads naturally to our main conclusion that the DM coefficient is given by the magnitude of the intrinsic spin current. We also develop a rigorous derivation of the coefficient based on an effective Hamiltonian method.

Let us start with an intuitive argument. The spin–orbit interaction with broken inversion symmetry is generally represented by a quantum mechanical Hamiltonian:

$$H_{\text{so}} = -\sum_{ia} \lambda_i^a \hat{p}_i \sigma_a,$$

where $\hat{p}$ is a momentum operator, $\sigma$ is a vector of Pauli matrices, and $\lambda_i^a$ is a coefficient specifying the amplitude of the spin–orbit field\cite{21}. In terms of a spin current operator, $\hat{j}_{ia} = \frac{1}{2m} \hat{p}_i \sigma_a$, the interaction is written as $H_{\text{so}} = -2m \sum_{ia} \lambda_i^a \hat{j}_{ia}$, and it thus generates an intrinsic spin current proportional to $\lambda_i^a$. The existence of an equilibrium spin current does not contradict the laws of thermodynamics since the current does not do work as far as it is static. A similar spin current but with a different origin is known to arise from non-collinear spin structures\cite{22}.

We are interested in the magnetic energy of localized spins arising from the electron carrying an intrinsic spin...
The electron is modified as follows. The existence of an intrinsic direction of the Doppler shift, the magnetic energy is modified to
\[ \mathbf{n} \cdot \nabla (\mathbf{n}) + O(\eta^2). \]
We see here that the DM interaction arises and that its magnitude is proportional to that of the intrinsic spin current, \( D^2 \propto j^{s,i} \). The Doppler shift interpretation of the DM interaction is natural since the nonreciprocal propagation of spin waves is naturally explained.

The picture presented above is a classical one. We present here a rigorous quantum mechanical derivation based on a continuum model, focusing on the metallic case. In the field representation, the Hamiltonian is

\[ H = \int d^3r \sum_{\alpha} c^\dagger_{\alpha} \left[ -\frac{\hbar^2 \nabla_i^2}{2m} - J_{\alpha} \mathbf{n} \cdot \mathbf{\sigma} + \frac{i}{2} \sum_{i} \lambda_i \cdot \mathbf{\sigma} \nabla_i \right] a_{\alpha}, \]

where \( c_{\alpha} \) and \( c^\dagger_{\alpha} \) are electron creation and annihilation operators for the orbit \( \alpha \), respectively, \( c^\dagger \nabla_i c = \sigma^i \nabla_i (\nabla_i c^\dagger) \) and the constant \( \lambda_i \) represents the spin–orbit interaction in the continuum with broken inversion symmetry. The local direction of the magnetization \( \mathbf{n}(\mathbf{r}) \), with \( \mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \), is static. We consider here a simplified model with the quadratic dispersion and the spin–orbit interaction linear in the momentum but the extension to general cases is straightforward as we shall demonstrate later. The effective model is derived from a multiband Hubbard model by introducing the magnetization by use of a Hubbard–Stratonovich transformation.

Considering the case of strong ferromagnets, i.e., large \( J_{s,i} \), we diagonalize the exchange interaction by introducing a unitary transformation in spin space as \( c_{\alpha}(\mathbf{r}) = U(\mathbf{r}) a_{\alpha}(\mathbf{r}) \), where \( U \) is a 2 \times 2 unitary matrix satisfying \( U^\dagger (\mathbf{n} \cdot \mathbf{\sigma}) U = \sigma^{26,27} \). Explicitly, \( U \) is chosen as \( U = \mathbf{m} \cdot \mathbf{\sigma} \) with \( \mathbf{m} = (\sin \frac{\theta}{2} \cos \phi, \sin \frac{\theta}{2} \sin \phi, \cos \frac{\theta}{2}) \). As a result of the unitary transformation, derivatives of the electron field become covariant derivatives as

\[ e_s = U^\dagger \mathbf{C} U, \]

where \( \mathbf{C} \) is the polarization of the spin current, the above expression indicates that the spatial derivative of the localized spin structure is modified when the electron spin media flow to be a “covariant derivative” as

\[ \mathbf{D}_i \mathbf{n} = \nabla_i \mathbf{n} + \eta (\mathbf{j}_{s,i} \times \mathbf{n}), \]

where \( \eta \) is a coefficient. This covariant derivative is interpreted as a result of the Doppler shift as seen from the argument above. Only the component of the spin current perpendicular to the localized spin leads to the Doppler shift, in contrast to the spin-transfer torque effect arising from the adiabatic (parallel) component. Similar Doppler shift for a vector in a moving medium has been known in the case of the velocity vector of sound waves.

When the spatial derivative of the localized spin is modified to the derivative described by Eq. (3), because of the Doppler shift, the magnetic energy is modified to be proportional to \( (\mathbf{D}_i \mathbf{n})^2 = (\nabla \mathbf{n})^2 + 2\eta \sum_i \mathbf{j}_{s,i} \cdot (\mathbf{n} \times \nabla \mathbf{n}) \). As a result of the unitary transformation, derivatives of the field are modified as

\[ \mathbf{D}_i \mathbf{n} = \nabla_i \mathbf{n} + \eta (\mathbf{j}_{s,i} \times \mathbf{n}), \]

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Our objective is to derive an effective Hamiltonian describing the magnetization by integrating out the conduction electrons. Here, we are interested in the DM interaction [1], and it is sufficient to consider the first order derivative terms. The effective Hamiltonian is therefore

$$H_{\text{eff}} = \int d^3 r \sum_{\alpha,i} j_{s,\alpha,i}^a A_{s,i}^a,$$  

(7)

where $j_{s,\alpha,i}^a$ is the expectation value of the spin current density in the rotated frame, which is related to the one in the laboratory as $j_{s,\alpha,i}^a = \sum_b R_{ab} j_{s,\alpha,b}^b$. By use of the identity $\sum_b R_{ab} A_{s,b}^b = (\nabla_i n \times n)^a + n^a A_{s,i}^a$, the effective Hamiltonian reads

$$H_{\text{eff}} = \int d^3 r \sum_{ia} D_{s,i,a}^a (\nabla_i n \times n)^a + \sum_i j_{s,i}^\parallel A_{s,i}^\parallel,$$  

(8)

where $j_{s,i}^\parallel \equiv \sum_{\alpha} j_{s,\alpha,i}^\parallel \equiv n \cdot \sum_{\alpha} j_{s,\alpha,i}$, and

$$D_{s,i,a}^a \equiv \sum_{\alpha} j_{s,\alpha,i}^{a,\alpha}$$  

(9)

with $j_{s,\alpha,i}^{a,\alpha} \equiv j_{s,\alpha,i} - n^a j_{s,\alpha,i}$. We see that the DM coefficient is simply given by the expectation value of the spin current density of the conduction electrons. Since $n \cdot (\nabla_i n \times n) = 0$, only the perpendicular component contributes to the DM interaction, which is consistent with the intuitive Doppler shift argument (Eq. (3)).

A great advantage of the present formulation for material design is that Eq. (9) enables the prediction of the DM coefficient based on the features of the band structure. Let us consider three typical spin configurations of a conduction electron in the momentum space, the Rashba (which arises in polar systems), the Dresselhaus and the Weyl (in chiral systems), represented by the Hamiltonians $H_R = \alpha (k_x \sigma_y - k_y \sigma_x)$, $H_D = \beta (k_x \sigma_x - k_y \sigma_y)$ and $H_W = \gamma (k_x \sigma_x + k_y \sigma_y)$, respectively. The schematic spin textures are shown in Fig. 2. The DM coefficients in those cases (denoted by $D_R$, $D_D$ and $D_W$, respectively) are

$$D_{R,i}^a = \alpha n_{el} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad D_{D,i}^a = \beta n_{el} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$D_{W,i}^a = \gamma n_{el} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$  

(10)

where $n_{el}$ is the electron density and the row and column correspond to spatial ($i$) and spin ($a$) indices, respectively. We therefore see that polar systems lead to antisymmetric DM coefficients while diagonal coefficients are expected in non-polar systems, as discussed also in Refs. [20] and [21] by a different approach.

As for the DM coefficient, our result Eq. (9) agrees with that of Ref. [15] derived by evaluating the energy increase when the magnetization is twisted by a local spin rotation. The expression for the energy increase turned out to be the expectation value of the anticommutator of the spin rotation operator and the hopping matrix element, which is essentially the spin current density. On the other hand, the expression discussed in Ref. [21], $D \propto \frac{\partial^2 \chi}{\partial q^2} |_{q=0}$ ($\chi$ is the spin correlation function with wave vector $q$), and the ones obtained by a Ruderman–Kittel–Kasuya–Yosida (RKKY) approach [22][23] are valid when the exchange interaction, $J_{s,n} \cdot c_{\alpha}^\dagger \sigma_{\alpha}$ in Eq. (1), is weak enough and can be treated perturbatively. In contrast, in our method that uses a unitary transformation, a strong exchange interaction is assumed.

To examine this approach quantitatively, we perform relativistic electronic-structure calculations for the B20 chiral ferromagnet, FeGe, using quantum-espresso code [25]. We treat exchange and correlation effects within the Perdew–Burke–Ernzerhof (PBE) generalized-gradient approximation [26] and use ultrasoft pseudopotentials [27] with plane-wave cutoffs of 50 Ry for wavefunctions and of 400 Ry for charge densities, respectively. Brillouin-zone (BZ) integration is carried out on a $8 \times 8 \times 8$ k-point mesh. To discuss the atomic composition dependence for Mn$_{1-x}$Fe$_x$Ge and Fe$_{1-x}$Co$_x$Ge, we compute the self-consistent charge densities for several different carrier densities by fixing the atomic geometries and the lattice constant to the experimental values of FeGe. In all cases, we assume the total magnetic moment in each unit cell to be aligned along the z-axis.

To calculate the DM coefficient using Eq. (9), from the first principles, we consider a general form of the spin current density as follows:

$$j_{s,\alpha,i}^a = \sum_k \frac{1}{4} \langle c_{k\alpha}^\dagger (v_i \sigma_a + \sigma_a v_i) c_{k\alpha} \rangle,$$  

(11)

where the velocity operator is defined as $v_i = dH_k/dk_i$ with $H_k = e^{-i \mathbf{k} \cdot \mathbf{x}} H e^{i \mathbf{k} \cdot \mathbf{x}}$. Due to the symmetry of B20 magnets, we focus on $D_{x,i}^a = \sum_{\alpha} j_{s,\alpha,i}^x$, and $D_{y,i}^a$. In fact, the other components of $D_{i}^a$ are found to be negligible compared to $D_{x,i}^a$ and $D_{y,i}^a$. For the BZ integration in Eq.
FIG. 3. The DM coefficients $D$ for $\text{Mn}_{1-x}\text{Fe}_x\text{Ge}$ and $\text{Fe}_{1-x}\text{Co}_x\text{Ge}$ calculated using the energies of helical spin structures, $E(q) = D_q + Jq^2$, and as expectation values of the equilibrium spin current $D = \langle j_s \rangle$. The error bars for each calculation indicate the fitting errors of $E(q)$ and the variances of $D_x^x$ and $D_y^y$, respectively.

FIG. 4. (a) Contribution of each band to the DM interaction, $D_{nk}$, with dominant band anticrossing points circled, and (b) the energy distribution of the DM interaction, $D(E)$ (black line), for FeGe. The Fermi energy dependence of the DM interaction, $D = \int E D(E') f(E')dE'$, within the rigid band approximation is also shown as the red line.

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Similar expression for the covariant derivative has been discussed for the particular case of the Rashba spin–orbit interaction in Ref. [30] but it was not associated with the intrinsic spin current.

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The spin current in the expression of Eq. (9) is the intrinsic part induced by the spin–orbit interaction in the absence of magnetization structures. Obviously, the spin current generated by the magnetization structure, $J_{\alpha}^{(m)} \propto (\partial_{\alpha} n \times n)$, results in only the terms with higher order derivatives in the effective Hamiltonian.

As in seen in Eq. (5), spin transfer effect arises if the adiabatic contribution $j_{\alpha}^{(a)}$ remains finite, but such spontaneous motion does not arise at least when the spin–orbit interaction is weak. We have checked that the adiabatic spin current vanishes to the third order of $\lambda$ in our model.