



Interplay of Dzyaloshinsky-Moriya and dipole-dipole interactions and their joint effects upon vortical structures on nanodisks



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ARTICLE INFO

Keywords:

Dzyaloshinsky-Moriya interaction

Dipole-dipole interaction

Magnetic vortices

Quantum simulation model

ABSTRACT

In transition metal oxides, magnetic dipole-dipole (DD) and chiral Dzyaloshinsky-Moriya (DM) interactions between nearest neighboring spins are comparable in magnitude. In particular, the effects of the DD interaction on the physical properties of magnetic nanosystems cannot be simply neglected due to its long-range character. For these reasons, we employed here a new quantum simulation approach in order to investigate the interplay of these two interactions and study their combined effects upon the magnetic vortical structures of monolayer nanodisks. Consequently, we found out from our computational results that, in the presence of Heisenberg exchange interaction, a sufficiently strong DD interaction is also able to induce a single magnetic vortex on a small nanodisk; a strong DM interaction usually gives rise to a multi-domain structure which evolves with changing temperature; In this circumstance, if a weak DD interaction is further considered, the multi-domains merge to form a single vortex in the whole magnetic phase. Moreover, if only the Heisenberg exchange and chiral DM interactions are considered in simulations, our results from calculations with different spin values show that the transition temperature T_M is simply proportional to $S(S+1)$; if the temperature is scaled with T_M , and the calculated magnetizations are divided by the spin value S , their curves exhibit very similar features in the whole temperature region below T_M .

1. Introduction

In 1989, Bogdanov and Yablonskii speculated theoretically [1] that skyrmions, which were originally introduced in particle physics to describe the localized, particle-like topological solitons [2], can exist in magnets when the chiral Dzyaloshinsky-Moriya (DM) interaction is present [3–5]. This prediction was later confirmed by experimental findings that magnetic skyrmions can be generated by the DM interaction in helical magnets, such as MnSi and $\text{Fe}_{1-x}\text{Co}_x\text{Si}$ [6–8]. The results suggest that this interaction favors canted spin configurations [6–16]. Most skyrmions found in helimagnets were induced by an external magnetic field at low temperatures [6–8,17]. However, Yu et al. [7] obtained a skyrmion lattice in FeGe with a high transition temperature around 280 K by applying an external magnetic field, as well.

The diameters of the skyrmion structures formed in a Fe monolayer on an Ir(111) surface are in the order of a few atomic spacings [10]. They can be easily manipulated by spin currents of only about 10^6 Am^{-2} [18,19], which is a factor of 10^5 to 10^6 weaker than those required to drive magnetic domain walls [20]. These unique properties

provide a possibility to fabricate novel high density, power-efficient spintronic storage and logic devices [17,21], for example, a racetrack-like memory [22] that uses skyrmions instead of magnetic domains [21,23].

Both magnetic skyrmions and vortices are usually induced by the DM interaction. Thus, they are closely related and have been mainly studied numerically with Monte Carlo and micromagnetic methods. Within the framework of both these methods, the spins and magnetic moments in the sample under consideration are treated as classical vectors with fixed lengths. In order to go beyond a classical treatment, we have developed a quantum simulation approach in recent years [24–27]. In this new method, all spins are taken as quantum operators, and all physical quantities are calculated strictly with quantum theory. Thus the computational code can quickly converges to the correct equilibrium states spontaneously at all temperatures.

Recently, we employed this quantum simulation approach to investigate the magnetic and thermodynamic properties of both ferromagnetic (FM) and antiferromagnetic (AFM) monolayer nanodisks in the presence of a chiral DM interaction [28,29]. In the first case, we found that the chirality of the FM vortices formed on a small

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nanodisk is solely determined by the sign of DM interaction parameter, and the applied magnetic field is able to stabilize the single vortical structure [6–8,17]. In the second case, we observed that the magnetic moments not only form in-plane AFM vortices, but also order antiferromagnetically in the perpendicular direction. In the both cases, the calculated average distances between two neighboring vortices agree well with a grid theory in the low temperature region [30].

On the other hand, in transition metal oxides, the DM interaction is of the order of 0.1 meV between a pair of nearest neighboring spins, while that for the dipole-dipole (DD) interaction is around $\mu_0\mu_B^2/4\pi a^3 \sim 0.1$ meV, which is comparable to the DM interaction [31]. Moreover, the dipolar interaction is a long-range interaction, so it plays an important role in the formation of long-range ordered spin structures. In particular, its co-existence with the Heisenberg exchange interaction can also generate magnetic vortices on nanodisks [32–37]. When this long-range interaction is sufficiently strong, the continuity of the effective magnetic field along the boundary of a two dimensional (2D) nanodot is able to force the magnetic moments to align tangent to the border [38–40], thus a vortex appears on the disk-plane [41].

So far, a great amount of works in this respect have been undertaken over the years, such as Monte Carlo simulations [41–44], micromagnetic simulations [45], computations for dynamics of vortex [46], theoretical studies on the effect of the DD interaction [47] and experimental studies [48–50]. Vortices and anti-vortices were observed experimentally [49] in 2D cobalt micro-dots; layers of magnetic dots on a superconducting film, which shows transport properties attributed to magnetic vortices, were also investigated [50].

In the present work, we employed our new quantum simulation approach to investigate the effects of the DM and DD interactions upon the vortical structures on circular magnetic monolayer nanodisks with the square unit cell structure consisting of $S=3/2$ spins. We found that, in presence of Heisenberg exchange interaction, a sufficiently strong DD interaction is also able to induce a single stable magnetic vortex on a small nanodisk; whereas a strong DM interaction usually gives rise to temperature-dependent multi-vortical structures – however, few people have paid attention to, or systematically studied the dynamic character of such phenomenon; and when a strong DM and a weak DD interactions are both involved, the above multi-domain structures merge to form a single vortex which prevails in the whole magnetic phase. Moreover, if only Heisenberg exchange and chiral DM interactions are considered, our results obtained for different spin values indicate that the transition temperature T_M is simply proportional to $S(S+1)$; and if the temperature is scaled with T_M , the calculated $\langle S_x \rangle$, $\langle S_y \rangle$ and $\langle S_z \rangle$ are divided by the spin value S , their curves only differ slightly in the whole magnetic phase.

2. Quantum model and computational algorithm

The Hamiltonian of the nanosystems that we consider here can be expressed as [30,51,52]

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j \neq i} [\mathcal{J}_{ij} \vec{S}_i \cdot \vec{S}_j - D_{ij} \vec{r}_{ij} \cdot (\vec{S}_i \times \vec{S}_j)] - \frac{d}{2} \sum_{i,j \neq i} \left[\frac{3(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{r_{ij}^5} - \frac{\vec{S}_i \cdot \vec{S}_j}{r_{ij}^3} \right], \quad (1)$$

where the first and second terms represent the Heisenberg exchange and DM interactions between every pair of neighboring spins with the strengths of \mathcal{J}_{ij} and D_{ij} , respectively. The last term denotes the DD interaction, where \vec{r}_{ij} is the vector from the i th to the j th sites, and d is the dipolar interaction strength. The last sum is taken over all spins within a circle of a cut-off radius r_c . To a satisfactory accuracy, r_c was set to $15a$ in all our simulations.

The nanodisks under consideration are assumed to be composed of $S=3/2$ spins. In light of quantum theory, the matrices of the spin components in a cartesian system are given by respectively.

$$S_x = \frac{1}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \quad S_y = \frac{1}{2i} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & 0 & 2 & 0 \\ 0 & -2 & 0 & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & 0 \end{pmatrix}, \quad S_z = \frac{1}{2} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}, \quad (2)$$

As described in our previously published papers [24,25,28,29], all simulations done in recent years are started from a random magnetic configuration above the magnetic transition temperature T_M , then they are carried out stepwise down to very low temperatures. At a temperature below T_M , convergence is considered to be reached if the difference $|\langle \vec{S}'_i \rangle - \langle \vec{S}_i \rangle|/|\langle \vec{S}_i \rangle|$ between two successive iterations for every spin is less than a very small given value τ_0 .

3. Simulated results

In order to clearly display the spin configurations, we considered here a very small circular monolayer nanodisk with radius $R=10a$, where a is the side length of the square crystal unit cell. For convenience, only the interactions between the nearest neighboring spins are considered and these spins are coupled uniformly with strengths $\mathcal{J}_{ij} = \mathcal{J} = 1$ K and $D_{ij} = D$. Therefore, all parameters used in this work are scaled with both Boltzmann constant k_B and the exchange strength \mathcal{J} .

3.1. Temperature dependence of vortical structure driven by a strong DM interaction

Firstly, to investigate how the vortical structure evolves with the changing temperature under a strong DM interaction, DD interaction was neglected, and D was assigned to a value of 0.3 K to perform simulations.

Fig. 1(a) and (b) display our calculated thermally averaged $\langle S_x \rangle$, $\langle S_y \rangle$ and $\langle S_z \rangle$ for the nanodisk. The DM interaction has indeed induced an out-plane magnetic moment $\langle S_z \rangle$ below the transition temperature $T_M \approx 5.15$ K [53–56], which is stronger than the other two components, $\langle S_x \rangle$ and $\langle S_y \rangle$, in the whole magnetic phase. The curves abruptly change at $T_{M1,2,3,4} \approx 1.65, 1.85, 2.45$, and 2.50 K, suggesting that a few spin configurations have been formed in the magnetic phase, as shown and described below. Above $T_{M4} (\approx 2.50$ K), all the three components decrease monotonously as temperature increases, and below $T_{M1} (\approx 1.65$ K), as expected, $\langle S_z \rangle$ increases gradually in magnitude, though not smoothly, as temperature decreases.

Under the strong DM interaction, ferromagnetic vortical structures are formed on the nanodisk, however, they are temperature dependent. Fig. 2 displays the magnetic structures, recorded at four temperatures, projected onto the disk-plane (the xy -plane) and the perpendicular z -direction.

As shown in Fig. 2(a) and (b), a single vortex is observed in the disk-plane in the temperature region $T_{M4} \leq T < T_M$. Inside the central circle of radius $r=8a$, the z -components of all spins are upward, outside of this circle, the spins are downward. Therefore, the chirality of the single vortex is clearly right-handed since $D > 0$. Obviously, the sizes of the marginal and central circular areas are affected by the disk size and temperature.

As temperature drops down, the spin configuration evolves. As shown in Fig. 2(c), at $T=2.5$ K, an elongated vortex centered at the origin of the nanodisk appears, accompanied by other two initially developed vortices on its both sides. Fig. 2(d) displays the z -projection of the spin structure. In the elongated area all spins are upward, others on its both sides are downward. Although the three vortices are deformed, their chiralities are still right-handed since D is positive.

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