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Effects of external magnetic field and magnetic anisotropy on chiral spin structures of square nanodisks investigated with a quantum simulation approach

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ABSTRACT

We employed a quantum simulation approach to investigate the magnetic properties of monolayer square nanodisks with Dzyaloshinsky-Moriya (DM) interaction. The computational program converged very quickly, and generated chiral spin structures on the disk planes with good symmetry. When the DM interaction is sufficiently strong, multi-domain structures appears, their sizes or average distance between each pair of domains can be approximately described by a modified grid theory. We further found that the external magnetic field and uniaxial magnetic anisotropy both normal to the disk plane lead to reductions of the total free energy and total energy of the nanosystems, thus are able to stabilize and/or induce the vortical structures, however, the chirality of the vortex is still determined by the sign of the DM interaction parameter. Moreover, the geometric shape of the nanodisk affects the spin configuration on the disk plane as well.

1. Introduction

Dzyaloshinsky-Moriya (DM) interaction [1,2] exists in systems with broken inversion symmetry, such as in the metallic alloys with B20 structure [3–7] and at the surface or interface of magnetic multi-layers [8,9]. This interaction can induce chiral spin structures like *skyrmions* [3–10] and exotic properties, which paves the way for developing spintronic devices. For instance, in confined structures such as magnetic nanodisks and nanostripes, DM interaction produces stable out-of-plane magnetizations and in-plane magnetic vortices [11,12] which can be classified as left-handed and right-handed [13,14]. The skyrmions have been observed in helical magnets, such as MnSi, $Fe_{1-x}Co_xSi$, and the monolayer Fe film [4]. The tiny size of magnetic skyrmions, as small as one nm [8], which can be easily moved by weak current, makes them good candidates for future data storage.

So far, magnetic vortices formed on nanodisks have been intensively investigated numerically by means of Monte Carlo [15–18] and micromagnetic methods [19–22]. But, in the present work, we employed a quantum simulation approach, which we developed in recent years, to systematically study the magnetic properties of monolayer nanodisks with the co-existence of DM, Heisenberg, uniaxial anisotropic interactions and external magnetic field, in order to understand how these

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interactions affect the chiral spin structures and other physical properties of the nanosystems. As done by previous authors, we focus our studies on small nanodisks [19,20].

The quantum simulation approach, which is facilitated by a self-consistent algorithm, so abbreviated as the SCA approach, is assumed to be based on the principle of the globally least free energy [23–28]. That is, as a code implemented with this algorithm runs, the orientations and magnitudes of all magnetic moments in the considered system are adjusted simultaneously by the local effective magnetic fields to minimize the total free energy of the whole system spontaneously, so that the code can finally converge to the equilibrium states at all temperatures. This hypothesis has been proved by our simulations performed for a ferromagnetic nanowire [27]. Until now, we have successfully applied this simulation approach to nanosystems consisting of rare-earth [23,24] and transition [25–28] elements. Especially, the simulated magnetic structures using the SCA approach for a $DyNi_2B_2C$ nanoball, assumed to be cut out of the body-centered tetragonal crystalline, were in good agreement with that observed in the bulk sample: below the transition temperature, the magnetic moments on an *ab*-plane inside the core aligned ferromagnetically (FM) in the [110] direction, two adjacent *ab* layers ordered antiferromagnetically (AFM), and the calculated transition temperature was very close to that of the bulk sample [24]. Moreover, recent simulations performed for an antiferromagnetic nanoparticle using the currently employed SCA approach has generated the same results as those calculated with a quantum Monte Carlo method we proposed, so that the two quantum simulation approaches have been verified by each other [28]; and the numerical results generated with the SCA approach for both FM and AFM Ising-like nanotubes are exactly identical with those calculated with the one-dimensional chain models based on quantum mean-field theory [29].

2. Quantum simulation model and computational algorithm

The Hamiltonian of the magnetic systems with square unit cell structure we consider here can be expressed as [17,18,22].

$$\mathcal{H} = -\frac{1}{2}\left[\sum_{i,j\neq i}\mathcal{J}_{ij}\vec{S}_i\cdot\vec{S}_j - \sum_{i,j\neq i}D_{ij}\vec{r}_{ij}\cdot\left(\vec{S}_i\times\vec{S}_j\right)\right] - K_A\sum_i\left(\vec{S}_i\cdot\hat{z}\right)^2 - \mu_B g\vec{B}\cdot\sum_i\vec{S}_i. \tag{1}$$

The first and second terms represent the Heisenberg exchange and DM interactions with strengths of $\mathcal{J}_{ij}$ and D_{ij} between each pair of neighboring spins $\vec{S}_i$ and $\vec{S}_j$, respectively, the third one denotes the magnetic uniaxial anisotropy of strength K_A along the *z*-axis, which is assumed here to be normal to the disk plane, and the last one is the Zeeman energy in the external magnetic field. In light of quantum theory, the spins appearing in the Hamiltonian are operators instead of classical vectors, and the thermal average of a physical quantity *A* at any temperature *T* must be evaluated with

$$\langle A\rangle = \frac{\sum_n\langle\varphi_n\left|\widehat{A}\exp(-\varepsilon_n/k_BT)\right|\varphi_n\rangle}{\sum_n\exp(-\varepsilon_n/k_BT)}, \tag{2}$$

where ε_n and φ_n are the eigenenergy and eigenfunction of the Hamiltonian of the considered spin, for instance.

In the present work, we consider monolayer square nanodisk with a side of length *L* and consisting of $S = 1$ spins, thus the matrices of the three spin components in the Cartesian coordinate system are given by

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

respectively. For convenience, it is assumed that the spins only interact with their nearest neighbors, the Heisenberg exchange and DM interactions are isotropic and uniform so that $\mathcal{J}_{ij} = \mathcal{J}$ and $D_{ij} = D$ over the whole nanodisk.

To solve the Hamiltonian, mean field theory must be employed, so that the computational code can run self-consistently. Moreover, our SCA simulations were all started above the transition temperatures from a random spin configuration, then carried out down to very low temperatures with an iteration step $\Delta T < 0$. This technique is crucial, since we believe that at high temperatures the magnitudes of all spins are sufficiently weak, the thermal disturbance is strong enough to help the spins tunnel through the energy barriers, so that the code can avoid being trapped in any local energy minima, and finally converge to the equilibrium states of the considered systems with globally lowest free energy. At any temperature, 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, which is equal to 10^{-6} in the present work, convergence is believed to be reached.

3. Calculated results

3.1. Chirality of single magnetic vortex

Using the SCA approach, we first carried out simulations for 20×20 square lattices assumed to be on the *xy*-plane in the absence of external magnetic field, with $\mathcal{J}$, *D* and K_A assigned to 1 K, 0.1 K and 0, respectively. We stress here that, for