Numerical Studies on Antiferromagnetic Skyrmions in Nanodisks by Means of A New Quantum Simulation Approach

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We employ a self-consistent simulation approach based on quantum physics here to study the magnetism of antiferromagnetic skyrmions formed on monolayer nanodisk planes. We find that if the disk is small and the Dzyaloshinsky-Moriya (DM) interaction is weak, a single magnetic vortex may be formed on the disk plane. In such a case, when uniaxial anisotropy normal to the disk plane is further considered, the magnetic configuration remains unchanged, but the magnetization is enhanced in that direction, and reduced in other two perpendicular orientations. Very similarly, a weak external magnetic field normal to the disk plane cannot obviously affect the spin structure of the nanodisk; however, when it is sufficiently strong, it can destroy the AFM skyrmion completely. On the other hand, by increasing DM interaction so that the disk diameter is a few times larger than the DM length, more self-organized magnetic domains, such as vortices and strips, will be formed in the disk plane. They evolve with decreasing temperature, however always symmetric about a geometric axis of the square unit cell. We further find that in this case introducing normal magnetic anisotropy gives rise to the re-construction of AFM single-vortex structure or skyrmion on the disk plane, which provides a way to create and/or stabilize such spin texture in experiment.

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I. INTRODUCTION

The concepts of skyrmions were originally introduced by a particle physicist, Tony Skyrme, to describe the localized, particle-like structures in the field of pion particles in the early 1960s \cite{1}. About 30 years later, Bogdanov and Yablonskii theoretically predicted \cite{2} that they could exist in magnets when a chiral Dzyaloshinsky-Moriya (DM) interaction \cite{3,4} is present. Indeed, it was later found in experiments that magnetic skyrmions exist in helical magnets, such as MnSi and Fe\textsubscript{1−x}Co\textsubscript{x}Si \cite{5,6}, and DM interaction favors canted spin configuration \cite{7}. Most skyrmions found in helimagnets were induced by an external magnetic field at low temperatures \cite{6–8,10}. For example, Heinze et al. \cite{11} observed a spontaneous atomic-scale magnetic ground-state skyrmion lattice in a mono-layer Fe film at a low temperature about 11 K. However, Yu et al. \cite{12} obtained a skyrmion crystal near room-temperature in FeGe with a high transition temperature (280 K) by applying a magnetic field.

So far, ferromagnetic (FM) skyrmions have been intensively investigated both theoretically and experimentally. However, the DM interaction is more generally found in antiferromagnetic (AFM) materials than ferromagnetic materials. Most recent experiments on FM skyrmions rely on the presence of the interfacial DM interaction to stabilize skyrmions. In contrast, bulk DM interaction is more prevalent in antiferromagnets \cite{2,3}, and they are considerably more abundant in nature than ferromagnets.

Skyrmions have been predicted to appear in the ground state of doped antiferromagnetic insulators \cite{13,20}. However, it is difficult to identify these isolated skyrmions. Neutron scattering, for example, would not be an effective probe, since these skyrmions do not form a lattice, whereas their signatures on transport may be screened by the insulating character of the carriers \cite{21}. Based on their experimental observation, Raičević et al. concluded that the low-temperature magnetic and transport properties of the AFM La\textsubscript{2}Cu\textsubscript{1−x}Li\textsubscript{x}O\textsubscript{4} provided the first experimental support for the presence of skyrmions in AFM insulators.

Recently, Huang et al. \cite{22} simulated the creation process of skyrmion in a two-dimensional (2D) antiferromagnetic system to investigate the dynamics of the created skyrmions, and observed stable skyrmions even at long time scales. So far, many researchers have done extensive studies on the static properties of 2D FM skyrmions. Therefore, it is obviously necessary and meaningful to investigate how the magnetism of the 2D AFM skyrmions are influenced by external magnetic field, Heisenberg exchange, anisotropic and DM interactions, so as to find ways to create or stabilize the AFM skyrmion in experiments. For the purpose, this work has been done.

In a just finished work \cite{23}, we investigated the magnetic and thermodynamic properties of mono-layer nanodisks with the co-existance of DM and FM Heisenberg interactions by means of a new quantum simulation approach we develop in recent years \cite{24,25}. We found there that the chirality of the single magnetic vortex on a small nanodisk is only determined by the sign of DM interaction parameter, no matter an external magnetic field is absent or applied normal to the disk plane; however the applied magnetic field perpendicular to the disk-plane is able to stabilize the vortex structure and induce

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skyrmions \[6, 8, 17\].

In the present work, the new quantum simulation approach is applied to AFM mono-layer nanodisks with the co-existence of Heisenberg and DM interaction as well. We find that for small disk of weak DM interaction, single AFM skyrmion is always formed on the disk plane. Further inclusion of uniaxial anisotropy or weak external magnetic field normal to the disk plane causes no obvious change in the spin configuration, but they do enhance the magnetization in that direction and reduce the other two in-plane components. However, if this applied magnetic field is strong enough, the in-plane AFM Skyrmion will be completely destroyed. Moreover, by increasing the DM interaction, more self-organized magnetic domains will appear on the disk plane. They evolve with varying temperature, but always symmetric about a geometric axis of the square unit cell. In this case, an uniaxial magnetic anisotropy normal to the disk plane is able to force the multi-domain structure merge to form a single AFM vortex. In another word, the anisotropy can induce and/or stabilize the AFM skyrmion, which the experimentalists may be very interested.

\section{II. MODELING AND COMPUTATIONAL ALGORITHM}

The Hamiltonian of this sort of nanosystems can be written as \[10, 26, 34\]

\[ \mathcal{H} = -\frac{1}{\tau} \sum_{i,j \neq i} \left[ J_{ij} \vec{S}_i \cdot \vec{S}_j - D_{ij} \vec{n}_i \cdot (\vec{S}_i \times \vec{S}_j) \right] - K_A \sum_i (\vec{S}_i \cdot \vec{n})^2 - \mu_B g S \mathcal{B} \cdot \sum_i \vec{S}_i , \tag{1} \]

where the first and second terms represents the Heisenberg exchange and DM interactions with strength of \( J_{ij} \) and \( D_{ij} \) between every pair of neighboring spins sitting at the \( i \)- and \( j \)-th sites, respectively, the third term denotes the uniaxial anisotropy along \( \vec{n} \), assumed to be normal to the disk plane here, and the last one is the Zeeman energy of the system within external magnetic field \( \mathcal{B} \). For simplicity, we consider in the current work a round mono-layer nanodisk consisting of \( S = 1 \) spins which interact antiferromagnetically only with their nearest neighbors uniformly, that is, \( J_{ij} = J \) and \( D_{ij} = D \), across the whole disk plane. In our model, the spins are quantum operators instead of the classical vectors. Since \( S = 1 \), the matrices of the three spin components are given by

\[ S_x = \frac{1}{2} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \quad S_y = \frac{1}{2i} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{2} \]

respectively.

Our simulation approach, which is facilitated by a self-consistent algorithm, so called as the SCA approach, was assumed to be based on the principle of the least (free) energy \[24, 25\]. Thus, as a computational code implemented with this algorithm runs, all magnetic moments in the sample are rotated and their magnitudes adjusted by the local effective magnetic field to minimize the total (free) energy of the whole nanosystem spontaneously according to the law of least (free) energy, so that the code can finally converge down to the equilibrium state automatically without the need to minimize the total (free) energy elaborately in every simulation step.

All of our recent simulations are started from a random magnetic configuration and from a temperature well above the magnetic transition temperature \( T_M \), then carried out stepwise down to very low temperatures with an iteration step \( \Delta T < 0 \). At any temperature, if the difference \( |\langle \vec{S}_i^z \rangle - \langle \vec{S}_i \rangle|/|\langle \vec{S}_i \rangle| \) between two successive iterations for every spin is less than a very small given value \( \tau_0 \), convergency is believed to be reached.

\section{III. CALCULATED RESULTS}

\subsection{A. Simulations for Nanodisk without Uniaxial Anisotropy and External Magnetic Field}

To investigate the effects of DM interaction, the magnetic anisotropy was neglected in simulations at the beginning. And to visualize the spin configuration clearly, we considered a very tiny round mono-layer nanodisk, its radius \( R = 10a \), where \( a \) is the side length of the square crystal unit cell, and the spins on the disks are assumed to be antiferromagnetically coupled uniformly. We performed simulations with the SCA approach by assigning \( J \) to -1 K and \( D \) to 0.1 K, respectively. To avoid misunderstanding, we indicate here that all parameters used in this paper are scaled with Boltzmann constant \( k_B \).

Under the DM interaction, magnetic vortex is formed on the nanodisk, and owing to the antiferromagnetic Heisenberg interaction, each pair of neighboring spins order oppositely both in-plane and out-plane below the transition temperature \( T_M \approx 2.65 \) K as shown in Figure 1(a,b).

Figure 2(a,b) display our calculated thermally averaged \( \langle S_z \rangle \), \( \langle S_x \rangle \) and \( \langle S_y \rangle \) for the nanodisk in the absence of external magnetic field. The DM interaction has induced out-plane magnetic moments \[33, 38\], which is much stronger than the other two components at all temperatures. The three components decay monotonously with increasing temperature until the transition point \( T_M \approx 2.65 \) K, and the saturated value of \( \langle S_z \rangle \) is approximately 0.85 at very low temperatures, much less than the maximum value \( S = 1 \).

To describe the detailed spin configuration on the nanodisk, two new quantities are introduced and defined as

\[ A_x = \langle S_x \rangle/N_z \quad \text{and} \quad A_{xy} = \sqrt{(A_x)^2 + (A_y)^2}/N_z \]

for the out- and in-plane components, respectively. Here \( N_z(r) \) is the spin number on the circle of radius \( r \) around the disk center. Figure 2(c,d) display their variations with changing \( r = |N_z| \) at four different temperatures. Natu-
rally, the larger the radius, the more spins on the circle. In the inner region of the disk, $A_{xy}$ is very weaker than $A_z$. That is, therein the spin are mainly oriented antiferromagnetically out of the plane, but slightly canted from the normal. Until $r < 6a$, while the radius increases, $A_z$ decreases but $A_{xy}$ grows gradually. That is, as $r$ increases the spins are rotated by the effective magnetic field towards the plane, so that finally, within the marginal region of the disk the magnitudes of $A_z$ and $A_{xy}$ become comparable.

The total free energy $F$, total energy $E$, magnetic entropy $S_M$ and specific heat $C_M$ of this sort of canonical magnetic systems can be calculated with following formulas

$$F = -k_B T \log Z_N, \quad E = -\frac{\partial}{\partial T} \log Z_N,$$

$$S_M = \frac{E}{T} + k_B \log Z_N, \quad C_M = T \left( \frac{\partial S_M}{\partial T} \right)_B,$$

(3)

successively, where $\beta = 1/(k_B T)$ and $Z_N$ is the partition function of the whole system. Figure 3(a,b) display the $F$, $E$, $S_M$ and $C_M$ curves obtained by means of the SCA approach for the AFM nanodisk. The slopes of $F$, $E$ and $S_M$ curves change suddenly near $T_M$, which are the signs of phase transition. However, the $C_M$ curve now varies smoothly around $T_M$, in contrast to the sharp peaks observed in the $C_M$ curves near $T_M$’s of bulk magnets. This fact suggests that the phase transition behavior of the nanosystem has been strongly modified by its finite size and the spiral DM interaction.

B. Effect of External Magnetic Field

In our previous simulations for FM nanodisks with DM interaction, we found that an applied magnetic field is able to induce or stabilize the in-plane vortical spin structures, so that the chiral configuration can maintain to a temperature well above $T_M$ as observed in experiments. So we naturally wonder if this rule still holds true in the case of AFM nanodisks.

For the purpose, by assuming a magnetic field exerted normal to the disk plane at $T = 0.25$ K, we did simulations for the AFM nanodisk with the spin structure calculated at that temperature in the absence of external magnetic field as the input data. In this circumstance, the nanosystem is able to sustain the external influence to maintain the vortical structure until $B_z = 0.3$ Tesla as shown in Fig.4(a). However, when $B_z$ is further increased to 0.4 Tesla, the spiral structure is thus completely overcome, whereas the in-plane components of the spins still order antiferromagnetically in the [-1,1,0] direction as depicted in in Fig.4(b). This behavior of the nanosystem is easy to understand. When the external magnetic field along the $z$ direction is strong enough, the spins are unable to align antiferromagnetically in the $z$ direction any longer, as a result, the in-plane components cannot form antiferromagnetic vortices either. That is, the formation of an FM (AFM) vortex in the disk plane depends strongly on the presence of a spatial region wherein the spins order ferromagnetically (antiferromagnetically) in the normal direction.

C. Effect of Uniaxial Anisotropy

So far, we have not considered the influence of magnetic anisotropy. To study its effects, it is now assumed to be along the $z$-direction to do further simulations. Since other parameters are kept unchanged, as expected, below $T_M$, $\langle S_z \rangle$ has been enhanced by the anisotropy, but both $\langle S_x \rangle$ and $\langle S_y \rangle$ are suppressed for the same reason, so that the maximum of $|\langle S_z \rangle|$ is now increased to 0.984, but that of $|\langle S_{x,y} \rangle|$ reduced to 0.100 as seen in Fig.5(a). In addition, all these curves changes gradually, though not smoothly due to relatively weak DM interaction, and
a single magnetic vortex is found on the nanodisk, which prevails in the whole magnetic phase as depicted in Figure 5(b).

D. Effect of DM Interaction Strength

To describe the multi-domain structures, a new quantity named DM length has been introduced and defined as \( \zeta = J / D \) which is related to the size of self-organized structures, where the distance between two unit grids is defined as the unity \([26]\). When the Monte carlo method is employed, each grid contains \( n \times n \) atomic sites. We adopt this theory by replacing the grid with a spin, and will see how the theory works. Thus, as the disk scale is a few times larger than \( \zeta \) in the unit of lattice parameter \( a \), more magnetic structures, such as strips and vortices, will be formed in the disk plane. This condition can be realized by either increasing DM interaction or the lattice size.

To test the idea, we then carried out simulations for the nanodisk by increasing the DM interaction to \( D = 0.3 \) K, but keeping other parameters unchanged. The calculated \( \langle S_z \rangle \), \( \langle S_x \rangle \) and \( \langle S_y \rangle \) in the absence of external magnetic field are plotted in Figure 6. These magnetization curves are not smooth in the whole low temperature range, reflecting the fierce competition between the Heisenberg and DM interactions. The sudden changes appearing around \( T \approx 1.25 \) K and \( 0.7 \) K especially in the \( \langle S_x \rangle \) and \( \langle S_y \rangle \) curves indicate that phase transitions happen nearby, leading to formations of different magnetic structures. According to the theory just described, now \( \zeta = J / D \approx 3.333 \), and \( 2R > \zeta \), so it is expected more self-organized magnetic domains will appear in the low temperature region. Above \( 1.4 \) K, a single magnetic vortex, as shown in Figure 7(a), occupies the whole disk. However, below \( T = 1.2 \) K, a few magnetic domains appear. The spin configuration evolves with decreasing temperature until \( T = 0.6 \) K, where we observe a very symmetric magnetic structure: a vertical strip appearing exactly in the middle of two AFM vortices, and this pattern remains unchanged down to very low temperature, as displayed in Figure 7(b). The two vortex centers are approximately \( 11a \) apart, three self-organized domains

Figure 2. Calculated spontaneous (a) \( \langle S_z \rangle \), and (b) \( \langle S_{x,y} \rangle \) for the mono-layer AFM nanodisk as functions of temperature; (c) \( A_x \), and (d) \( A_{xy} \) as functions of the distances from the center of the nanodisk at four different temperatures. Here \( R = 10a \), \( J = -1 \) K, and \( D = 0.1 \) K, respectively.
are involved between, thus the averaged distance of two neighboring structures is about 3.67\(a\), slightly larger than \(\zeta\) due to the influence of the disk boundary. Therefore, our simulated results agree well with the adopted grid theory.

E. Joint Effects of Uniaxial Anisotropy and Strong DM Interaction

As described above, a strong DM interaction usually leads to a multi-domain structure on the disk plane. On the other hand, as described above, the formation of an in-plane AFM skyrmion requires the spins to order also antiferromagnetically in the normal direction, and the magnetic anisotropy perpendicular to the disk-plane has such an effect. Therefore, we expect that when a strong DM interaction is present in the nanosystem, which gives rise to multi-domain configuration, introducing the uniaxial anisotropy normal to the disk plane will recover the single vortex structure.

To test this idea, we carried out simulations by using the parameters given in Figure 7, but increasing the anisotropy strength \(K_A\) from zero to 0.1 K. This anisotropic interaction effectively suppresses the strong DM interaction, consequently, the three components of the magnetization change smoothly and fade gradually with increasing temperature below \(T_N\) as shown in Figure 8(a), foretelling the appearance of a single magnetic vortex on the disk plane. This prediction is confirmed by the spin structure that is stable in the whole magnetic phase, as displayed in Figure 8(b).
can be formed on the disk plane. The spin configuration evolves with varying temperature, but is always symmetric about a geometric axis of the square unit cell. In this case, a moderate uniaxial magnetic anisotropy normal to the disk-plane is able to suppress the DM interaction, so that the multi-domains merges to a single AFM skyrmion that occupies the whole disk plane below the transition temperature.

We have adopted a grid theory [26] to describe the multi-domain structures on the nanodisks. The sizes of the magnetic domains and the average distance between a pair of them agree approximately with this modified theory, as already achieved in our recent simulations for FM nanodisks [23].

We would like to stress finally that our simulation approach is based on quantum physics – the spins appearing in the Hamiltonian are treated as quantum operators instead of classical vectors, the thermal expectation values of all physical quantities are calculated with quantum operators in the Hamiltonian are treated as quantum operators instead of classical vectors, the thermal expectation values of all physical quantities are calculated with quantum operators.
formulas. Consequently, the computational program is able to run self-consistently, and quickly converge down to equilibrium state of the magnetic system automatically. Frequently, we find that the computational code only takes a few loops, or even one loop, to converge in low temperature region. And especially, the approach has produced good agreements with experimental and our theoretical results \[23, 39\].

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