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Correlated band theory of spin and orbital contributions to Dzyaloshinskii-Moriya interactions

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A distinct approach for calculations of Dzyaloshinskii-Moriya interactions in molecules and crystals is proposed. It is based on the exact perturbation expansion of the total energy of weak ferromagnets in the canting angle with the only assumption of local Hubbard-type interactions. This scheme leads to a simple and transparent analytical expression for the Dzyaloshinskii-Moriya vector with a natural separation into spin and orbital contributions. The main problem was transferred to calculations of effective tight-binding parameters in the properly chosen basis including the spin-orbit coupling. Test calculations for La_2CuO_4 give the value of the canting angle in agreement with experimental data.

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The Dzyaloshinskii-Moriya interactions (DMI) (Refs. 1 and 2) were introduced in the theory of weak ferromagnetism to explain the canting of the magnetic moments of some antiferromagnets (such as α-Fe_2O_3, $MnCO_3$, $CoCO_3$, and others[3]). It was shown later that the DMI are of crucial importance for many others classes of magnetic systems, such as spin glasses,[4] molecular magnets,[5–7] multiferroics systems,[8] magnetic surfaces and clusters on the surfaces,[9–12] and Jahn-Teller systems.[13] In a sense, DMI is the simplest example of relativistic magnetic interactions, since it appears already in the first order in the spin-orbit (SO) coupling, whereas the magnetic anisotropy is at least of the second order.[2] On the other hand, the DMI vanish for systems with inversion symmetry, which explains their special relevance for low symmetric cases such as molecules, clusters, surfaces, and disorder systems.

The microscopic origin of the DMI was clarified by Moriya for model systems.[2] For that he used the idea of Anderson[14] about the superexchange interaction mechanism. However, the original formulation of the Dzyaloshinskii-Moriya interaction is not suitable for quantitative calculations of the DMI parameters for specific compounds based on real electronic structures. Numerous attempts of more convenient and general formulations have been made afterward.[15–21]

Yildirim *et al.*[15] have developed a perturbative approach in the spin-orbit coupling for Mott insulators within the Hubbard-type model. A similar approach has been developed in Ref. 21 within the local-density approximation plus U (LDA+U) method. In Refs. 16–18 the magnetic force theorem[22] has been applied but only for spin rotations. The authors of Ref. 23 presented a computationally efficient method to determine the strength of the DMI from the spin-orbit induced corrections to the energy of long-ranged spin spirals. A general first-principles approach for the DMI was suggested in Ref. 19 in a similar but fully relativistic formalism, that takes into account both spin and orbital contributions. This is probably the best possible way if one starts to calculate the DMI from the true noncollinear ground-state magnetic structure.

The results of previous theoretical investigations[15] have demonstrated that in the real transition-metal compounds there are a lot of different microscopic mechanisms for the anisotropic exchange interactions. For instance, to take into account the metal-oxygen hybridization one should consider high-order hopping processes between metal and oxygen orbitals. It strongly complicates the formulation and solution of the problem. In this Rapid Communication, we return to the original Anderson's idea[14] about the superexchange interaction in the Wannier function basis. We use the main advantage of such an approach which is that all the important hybridization effects can be captured by constructing the Wannier function. As we will show it simplifies dramatically the formalism without any essential loss of accuracy.

Since the canting angles are normally quite small it allows us to proceed with the corresponding collinear structures and use advantage of first-order perturbation treatment for the magnetic torque. The application of the magnetic force theorem to equilibrium configurations, involves additional assumptions such as neglecting of vertex corrections.[24] First-order variation in the total energy near the collinear states leads to an expression for the DMI formally exact in the many-body sense.

We start with the general Hamiltonian of interacting electrons in a crystal,

$$\hat{H} = \hat{H}_t + \hat{H}_u = \sum_{12} c_1^+ t_{12} c_2 + \frac{1}{2} \sum_{1234} c_1^+ c_2^+ U_{1234} c_3 c_4, \qquad (1)$$

where $1=(i_1, m_1, \sigma_1)$ is the set of site (i_1), orbital (m_1), and spin (σ_1) quantum numbers, and t_{12} are hopping integrals that contain the spin-orbit coupling. These transfer couplings can be found by the Wannier parametrization of the first-principles band structure with the spin-orbit coupling.[25] In this case the real-space site-centered spinor Wannier function can be written as

$$W_n(\mathbf{r}) = \sum_{\mathbf{T}\mu} \omega_{n\mu\mathbf{T}} \psi_\mu(\mathbf{r}-\mathbf{T}), \qquad (2)$$

where $\mathbf{T}$ is a lattice translation vector, $\psi_\mu(\mathbf{r}-\mathbf{T})$ are the site-centered spinor atomic-like orbitals [in our case they were linear muffin-tin orbitals (LMTO)], and $\omega_{n\mu\mathbf{T}}$ are expansion

coefficients of the Wannier functions in terms of the corresponding LMTO orbitals.

We will take into account only the local Hubbard-type interactions, keeping in $\hat{H}_u$ only terms with $i_1=i_2=i_3=i_4$. This assumption corresponds to the LDA+U Hamiltonian[26] that is also a starting point for the LDA plus dynamical mean-field theory (DMFT).[27,28] It is crucially important for the later consideration that the interaction term $\hat{H}_u$ is supposed to be rotationally invariant.

Let us start with a collinear magnetic configuration (e.g., the Neel antiferromagnetic state), which is close to the real ground state (weak ferromagnet), but does not coincide with it due to the Dzyaloshinskii-Moriya interactions. The phenomenological Hamiltonian of the DMI is given by

$$H_{\mathrm{DM}} = \sum_{ij} \vec{D}_{ij}[\vec{e}_i \times \vec{e}_j], \tag{3}$$

where $\vec{e}_i$ is a unit vector in the direction of the ith site magnetic moment and $\vec{D}_{ij}$ is the Dzyaloshinskii-Moriya vector. We analyze the magnetic configuration that is slightly deviated from the collinear state,

$$\vec{e}_i = \eta_i \vec{e}_0 + [\delta\vec{\varphi}_i \times \eta_i \vec{e}_0], \tag{4}$$

where $\eta_i = \pm 1$, $\vec{e}_0$ is the unit vector along the vector of antiferromagnetism and $\delta\vec{\varphi}_i$ are the vectors of small angular rotations.

Substituting Eq. (4) into Eq. (3) one finds for the variation in the magnetic energy,

$$\delta E = \sum_{ij} \vec{D}_{ij}(\delta\vec{\varphi}_i - \delta\vec{\varphi}_j). \tag{5}$$

Now we should calculate the same variation for the microscopic Hamiltonian (1). Similar to the procedure used in Ref. 24 to derive exchange interactions for the LDA+DMFT approach, we consider the effect of the local rotations

$$\hat{R}_i = e^{i\delta\vec{\varphi}_i \hat{\vec{J}}_i} \tag{6}$$

on the total energy; here $\hat{\vec{J}}_i = \hat{\vec{L}}_i + \hat{\vec{S}}_i$ is the total moment operator, $\hat{\vec{L}}_i$ and $\hat{\vec{S}}_i$ are the orbital and spin moments, respectively. We would like to stress that the operator $\hat{R}_i$ acts on ith Wannier state. In the supplementary materials[29] we demonstrate that the rotation of the orbital part of $\hat{\vec{J}}_i$ in Wannier function basis results in independent rotations of the atomic orbital moments.

The interaction part of the Hamiltonian $\hat{H}_u$ is rotationally invariant and is not changed under this transformation, opposite to the hopping part $\hat{H}_t$,

$$\delta\hat{H}_t = \sum_{ij} c_i^+(\delta\hat{R}_i^+ \hat{t}_{ij} + \hat{t}_{ij}\delta\hat{R}_j)c_j = -i\sum_{ij} c_i^+(\delta\vec{\varphi}_i \hat{\vec{J}}_i \hat{t}_{ij} - \hat{t}_{ij}\hat{\vec{J}}_j \delta\vec{\varphi}_j)c_j$$

$$= -\frac{i}{2}\sum_{ij} c_i^+(\delta\vec{\varphi}_i - \delta\vec{\varphi}_j)(\hat{\vec{J}}_i \hat{t}_{ij} + \hat{t}_{ij}\hat{\vec{J}}_j)c_j - \frac{i}{2}\sum_{ij} c_i^+(\delta\vec{\varphi}_i + \delta\vec{\varphi}_j)$$

$$\times(\hat{\vec{J}}_i \hat{t}_{ij} - \hat{t}_{ij}\hat{\vec{J}}_j)c_j. \tag{7}$$

Assuming that $\hat{\vec{J}}_i = \hat{\vec{J}}_j = \hat{\vec{J}}$ the change in the total energy takes the form

$$\delta E = -\frac{i}{2}\sum_{ij} (\delta\vec{\varphi}_i - \delta\vec{\varphi}_j)\mathrm{Tr}_{m,\sigma}\langle c_i^+[\hat{\vec{J}}, \hat{t}_{ij}]_+ c_j\rangle$$

$$-\frac{i}{2}\sum_{ij} (\delta\vec{\varphi}_i + \delta\vec{\varphi}_j)\mathrm{Tr}_{m,\sigma}\langle c_i^+[\hat{\vec{J}}, \hat{t}_{ij}]_- c_j\rangle, \tag{8}$$

where $\mathrm{Tr}_{m,\sigma}$ is a trace over orbital (m) and spin (σ) quantum numbers.

The first term in the right-hand side of Eq. (8) is responsible for *relative* deviations of the magnetic moments on sites i and j (DMI) whereas the second one is related with the rotation of the magnetic axis as a whole (magnetic anisotropy). Assuming that $\delta\vec{\varphi}_i = \delta\vec{\varphi}$ is independent on site index one finds the following expression for the magnetic anisotropy torque:

$$\frac{\delta E}{\delta\vec{\varphi}} = -i\sum_{ij} \mathrm{Tr}_{m,\sigma}\langle c_i^+[\hat{\vec{J}}, \hat{t}_{ij}]_- c_j\rangle. \tag{9}$$

In contrast with the previous results[17,18] expression (9) contains both spin and orbital contributions. Application of this expression to real systems will be considered elsewhere. Here we will focus on the DMI.

Comparing Eq. (8) with Eq. (5) one finds

$$\vec{D}_{ij} = -\frac{i}{2}\mathrm{Tr}_{m,\sigma}\langle c_i^+[\hat{\vec{J}}, \hat{t}_{ij}]_+ c_j\rangle = -\frac{i}{2}\mathrm{Tr}_{m,\sigma} N_{ji}[\hat{\vec{J}}, \hat{t}_{ij}]_+, \tag{10}$$

where $N_{ji} = \langle c_i^+ c_j\rangle = -\frac{1}{\pi}\int_{-\infty}^{E_f} \mathrm{Im}\, G_{ji}(E)dE$ is the occupation matrix and $\hat{G}$ is the Green function, E_F is the Fermi energy. Assuming that the occupation matrix is known exactly the expression for DMI, Eq. (10), is exact due to the Hellmann-Feynman theorem. Note that the occupation matrix is calculated in the corresponding collinear states, which strictly speaking can be done self-consistently only within constrained calculations.[30] Using the decomposition of the total moment $\hat{\vec{J}}$ into orbital and spin moments, we have a natural representation of the Dzyaloshinskii-Moriya vector, Eq. (10), as a sum of the orbital and spin contributions, which are related with the rotations in orbital and spin space, respectively.

To test the developed method we consider weak ferromagnetism phenomena which result from DMI. The problem of the theoretical description of weak ferromagnetism in antiferromagnets can be solved by calculating the canting angle. As an example of the system demonstrating weak ferromagnetism we have chosen La_2CuO_4 in the low-temperature orthorhombic phase presented in Fig. 1. For this system the Wannier functions can be qualitatively analyzed by using a one-band Hubbard model with the spin-orbit coupling proposed in Refs. 31 and 32,

$$H = \sum_{ij\alpha\beta} c_{i\alpha}^+(t\delta_{\alpha\beta} + i\vec{\lambda}_{ij}\vec{\sigma}_{\alpha\beta})c_{j\beta} + U\sum_i n_{i\uparrow}n_{i\downarrow}. \tag{11}$$

Here t is a nearest-neighbor hopping parameter and the vector $\vec{\lambda}_{ij}$ depends on the tilting pattern of oxygen octahedra

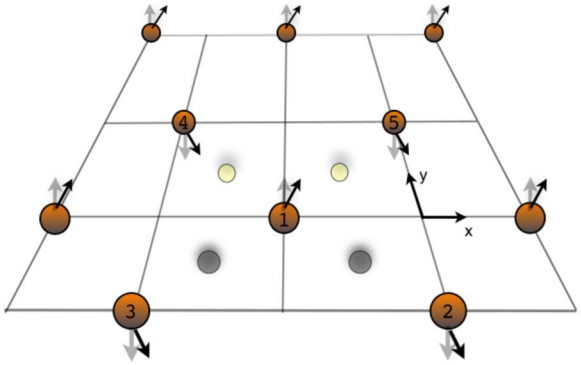

FIG. 1. (Color online) Magnetic structures of La_2CuO_4. Black and gray arrows denote noncollinear and fixed collinear ground states, respectively. Gray (dark) and yellow (light) small circles represent oxygen atoms that are above and below the copper oxide plane, respectively.

surrounding the copper atom. Substituting Eq. (11) into Eq. (10) we obtain

$$\vec{D}_{ij} = \vec{\lambda}_{ij}\,\mathrm{Tr}_\sigma\, N_{ji}. \tag{12}$$

Therefore the symmetry of the Dzyaloshinskii-Moriya vector is fully described by the vector $\vec{\lambda}_{ij}$. If there is the inversion center between copper atoms then $\vec{\lambda}_{ij}=0$ and DMI vanishes.

Using the definitions introduced in Refs. 31 and 32 we obtain $\vec{\lambda}_{12}=\vec{\lambda}_{14}=\frac{1}{2}(\lambda_1-\lambda_2,\lambda_1+\lambda_2,0)$ and $\vec{\lambda}_{13}=\vec{\lambda}_{15}=\frac{1}{2}(\lambda_1-\lambda_2,-\lambda_1-\lambda_2,0)$. It is easy to show that the total Dzyaloshinskii-Moriya vector $\Sigma_{j=2}^{5}\vec{D}_{1j}$ has only nonzero x component. It means that the canting exists if the magnetic moments are in yz plane. This fully agrees with the results of previous works.[31,33,34]

Unfortunately, the performed microscopic analysis is only qualitative. The most straightforward way to obtain a reliable numerical estimation of the canting angle would be to perform relativistic first-principles calculations for the corresponding noncollinear magnetic structure. However, this is a very challenging computational problem. Since in the case of $3d$-metal compounds the spin-orbit coupling is small one should run many thousands of iterations to relax the magnetic structure.[35] On the other hand, to solve the weak ferromagnetism problem we only need to know the magnitude and the direction of the Dzyaloshinskii-Moriya vector. It can be done by using the developed method for the fixed collinear magnetic configuration. Such an approach seems to be preferable since it requires much less computational efforts.

We have performed the LDA+U+SO calculations for the collinear antiferromagnetic structure where the magnetic moments were fixed along z axis. The computational details are the same as in Ref. 21. The obtained results are presented in Table I.

In order to calculate the Dzyaloshinskii-Moriya interaction, Eq. (10), one needs to define the occupation matrix N_{ji} and the kinetic part $\hat{t}_{ij}$ of the Hamiltonian in a Wannier function basis. The construction of a reliable Wannier basis can be performed in different schemes.[36–39] As a first attempt we will use the simplest choice related with orthogonalized

TABLE I. Calculated magnitude (in μ_B) and orientation of the spin and orbital copper moments in La_2CuO_4.

Atom	Spin moment	Orbital moment
1	$0.65\times(0,0,-1)$	$0.04\times(0,0,-1)$
2	$0.65\times(0,0,1)$	$0.04\times(0,0,1)$

minimal basis LMTO scheme[36,38] including the spin-orbital coupling. Note that, since the trace in Eq. (10) is only over orbital indices and not on the site ones, the resulting $\vec{D}_{ij}$ is Wannier-gauge dependent. The Wannier functions are normally constructed using a truncated basis, therefore it will be important to investigate in the future a sensitivity of the results with respect to a choice of the Wannier states.

Since in our investigation we used the LMTO-atomic-sphere approximation (LMTO-ASA) (Ref. 36) it was natural to associate N_{ji} and $\hat{t}_{ij}$ with the occupation matrix and kinetic energy of the $3d$ states of the copper atoms. We consider such an approximation as a reasonable one since the magnetic moments in La_2CuO_4 are due to the $3d$ states of copper.[40] Another fact supported our approximation is good agreement between the isotropic exchange interaction calculated by using the Green's-function method in the framework of LMTO-ASA and the model kinetic exchange estimated as $J_{ij}=\frac{4t_{ij}^2}{U}$.[41]

The DMI parameters between neighboring copper atoms calculated via Eq. (10) are presented in Table II. One can see that the orbital contribution to the Dzyaloshinskii-Moriya interaction is one order of magnitude larger than the spin one. The obtained magnetic torque is directed along x axis. This agrees with the results of our microscopic analysis. Summarizing all the vectors we can calculate the canting angle of the magnetic moment which is given by

$$\delta\theta = \frac{\left|\sum_j \vec{D}_{1j}\right|}{\sum_j J_{1j}} = 0.005, \tag{13}$$

where the total exchange interaction $\Sigma_j J_{1j}$ was taken to be 58.3 meV.[21] The obtained value of the canting angle is in a reasonable agreement with the experimental estimate of 0.003.[40]

To conclude, we have proposed a distinct method for calculation of the Dzyaloshinskii-Moriya interaction parameters which, conceptually, is much simpler than approaches known

TABLE II. Different contributions to the Dzyaloshinskii-Moriya vectors (in meV).

$\vec{R}_{1j}$	$\vec{D}_{1j}^{spin}$	$\vec{D}_{1j}^{orb}$
(1,2)	(−0.005;−0.006;0)	(−0.07;−0.03;0)
(1,3)	(−0.005;0.006;0)	(−0.07;0.03;0)
(1,4)	(−0.005;−0.006;0)	(−0.07;−0.03;0)
(1,5)	(−0.005;0.006;0)	(−0.07;0.03;0)

before. This method represents, in a natural way, the Dzyaloshinskii-Moriya vector as a sum of the spin and orbital contributions which may give a deeper insight into microscopic mechanisms of the DMI for a given system. In our approach, the crucial point is the construction of a reliable tight-binding parametrization of the Hamiltonian with the spin-orbit interaction taken into account. We have performed the corresponding calculations for the weak ferromagnet La_2CuO_4, and the results look quite promising.

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