Magnetic Vortices Induced by Dipole-Dipole Interaction in Monolayer Nanodisks

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Abstract. In transition metal oxides, the magnetic dipole-dipole interaction (DDI) and chiral Dzyaloshinsky-Moriya interaction (DMI) between the nearest neighboring spins can be comparable in magnitude sometimes. Moreover, the DDI is of long range character, its co-existence with the Heisenberg exchange can also induce magnetic vortices on nanodisks as the DMI does. For these reasons, we employ here two quantum computational approaches, which we develop in recent years, to simulate the vortical spin structures in magnetic nanodisks induced primarily by the dipolar interaction. Our calculated results indicate that, in the presence of Heisenberg exchange interaction: A sufficiently strong dipolar interaction is able to induce a single stable magnetic vortex on the disk-plane, meanwhile the spins in the core region have nonzero components in the perpendicular direction; Further increasing the dipolar interaction leads to the formation of a well symmetric multi-vortex structure in the disk-plane, whereas the out-of-plane spin components completely vanish; An external magnetic field or magnetic anisotropy both normal to the disk-plane can help to induce a vortical structure when the dipolar interaction is not sufficiently strong to induce that kind of structure by itself, providing new techniques to create and annihilate magnetic vortices by either an external magnetic field or electric field for nanomagentic data storage and computing; A DDI-induced vortex shows no chirality even within external magnetic field; Under strong dipolar interactions, the calculated multi-vortex textures with the two quantum simulation approaches are well consistent with each other, so the two methods are verified by each other once again. Overall, our computational results agree well with the findings of previous authors in principle, and our simulated multi-vortex structure

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are very symmetric. Therefore, the phenomena and mechanisms revealed here might stimulate extensive interest of theorists and experimentalists.

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1. Introduction

The long-range ferromagnetic order in a magnetic device tends to disappear when the energy due to thermal fluctuation becomes comparable to the anisotropic and exchange energy terms. This is a well known super-paramagnetic limit imposed on the miniaturization of magnetic devices [1]. Fortunately, recent studies on nanomagnetic materials have shown that a vortical structure, such as magnetic vortices and skyrmions, in quasi-two-dimensional nanomagnets can help overcome this limit. Its possible applications include magnetic random access memory systems, magnetic sensors, high density magnetic recording media, magnetic reading and writing heads [2, 3, 4].

Magnetic vortices and skyrmions are usually induced by the chiral Dzyaloshinsky-Moriya interaction (DMI) [5]. However, in transition metal oxides, the DMI is in the order of 0.1 meV per pair of atoms, while the dipole interaction energy between a nearest neighboring pair expressed as $\mu_0 g \mu_B^2 / 4\pi a^3$ (where μ_0 is the permeability of the vacuum, g the Landé factor, μ_B the Bohr magneton and a the lattice constant) is in the same order as DMI [6]. Especially, the DDI is of long range character, its co-existence with the Heisenberg exchange can also induce magnetic vortices on nanodisks [7, 8, 9]. When the DDI term is sufficiently strong, the continuity of the effective magnetic field along the disk border forces the magnetic moments to be tangent to its boundary [10, 11]. As a result, a magnetic vortex is induced around the center of the nanosystem. Therefore, to study the formation mechanism of vortical spin structures and to understand the properties of magnetic nano- and sub-micro-dots, it is necessary to make thorough studies on the effects of DDI [7, 8, 9, 12, 13, 14, 15].

The competition between the Heisenberg exchange and DDI with conflicting symmetries gives rise to complex physical behaviors in magnetic nanosystems. For this reason, the dipolar interaction is very difficult to treat in both analytical and computational studies. Various methods have been applied over the years to deal with it, such as Monte Carlo simulations [14, 15, 16, 17, 18, 19], micromagnetic simulations [20, 21, 22], computations for dynamics of vortices [23], as well as theoretical [24] and experimental studies [25]. Vortices and anti-vortices were observed experimentally [26] in two-dimensional (2D) cobalt micro-dots. Layers of magnetic dots on a superconducting film were also investigated, which shows transport properties attributed to magnetic vortices [27]. The above works, though not extensive, give us an idea of the amount of the research activity and passionate interest involved.

In particular, it is worth mentioning the work of Rocha et al. who performed systematic Monte Carlo simulations to investigate the formation conditions of vortices in 2D nanodisks with triangular, square and hexagonal structures [16]. They found that there is a transition line which separates the vortical state from the capacitor-like state. This line is obeyed by all three types of lattices. The critical value of the DDI strength parameter is given by

$$D_c = D_0 + 1/\left[A(1 + BL^2)\right] \ , \tag{1}$$

where the values of D_0, A and B depend on the type of the lattice under consideration, and L is the disk diameter. With the exception of the triangular lattice, two types of vortices, with and without out-of-plane components, are identified when the DDI strength is given different values. Vedmedenko et al. have also investigated the magnetic structure of 2D films by means of Monte Carlo simulations [14]. It was found that, when the magnetic anisotropy perpendicular to the film dominates, the out-of-plane domains are stabilized, while the in-plane vortices are formed for a vanishing anisotropy. On the other hand, if the anisotropic and dipolar interactions are comparable, a complex domain pattern evolves, yielding a continuous transition between the two sorts of structures. In another study, Depondt et al. simulated 2D magnetic disks of finite sizes by integrating the Landau-Lifshitz equation for an isotropic Heisenberg model with the dipolar interaction of various strengths at low temperatures, magnetic structures with or without vortices were generated in their simulations [22].

In the present work, we utilize two quantum computational approaches which we develop in recent years [28, 29, 30, 31, 32] to simulate the vortical structures that are induced primarily by the dipolar interaction in monolayer nanodots. Our simulated results suggest that: (a) A moderately strong DDI is able to induce a single stable magnetic vortex that occupies the whole disk-plane, while the spins also order, though quite weakly, in the perpendicular direction in the central region [16]; (b) A considerably strong DDI usually gives rise to a well symmetric multi-vortex structure in the disk-plane, however the out-of-plane spin components completely disappear; (c) An external magnetic field or magnetic anisotropy both perpendicular to the disk-plane can help induce a single vortical structure when the DDI is not sufficiently strong, providing new techniques to manipulate magnetic vortices for nanomagnetic data storage and computing by applying either external magnetic or electric field; (d) A DDI-induced vortex has no chirality even being placed inside an external magnetic field, this character makes a DDI-induced vortex distinguishable from other sorts of vortices; (e) Under strong DDI interactions, the calculated multi-vortex textures with the two quantum approaches are well consistent, thus the two methods are verified by each other once again. In brief, our computational results agree well with the findings of Rocha et al. in principle [16], so the phenomena and mechanisms revealed in the present work might stimulate extensive theoretical and experimental studies.

2. Methods: the Two Quantum Computational Approaches

The two quantum computational approaches we develop so far have been described in details in our published papers [28, 29, 30, 31, 32]. The spins appearing in Hamiltonians are treated as quantum operators instead of classical vectors, and all physical quantities are strictly evaluated with quantum formulas. In the first approach, the self-consistent algorithm is employed, thus the method is abbreviated as the SCA approach [28, 29, 30, 31]. Whereas, in the second one, Metropolis algorithm is incorporated with quantum theory, so it is a kind of quantum Monte Carlo (QMC) method [32]. All of our recent simulations are started from a random magnetic configuration above the magnetic transition temperature, T_M, then carried out stepwise down to very low temperatures with a reducing step $\Delta T < 0$.

For simplicity, we now consider a round monolayer nanodisk with the square crystal structure. The Hamiltonian of the magnetic nanosystem can be expressed as [14, 15, 16, 22]:

$$\begin{aligned}\mathcal{H} = & -\frac{1}{2}\sum_{i,j\neq i}\mathcal{J}_{ij}\vec{S}_i\cdot\vec{S}_j - K_A\sum_i\left(\vec{S}_i\cdot\hat{n}_i\right)^2 - \mu_B g_S \vec{B}\cdot\sum_i\vec{S}_i \\ & -\frac{D}{2}\sum_{i,j\neq i}\left[\frac{3\left(\vec{s}_i\cdot\vec{r}_{ij}\right)\left(\vec{s}_j\cdot\vec{r}_{ij}\right)}{r_{ij}^5}-\frac{\vec{s}_i\cdot\vec{s}_j}{r_{ij}^3}\right].\end{aligned} \tag{2}$$

Here, the first term in the right hand side represents the Heisenberg exchange interaction; the second term denotes the magnetic anisotropy, where $\vec{n}_i$ is a unit vector normal to the disk-plane at the i-th site; the third one is the Zeeman energy of the system within an external magnetic field; whereas the last summation stands for the long distance dipolar interaction among the spins. The strengths of the three intrinsic interactions are $\mathcal{J}_{ij}$, K_A and D, respectively. In the dipolar interaction term, $\vec{r}_{ij}$ is the vector from the i-th to the j-th lattice sites, and the summation is taken over all spins within a circle around the considered spin with a cut-off radius r_c. To a satisfactory accuracy, r_c was assigned to $15a$ in all our simulations.

The nanodisks are assumed to be composed of $S = 1$ spins, thus the matrices of the three spin components are given by

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

respectively, in light of quantum theory.

3. Computational Results

Firstly, we performed extensive simulations with the SCA approach for round monolayer nanodisks of different sizes, and all of them are assumed to lie in the xy-plane. However, only the results for nanodisks with radius $R = 30\,a$ are presented in this article for comparison purpose. To simplify the model, all the spins on the disks are considered to be ferromagnetically coupled with a uniform strength $\mathcal{J}_{ij} = \mathcal{J} = 1$ K. That is, all parameters used in this article are scaled with the Boltzmann constant k_B and exchange strength $\mathcal{J}$.

3.1. Single Vortex Formed with Out-of-Plane Magnetization

Firstly, we carried out SCA simulations for a monolayer nanodisk by using values of $\mathcal{J} = 1$ K and $D = 0.1$ K. The calculated spin configurations are projected onto the

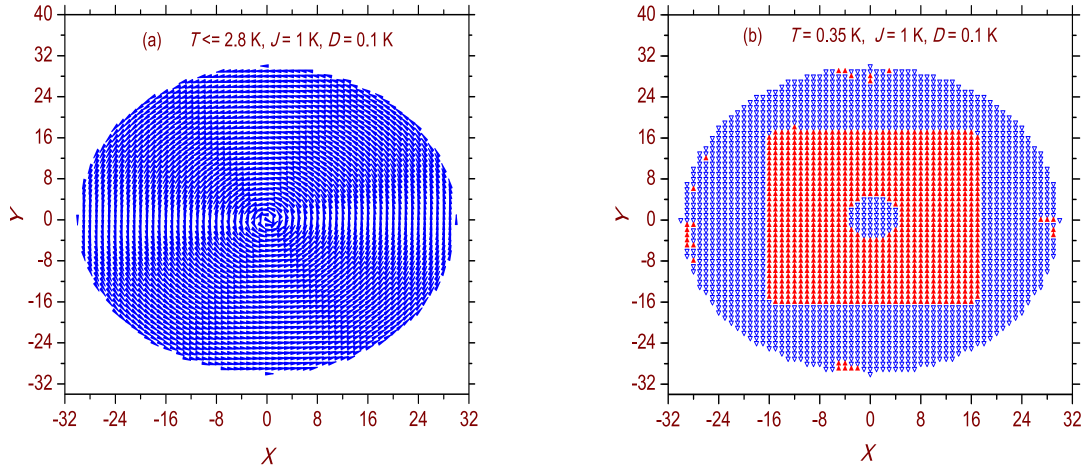

Figure 1. Calculated spin configurations with the SCA approach projected onto (a) the disk-plane in the temperature region $T \leq 2.8$ K, and (b) the perpendicular direction at $T = 0.35$ K, where the upward and downward triangles represent spins with positive and negative z-components respectively. Here $R = 30$a, $\mathcal{J} = 1$ K, and $D = 0.1$ K are used in simulations.

xy-plane and the z direction as shown in Figure 1 (a) and (b), respectively. We can see there that a single vortex with out-of-plane component is formed on the disk-plane in the low temperature range. This is consistent with Eq.(1) of Rocha et al. [16]. In the central and boundary areas, the out-of-plane spin components are downward, however these two regions are separated by a hollow square, where the z-components of all spins are upwards, showing the influence of the square crystal structure. Therefore, it is completely meaningless to talk about the chirality of a magnetic vortex induced by the dipolar interaction.

The dipolar interaction in the Hamiltonian can be divided into two parts: the first part tends to rotate the spins towards the direction of $\vec{r}_{ij}$ that is completely in the monolayer disk-plane, whereas the second part attempts to align the spins antiferromagnetically. When the magnetic moments in the border of a nanodisk are all aligned tangent to the boundary, both the Heisenberg exchange energy and the second part of the dipolar energy are minimized. As a result, a single magnetic vortex can be formed, as shown in Figure 1(a).

Due to the long range nature, up to seven hundreds of spins are involved in the dipolar interaction. Since all spins are on the disk plane, this interaction forces the magnetic moments towards the xy-plane. So we get large $\langle S_x \rangle$ and $\langle S_y \rangle$, but considerably weak $\langle S_z \rangle$, as shown in Figure 2(a,b). There, the out-of-plane component is three orders weaker than the in-plane components in magnitude. Especially, $\langle S_z \rangle$ is only appreciable in the temperature range $T < 0.65$ K, which is far below the transition temperature $T_M \approx 3$ K. The calculated three spin components fall down monotonously and smoothly with increasing temperature, suggesting that the single-vortex structure is stable in the

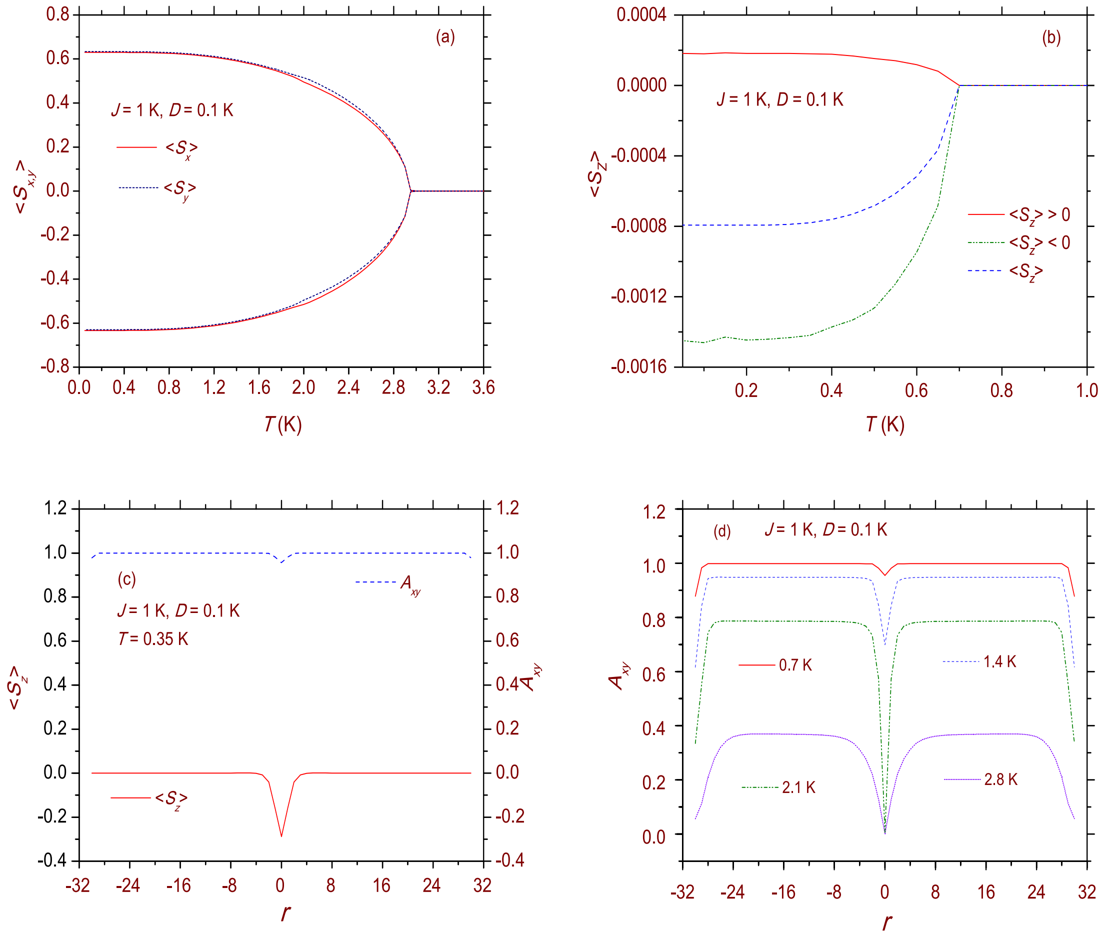

Figure 2. Calculated (a) $\langle S_x \rangle$, $\langle S_y \rangle$, and (b) $\langle S_z \rangle$ as functions of temperature, (c) $S_z(r)$ and $A_{xy}(r)$ at $T = 0.35$ K, and (d) $A_{xy}(r)$ at other four temperatures, as functions of r. Simulations were done with the SCA approach. Here $R = 30$a, $\mathcal{J} = 1$ K, and $D = 0.1$ K, respectively.

whole temperature range below T_M.

To describe the detailed spin configurations on the nanodisk, two quantities are introduced and defined here as:

$$A_z(r) = \frac{1}{N_c(r)} \sum_i |\langle S_{iz} \rangle|, A_{xy}(r) = \frac{1}{N_c(r)} \sum_i \sqrt{\langle S_{ix} \rangle^2 + \langle S_{iy} \rangle^2}\,, \tag{4}$$

for the out-of and in-plane components of the spins, respectively. Here, the quantity $N_c(r)$ is the number of the spins on a circle of radius r around the disk center. Naturally, the larger the radius, the more spins on the circle. Figure 2(c,d) display them as the functions of r at different temperatures. In Figure 2(c), we depict $\langle S_z \rangle$ at 0.35 K since it is now sizable, where the spins with appreciable out-of-plane components are found only inside a small central region and they all order downward. However, when $T > 0.65$ K, $A_z(r)$ is negligible. So only the $A_{xy}(r)$ curves are plotted in Figure 2(d) at four high temperatures. In each of these cases, $A_{xy}(r)$ decreases in both the central and boundary regions. Especially, its magnitude drops considerably with increasing temperature.

3.2. Multi-Vortices Induced by a Strong Dipolar Interaction

By successively increasing DDI strength in simulations, we found out that only a single vortex can be formed in the disk-plane for the D value up to 0.4 K, while the out-of-plane spin components vanish as $D > 0.125$ K [16]. In particular, multi-vortices are generated in the disk-plane if D is further increased as shown in Figure 3(a,b) where D is 0.5 K and 0.8 K, respectively.

It should be emphasized here that these large D values are reasonable, since the magnetic DDI and DMI between the nearest neighboring spins can be comparable in magnitude in transition metal oxides sometimes [6], and previous authors have increased $D/\mathcal{J}$ up to 0.4 [15, 33] and 0.7 [22] in their studies, respectively. Moreover, MacIsaac et al. found, in Monte Carlo simulations for ultrathin magnetic films, that when the dipolar and exchange interactions are of comparable strength there exists a reorientation transition from a planar ferromagnetic phase at low temperature to either an orientationally ordered striped phase or a tetragonal phase at higher temperature [12].

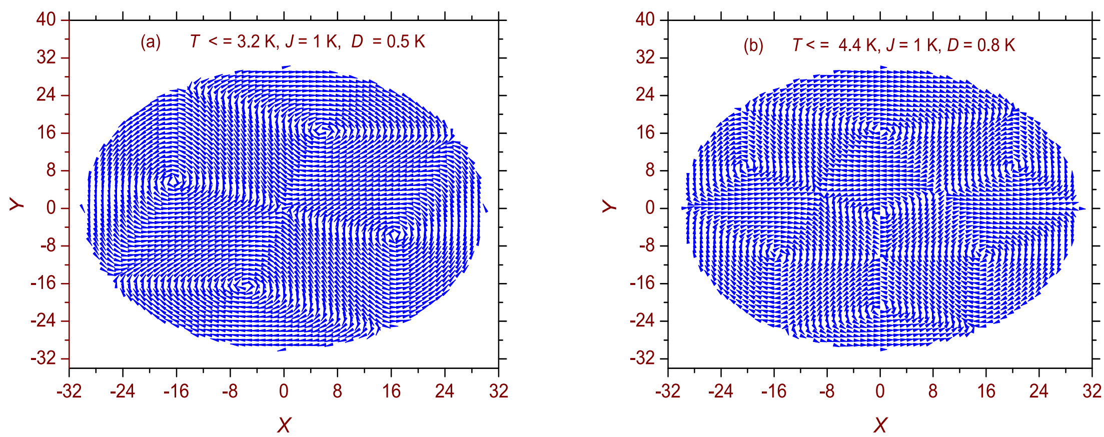

Figure 3. Spin configurations calculated with the SCA approach is projected onto the disk-plane (a) as $T \leq 3.2$ K, $D = 0.5$ K, and (b) while $T \leq 4.4$ K, $D = 0.8$ K. Other parameters are $R = 30$a, $\mathcal{J} = 1$ K, respectively.

In our simulations, when $D = 0.5$ K an anti-vortex is observed in the central region, it is surrounded by four vortices. The whole spin configuration shows two-fold rotational symmetry about the z-axis which passes through the disk center. Each pair of neighboring vortices curl in the opposite directions, one is clockwise and another is anti-clockwise, to minimize the total energy of the whole magnetic system.

In another case as $D = 0.8$ K, a vortex is formed in the central area, it is separated by three anti-vortices around it from other six outer vortices, and each pair of neighboring vortices swirl in the opposite directions as well. In addition, the whole spin structure looks quite symmetric. At least, the positions of the vortex centers show mirror symmetry about the y-axis.

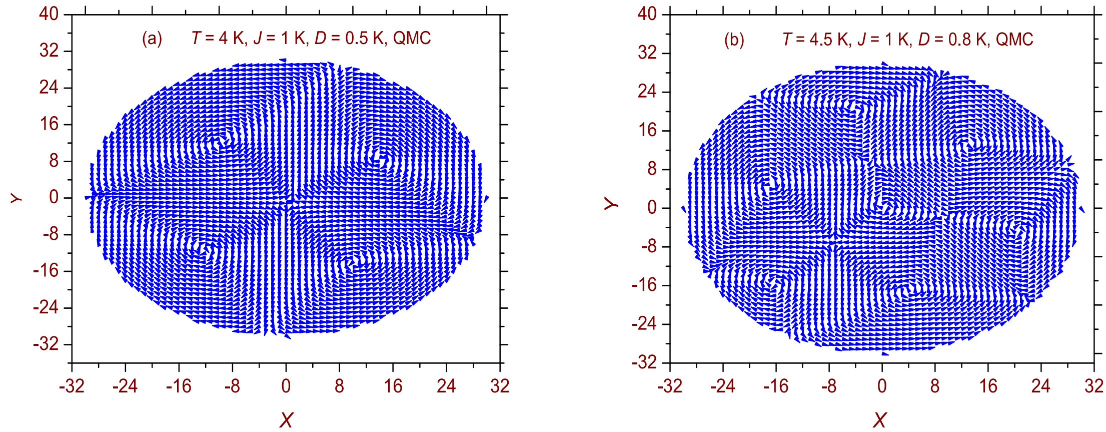

Figure 4. Spin configurations calculated with the QMC approach projected onto the disk-plane (a) as $T = 4$ K, $D = 0.5$ K, and (b) while $T = 4.5$ K, $D = 0.8$ K. Other parameters are $R = 30$a, $\mathcal{J} = 1$ K, respectively, as before.

Actually, in the above two cases, slightly different multi-vortex structures can be observed at higher temperatures in the magnetic phase. However, as temperature drops down below 3.2 K and 4.4 K, respectively, the spin textures become stable, so only in those temperature regions they are displayed in Figure 3.

When comparing the two interactions involved, the strong dipolar interaction is now the dominating one, so the multi-vortex structure induced by this interaction is very stable in the whole magnetic phase. The stability of the state is further evidenced by the smoothly changing $\langle S_x \rangle$, $\langle S_y \rangle$ curves in the low temperature region, for example, as $T \leq 5$ K in the latter case. For the purpose of brevity, these curves are not shown here.

To check these results, we performed simulations with our quantum Monte Carlo approach [32], the calculated spin configurations are displayed in Figure 4. By comparing them with those displayed in Figure 3, we can find that, though now the two spin configurations were calculated at higher temperatures, the two sets of corresponding spin textures look quite similar: if one of them is rotated around the z-axis passing through the disk-center for a certain angle, it will coincide with the corresponding one. Thus the two quantum simulation approaches were verified with each other here once again.

3.3. Effects of an External Magnetic Field

According to Eq.(1) given by Rocha et al. [16], for the nanodisk of this size, the vortical structure can not be formed in the disk-plane if the dipolar interaction strength D is less than 0.0386 K. This point has been confirmed by our simulations performed with D assigned to 0.03 K.

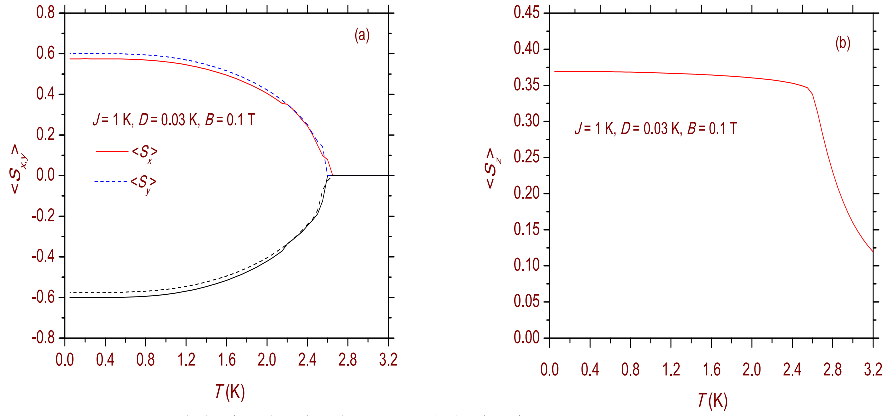

Figure 5. Calculated (a) $\langle S_x \rangle$, $\langle S_y \rangle$, and (b) $\langle S_z \rangle$ versus changing temperature with the SCA approach. Here $R = 30$a, $\mathcal{J} = 1$ K, $D = 0.03$ K and $B = 0.1$ T respectively.

Under this circumstance, we wonder whether an external magnetic field can help to induce a magnetic vortex. To test this idea, we carried out simulations by considering an external magnetic field of 0.1 T exerted along the z-axis. Consequently, a single magnetic vortex was indeed observed in the disk-plane, and it was quite stable below $T_M \approx 2.55$ K. To avoid repetition, the spin configuration is not displayed here.

The good stability enhanced by the external magnetic field is also verified by the smoothly and gradually changing $\langle S_x \rangle$, $\langle S_y \rangle$ and $\langle S_z \rangle$ curves as shown in Figure 5(a,b), respectively. The two in-plane components, which decay monotonically with increasing temperature until T_M, seem not obviously affected by the exerted field. However, the out-of-plane component is enhanced by a few orders in the whole low temperature range when compared with Figure 2(b), and this effect persists far above T_M.

Moreover, we also performed simulations by considering an external magnetic field of the same strength applied in the opposite direction. However, if such calculated $\langle S_x \rangle$, $\langle S_y \rangle$ and -$\langle S_z \rangle$ are plotted, we can get almost the same set of curves as shown in Figure 5(a,b). Though all spins are now reversed in the z-direction by the applied magnetic field, the simulated vortex still curls in the same direction as before. This phenomenon suggests once again that it is meaningless to talk about the chirality of a vortex induced primarily by the dipolar interaction.

3.4. Effects of Magnetic Anisotropy

We found in our previous simulations that, when Heisenberg exchange and Dzyaloshinsky-Moriya interactions co-exist, the magnetic anisotropy normal to the nanodisk is able to stabilize the vortex structure [30]. Thus, it is reasonable to speculate whether such a magnetic anisotropy plays the similar role in the present case when D is less than the threshold value. To test this hypothesis, we carried out SCA simulations by taking account of perpendicular anisotropy with a strength of $K_A = 0.2$ K while $\mathcal{J} =$ 1 K and $D = 0.03$ K. The co-existence of the latter two interactions of the strengths is inadequate to generate a magnetic vortex [16]. However, further including the magnetic anisotropy in simulations indeed dramatically changed the spin configuration: a stable single magnetic vortex is formed on the disk-plane in the low temperature range $T \leq$ 1.95 K. Above this temperature, magnetic vortices can also be observed at $T = 2.45$ K, 2.3 K, for instance. However they are easily to be destroyed at other high temperatures due to thermal disturbance. The reasons can be found from Figure 6(a,b), where both $\langle S_x \rangle$ and $\langle S_y \rangle$ oscillate wildly above 2.2 K, and as $T > 1.95$ K, $\langle S_z \rangle$ is too weaker than the two in-plane components to stabilize the magnetic vortex. Moreover, it is very interesting to find that $\langle S_z \rangle$ has a much lower transition temperature than $\langle S_x \rangle$ and $\langle S_y \rangle$.

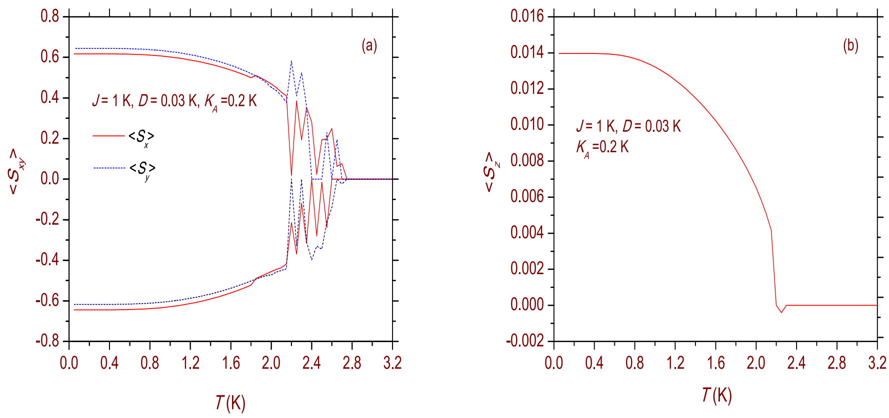

Figure 6. Calculated (a) $\langle S_x \rangle$, $\langle S_y \rangle$, and (b) $\langle S_z \rangle$ versus changing temperature with the SCA approach. Here $R = 30$a, $\mathcal{J} = 1$ K, $D = 0.03$ K and $K_A = 0.2$ K, respectively.

Afterwards, we performed simulations by reducing K_A to 0.1 K, but keeping $\mathcal{J}$ and D unchanged. Consequently, a single magnetic vortex was also observed on the disk-plane in lower temperature range which exhibits similar features as described in this subsection.

4. Discussion and Conclusions

To summarize, we have successfully simulated the spin vortical structures induced primarily by dipole-dipole interaction in monolayer nanodots by means of our quantum computational approaches. The methods enabled us to investigate the effects of magnetic anisotropy and external magnetic field both considered to be normal to the disk-plane. As noticed in earlier Monte Carlo simulations [16], our results show once again that a moderately strong dipolar interaction is able to induce a single stable magnetic vortex on the disk-plane, meanwhile inside the core region the spins also order in the z-direction with appreciable magnitude. It is also found that, when the DDI is substantially strong, more vortices are generated in the disk-plane, and the whole spin configuration exhibits excellent symmetry. In such a case, all spins only order in the disk-plane and the out-of-plane component completely vanishes. Moreover, if the dipolar interaction is not strong enough, an external magnetic field or magnetic anisotropy perpendicular to the disk-plane can help to induce the vortical structure. However, in the latter case, the single vortex is easy to be destroyed by thermal disturbance at high temperatures, since there the out-of-plane spin components are too weak to stabilize the in-plane magnetic vortex. Therefore, the external magnetic field is able to induce and stabilize the single vortex structure more efficiently, and this can be easily manipulated and realized in experiments.

Interestingly, the DDI-induced vortex shows no chirality even being placed within an external magnetic field. This distinct character makes it easy to judge if the DDI is dominating over the DMI in a nano-dot.

In fact, the uniaxial magnetic anisotropy of some nanomagnets can be increased or reduced by applied electric field [34]. Thus, when DDI strength D is slightly weaker than the threshold value, magnetic vortices can be easily created and annihilated by an applied electric field. This technique can be utilized to fabricate energy-efficient nanomagnetic memory for data storage and logic devices for nanomagnetic computing.

On the other hand, the perpendicular magnetic anisotropy of multi-layer systems can be enhanced, for example, by reducing the Fe/Co ratio and the overall FM thickness in Ir/Fe/Co/Pt [35]. This gives us another technique to create and stabilize magnetic vortices in nanodots where the dipolar interaction is appreciable.

The multi-vortex spin textures under strong DDI interaction obtained by means of our two quantum computational approaches agree well with each other: If the spin configurations obtained with the QMC method are rotated around the z-axis passing though the disk-center for certain degrees, they will coincide with those obtained with the SCA approach correspondingly, hereby verifying the two simulation approaches.

In short, our calculated results presented in this paper are in good agreement with the findings of Rocha's group [16] in principle, and our simulated multi-vortex structures exhibit good symmetry. Thus the phenomena and mechanisms revealed in our simulations may stimulate extensive theoretical and experimental studies in the field.

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