Dzyaloshinskii-Moriya–type interaction and Lifshitz invariant in Rashba 2D electron gas systems

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Abstract – The origin of chiral magnetic structures in ultrathin films of magnetic metals is analyzed. It is shown that the Lifshitz-type invariant term in the macroscopic thermodynamic potential can be derived from the spin-orbit Rashba Hamiltonian in two-dimensional electron gas (2DEG). The former is the prerequisite for the existence of spin cycloids, skyrmions and other chiral phenomena observed in thin films. The estimation of the period of spin cyclod gives the value of an order of 10 nm typical for structures reported in the literature.

Introduction. – Spatially modulated spin structures have been inspiring researchers for several decades due to the rich diversity of extra-functionalities which they render: ferroelectricity [1–3], sensitivity to mechanical stress [4], magnetic and electric fields [5,6], spin current [7,8], etc.

Dzyaloshinskii has shown [9] that the symmetry of some crystals allows the existence of the contributions to the thermodynamic potential linear with respect to the first spatial derivatives of magnetic order parameter. This macroscopic Dzyaloshinskii-Moriya interaction (mDM) is responsible for the formation of long-periodic spatially modulated magnetic structures with fixed sense of spatial rotation of spin (chiral spin structures) [9–11].

It should be noted that the mDM is often confused with the microscopic Dzyaloshinskii-Moriya interaction (μDM), i.e. antisymmetric exchange coupling proportional to the vector product of the localized spins \( \mathbf{S}_1 \times \mathbf{S}_2 \). The μDM is related to the local violation of the inversion symmetry in the geometric center of two neighbouring atoms and results in canting of their spins [12]. At the same time the existence of the macroscopic Dzyaloshinskii-Moriya interaction requires the inversion symmetry violation in the whole crystal. Thus, the presence of μDM is the necessary condition but not a sufficient one for the existence of the mDM and long-periodic spin modulation. There is a class of materials known as weak ferromagnets (hematite \( \alpha\text{-Fe}_2\text{O}_3 \), MnCO\(_3\), YFeO\(_3\) etc.) in which the μDM plays the key role but the presence of the spatial inversion in the symmetry group of crystal forbids the mDM and the chiral structures.

The violation of the inversion symmetry of crystal in magnetic ferroelectrics can give rise to both the microscopic exchange coupling and the macroscopic Dzyaloshinskii-Moriya interaction [13] in the form of the Lifshitz invariant for uniaxial crystal \( \left[ (\mathbf{P} \cdot \mathbf{m}) \text{div} \mathbf{m} - \mathbf{P} \cdot (\mathbf{m} \cdot \nabla) \mathbf{m} \right] \), where \( \mathbf{m} \) is a magnetic order parameter, \( \mathbf{P} \) is a polar vector corresponding to the displacement of ions in the crystal from the centroymmetric position [14]. As was shown in [15] the presence of the Lifshitz invariant term (1) in the thermodynamic potential leads to the spin cycloid ordering, i.e. spatially modulated magnetic structure with modulation direction lying in the magnetization rotation plane.

Another interesting possibility for the spin cycloid formation is the central symmetry breaking at the surface and interfaces [16,17]. In this case the role of polar direction \( \mathbf{P} \) is played by surface normal \( \mathbf{Z} \) that physically corresponds to the surface electric field [17]. The experimental evidences of the formation of the chiral structures...
in thin magnetic films are numerous: the spin cycloid with a period about 10 nm in single atomic layer of Mn [18]; the stripe domains with Neel-type domain walls in the double atomic Fe layers of iron [19] and Co/ Ni multilayers [8,20]; and the skyrmions in Fe monolayers [21]. However, the origin of chiral structures in the case of thin films is not quite clear.

In this paper the mechanism that induces the chiral spin structures in the 2D electronic gas (2DEG) is analyzed. It is shown that starting from a basic formula for the exchange interaction in the 2DEG with Rashba spin-orbit coupling the macroscopic Dzyaloshinskii-Moriya interaction described by the Lifshitz invariant can be obtained.

**RKKY interaction in 2DEG system.** – The conventional approach to the microscopic analysis of the origin of the chiral magnetic structures is based on the super-exchange interaction [12]. The metallic systems were previously considered in the context of the three-site indirect exchange interaction via high anisotropic ligand in amorphous magnets [22]. The presence of the spin cycloid structure in thin magnetic films can be understood from the perspective of the new variety of the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange coupling between localized spins. The spin precession of the conduction electrons in thin magnetic films can be understood from the perspective of the new variety of the spin-cycloid structure in thin magnetic films can be understood from the perspective of the new variety of the Rashba-type spin-orbit coupling: a “twisted” spin space where the spin quantization axis is normal to the film plane that represents the asymmetry of the confining potential in 2D structure. The twisted RKKY interaction results in the slight canting of their spins ordering. From the mathematical standpoint the product of spins in eq. (2) implies not only the scalar product of the spins but also the vector product:

\[ \mathbf{S}_1 \cdot \mathbf{S}_2(\theta) = \cos \theta \mathbf{S}_1 \mathbf{S}_2 + \sin \theta [\mathbf{S}_1 \times \mathbf{S}_2]_y + (1 - \cos \theta) \mathbf{S}_1^n \mathbf{S}_2^n, \]  

where \( \theta = 2k_R (x_1 - x_2) \) (spins are supposed to be located in the positions \( x_1 \) and \( x_2 \) on the \( x \)-axis [23]), \( k_R \) is the Rashba splitting proportional to the spin-orbit coupling \( \alpha \):

\[ k_R = \frac{m \alpha}{\hbar^2} . \]  

In the case of the ultrathin film the 2D array of atoms should be considered. For this case the second term of eq. (3) takes the form \( \sin \theta (\mathbf{Z} \times \mathbf{r}) \cdot [\mathbf{S}_1 \times \mathbf{S}_2] \), where \( \mathbf{r} = \mathbf{R}_{12}/R_{12} \) is the unit vector connecting the exchange coupled ions and \( \mathbf{Z} \) is the surface normal.

The range function of the twisted RKKY interaction can be expressed in the following way [23]:

\[ F(R) = -\frac{\theta}{2\pi^2 \hbar^2} e^{-R/L}, \]

\[ k_F = \sqrt{\frac{2m \varepsilon_F}{\hbar^2} + k_R^2}, \]

where \( j \) is the strength of the \( s-d \) interaction, \( L \) is the mean free path of the conduction electrons that shows the self-damping of the exchange interaction [24,25].

The range function dependence on the distance for Mn lattice is shown in fig. 1. It can be seen that for the neighbouring atoms its value is positive. For symmetric exchange (the first term in eq. (3)) this means antiparallel orientation of the spins of the neighbouring atoms. However, the second \( \mu \)DM-type term in the spin product in eq. (3) results in the slight canting of their spins \( \delta S \ll S \) since \( \mu \)DM term is the first order of smallness in \( \theta \) (\( \theta \ll 1 \) for neighbouring atoms): \[ [\mathbf{S}_1 \times \mathbf{S}_2] = [\mathbf{S}_1 \times (-\mathbf{S}_1 + \delta \mathbf{S})] = [\mathbf{S}_1 \times \delta \mathbf{S}] . \]

The third term in eq. (3) corresponds to the anisotropy of the exchange interaction. It is the second order of smallness in \( \theta \) and in the following discussion it will be neglected.

![Fig. 1: (Colour on-line) The range function \( F(R) \) for Mn single-atom layer: \( j = 9.4 \text{eV} \cdot \text{Å}^2 \) [18], the positions of atoms in the lattice are shown by the grey balls on the graph (period of the lattice is taken as \( a = 4.7 \text{Å} \)). The corresponding energies are written at the atom position.](image-url)
To calculate the $\mu$DM contribution to the exchange energy per atom with a spin $S_0$ we should take the summation over its neighbours. For simplicity we consider the square lattice (generalization on the lower symmetry case is straightforward). The surface density of the $\mu$DM energy will be

$$V = \frac{1}{2a^2} \sum_{n,m} \left( F(R_{n,m}) \sin(\theta_{n,m}) \cdot ([Z \times r] \cdot [S_0 \times \delta S_{n,m}]) \right),$$

(6)

$$\theta_{n,m} = 2akR\sqrt{n^2 + m^2}$$ is the angle between the spin quantization axes of the $(0,0)$-ion with spin $S_0$ and the $(n, m)$-ion, $a$ is the lattice parameter.

The vector $\delta S_{n,m}$ can be expanded in the Taylor series: $\delta S_{n,m} = a(\nabla S \cdot n + \nabla S \cdot m) + \ldots$. We restrict ourselves to the first term of the expansion:

$$V = \frac{1}{2a^2} \sum_{n,m} F \left( a \cdot \sqrt{n^2 + m^2} \right) \sin(\theta_{n,m}) \cdot ([Z \times r] \cdot [S_0 \times (an \cdot \nabla)S]),$$

(7)

where vector $n = (n, m)$.

To elicit the Lifshitz invariant we need to group the terms in the sum (7) in complimentary pairs $(n, m)$ and $(m, n)$, that add up into $(n+m)$ Lifshitz invariants (for the case $n \neq m$). Thus, the transition from the microscopic representation to the continuous one in Lifshitz invariant form could be obtained:

$$V = V_D([Z \cdot S] \text{div} S - Z \cdot (S \cdot \nabla)S),$$

(8)

where $V_D = \frac{1}{2a^2} \sum_{n,m=1}^{\infty} \sum_{n=0}^{n=m} C_{n,m} F(a \cdot \sqrt{n^2 + m^2}) \sin(\theta_{n,m})$ and coefficients $C_{n,m}$ are determined as follows:

$$C_{n,m} = \begin{cases} 2n, & m = 0, \\ 4(n + m), & 0 < m < n, \\ 4n, & n = m. \end{cases}$$

(8a)

As can be seen from eqs. (8) and (5a) the constant $V_D$ depends not only on the Rashba splitting $kR$ characterizing the $\mu$DM but also on 2DEG system parameters like lattice constant, Fermi momentum and the mean free path of electrons.

Thus, the $\mu$DM-type term in the spin product eq. (3) leads us to the Lifshitz invariant in the thermodynamical potential and, as a consequence, to the spin cycloid structure.

**Spin cycloid in 2DEG system.** – Let us assume without loss of generality that the spin cycloid is running along the $x$-axis. The spin spatial modulation is described by the dependences of spin components:

$$S_x = S \cdot \sin \varphi; \quad S_y = 0; \quad S_z = S \cdot \cos \varphi,$$

(9)

where $\varphi = \varphi(q\bar{x})$ is the angle between the spin and the $z$-axis that is normal to the film, and $q$ is the wave vector of the cycloid $q = (q, 0, 0)$ (fig. 2).

![Fig. 2: (Colour on-line) The cycloid structure in the single-layer of magnetic metal atoms. The $\varphi$ is the angle of spin spatial rotation. The indexes $(n, m)$ of neighbouring atoms are shown in the inset.](Image 320x667 to 528x756)

For the case of the homogeneous ferromagnetic state the perturbation that is introduced to the surface energy of the symmetric exchange energy by the spin cycloid is described in this case as follows:

$$V_{\text{exch}} = \frac{1}{2a^2} \sum_{n,m} F \left( a \cdot \sqrt{n^2 + m^2} \right) S (S + 1) \cdot \cos(\theta_{n,m}) \cdot \frac{(gan)^2}{2} = A \left( \frac{\partial \varphi}{\partial x} \right)^2,$$

(10)

where $A$ is the exchange stiffness that can be found as a sum

$$A = \frac{1}{4} \sum_{n=1}^{\infty} \sum_{m=0}^{n} B_{n,m} \cdot S (S + 1) F(a \cdot \sqrt{n^2 + m^2}) \cos(\theta_{n,m}),$$

$$B_{n,m} = \begin{cases} 2n^2, & m = 0, \\ 4(n^2 + m^2), & 0 < m < n, \\ 4n^2, & n = m. \end{cases}$$

The surface energy corresponding to the mDM interaction can be found in an analogous way for the continuous approach:

$$V = V_D S (S + 1) \cdot \frac{\partial \varphi}{\partial x}.$$

(11)

To estimate the period of the cycloid it is sufficient to use the harmonic approximation ($\varphi = q \cdot x$); the free-energy density of the magnetic system can be written in the following way:

$$W = A \left( \frac{\partial \varphi}{\partial x} \right)^2 + V_D S (S + 1) \cdot \frac{\partial \varphi}{\partial x} = Aq^2 + V_D S (S + 1)q.$$

(12)

Since the symmetric exchange scales as the second power of wave number $q$ while the mDM-term is linear in $q$, there is an optimum value of the wave number $q_0$ that corresponds to the minimum of energy of the system:

$$q_0 = \frac{V_D S (S + 1)}{2A} = \frac{1}{A} \sum_{n=1}^{\infty} \sum_{m=0}^{n} C_{n,m} F(a \cdot \sqrt{n^2 + m^2}) \sin(\theta_{n,m}) \sum_{n=1}^{\infty} \sum_{m=0}^{n} B_{n,m} F(a \cdot \sqrt{n^2 + m^2}) \cos(\theta_{n,m}).$$

(13)
ties for low-dissipation spintronics. The possibility of the voltage-tuned spin cycloids is a direct consequence of the twisted RKKY interaction. Thus, the presence of spin cycloids as well as other chiral structures like Neel-type domain walls and skyrmions is a direct consequence of the twisted RKKY interaction. The possibility of the voltage-tuned Rashba interaction reported in [26,27] provides the means for modulation of mDM which gives new intriguing opportunities for low-dissipation spintronics.

**Conclusion.** – Thus, in contrast to the conventionally proposed mechanism that is based on the super-exchange [12] model of the Dzyaloshinskii-Moriya interaction in thin films, another scenario can be realized originating from the twisted RKKY interaction in the 2DEG system with the Rashba spin-orbit coupling. This type of asymmetrical exchange between localized spins mediated by the conduction electrons looks more natural for the case of metallic ultrathin films than the super-exchange which is typical for dielectrics. Note that the idea of the polar direction is inherent for the twisted RKKY interaction. Thus, the presence of spin cycloids as well as other chiral structures like Neel-type domain walls and skyrmions is a direct consequence of the twisted RKKY interaction.

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