Vortex ground state for small arrays of magnetic particles with dipole coupling

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We show that a magnetic vortex is the ground state of an array of magnetic particles shaped as a hexagonal fragment of a triangular lattice, even for a small number of particles in the array \( N \leq 100 \). The vortex core appears and the symmetry of the vortex state changes with the increase of the intrinsic magnetic anisotropy of the particle \( \beta \); the further increase of \( \beta \) leads to the destruction of the vortex state. Such vortices can be present in arrays as small in size as dozens of nanometers.

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I. INTRODUCTION

Topological defects of vortex type play a paramount part in the general physics of ordered media such as superfluidity, superconductivity and magnetism. In particular, vortices and vortex pairs are important in two-dimensional (2D) magnetism. Recently, the ground state of soft ferromagnetic particles of micron and sub-micron size has been shown to be of a vortex type, which has received much attention from the research community.\(^1,2\)

Compared to vortices in superfluid systems, magnetic vortices in 2D ferromagnets and antiferromagnets have a richer behavior, since they may be divided into two different classes, in-plane and out-of-plane vortices.\(^3,4\) For in-plane vortices all spins lie in the vortex plane. Out-of-plane vortices have nonzero spin components orthogonal to the vortex plane localized within the so-called vortex core, a small region near the vortex center. Vortices with a core are described by several different types of topological charge vorticity \( q \), which is similar to circulation in a supercurrent systems, one can introduce \( \pi_2 \)-topological charge, the polarity or polarization \( p = \pm 1 \) of the vortex core, which is the spin direction in the core and is connected to the \( \pi_2 \) topological charge of the magnetization field. In-plane vortices can be associated with the value \( p = 0 \). Further, vortices found in the ground state of soft magnetic particles should have \( q = 1 \) only \( (q = -1 \) corresponds to antivortices that can be connected to “antidots”, small holes in a patterned magnetic film\(^5,6\)), but they are additionally classified by the discrete number chirality \( C = \pm 1 \), which is the sense of rotation of magnetization far from the vortex core. For a single vortex in a bulk 2D magnet with easy-plane magnetic anisotropy, there is a transition from coreless in-plane vortex structure to the vortex with a well defined core, as the anisotropy strength decreases below a certain critical value.\(^7,8\) The presence of a core plays a crucial role in the dynamic properties of magnetic vortices. In particular, the value of \( \pi_2 \)-topological charge determines special gyroscopic properties of the vortex dynamics and the presence of low-frequency dynamics, essential for possible applications of magnetic vortices in perspective spintronic\(^9,10,11\) and magnonic\(^12,13\) devices.

The presence of vortices in the ground state of soft ferromagnetic particles is determined by the balance between magnetostatic and exchange energies. For disk-shaped particles with negligible magnetocrystalline anisotropy and typical thicknesses about 20 ÷ 50 nm, the vortex state is stable if the disk radius exceeds some critical value \( R_c \sim 150 ÷ 200 \) nm. Vortices in the ground state of soft magnetic particles possess a core with the size of the order of the exchange length of the material \((\sim 15 \) nm in Permalloy). It has been recently shown that magnetic vortices of different structure can be the ground state for magnetic particles with comparable energies of the exchange and dipolar interactions, even for small \((\sim 10^3 \) number of magnetic moments in the particle\(^14,15\))

Highly non-uniform ground state is found for small particles with a sufficiently high surface anisotropy as well.\(^16,17\)

From the perspective of a search for vortex states, the promising magnetic systems are those in which the exchange interaction suppressed or non-existent and the main source of interaction among structural elements is the dipole-dipole interaction of their magnetic moments. These are so-called dipolar magnets, i.e. such spin systems where a long-range magnetic dipole interaction prevails. Dipolar magnets have been attracting persistent interest during decades as objects of the fundamental physics of magnetism possessing some unusual properties. One may mention the presence of an ambiguous ground state with non-trivial continuous degeneracy even for simple cubic\(^18,19\) or 2D square lattices\(^20,21\) and the existence of special phase transitions induced by an external magnetic field.\(^22,23\) Magnon spectra of such systems have a non-analytic behavior at small wave vectors.\(^24,25\)

The interest in systems with the dominant magnetic dipole interaction has significantly increased in last years, mainly in the context of artificial magnetic materials such as arrays of magnetic nanoparticles.\(^26\) Magnetic systems with the dominant dipole interaction possess interesting physical properties important for applications. Among those properties, one can highlight the fact that the ground state of an infinite system of magnetic moments constituting a lattice and coupled by the dipole-
dipole interaction depends essentially on the lattice structure and in the presence of the intrinsic (intra-particle) anisotropy it depends on the orientation of the easy axis of this anisotropy with respect to the lattice axes as well.

Let us discuss 2D lattices, which will be the object of our study. For the lattices of particles with a high perpendicular anisotropy, the ground state corresponds to various types of two-sublattice antiferromagnetic order, particularly, a chessboard structure is realized for a square lattice and a layered one for a triangular lattice. For finite fragments of such lattices these structures vary insignificantly being compared to the infinite case. In the case of systems with an in-plane anisotropy, the role of the boundaries is more essential. For an infinite square lattice, the ground state has four-sublattice antiferromagnetic order and has a high (continuous) degeneracy, while for the triangular lattice a ferromagnetic order is realized. The presence of a boundary, however, may change significantly the state of such a system. For finite fragments of the square lattice the aforementioned continuous degeneracy is removed, but the state remains finite square lattice, the ground state has four-sublattice order is realized.

In the case of systems with an in-plane anisotropy, the ground state is of great interest. In particular, it is interesting what is the minimal size of a system carrying a vortex and whether that size can be made significantly smaller than the critical size $R_c$ indicated above.

In this paper, we will demonstrate that for an array of particles shaped as a fragment of a triangular lattice with a high hexagonal symmetry, see Fig. the ground state is a vortex state even for a small number of particles in the array. Even for an extremely small array of such type, which consists of 7 particles, the vortex state energy is almost two times lower than that of a quasi-homogeneous state. We show further, that such arrays have very interesting behavior: their ground state structure is highly sensitive to the change of the anisotropy of a single particle. In particular, for a particle made of a soft magnetic material this anisotropy could be varied by changing the particle shape.

II. MODEL AND RESULTS

Consider an array of particles placed at the sites of a finite hexagonally shaped fragment of a 2D triangular lattice. The energy of the this system contains contributions from the energy of the magnetic dipole interaction and from the energy of the anisotropy:

$$W = \sum_{\ell \neq \ell'} \vec{\mu}_\ell \vec{\mu}_{\ell'} - \frac{3(\vec{\mu}_\ell \vec{\nu}_\ell')(\vec{\mu}_{\ell'} \vec{\nu}_{\ell'})}{|\vec{l} - \vec{l}'|^3} + \frac{\beta}{a^3} \sum_\ell [(\vec{\mu}_\ell \cdot \vec{e}_x)^2 + (\vec{\mu}_\ell \cdot \vec{e}_y)^2],$$

where $\vec{\mu}_\ell$ is the magnetic moment of the particle at site $\ell$, $|\vec{\mu}| = \mu_0$, $\mu_0$ is the magnetic moment of a single particle, $\vec{\nu} = (\vec{l} - \vec{l}')/|\vec{l} - \vec{l}'|$, $a$ is the lattice constant (the distance between closest particles in the array plane), and $\beta$ is a dimensionless constant determining the magnetic anisotropy strength of a particle. This anisotropy is assumed to be uniaxial, of the easy-axis type (so that $\beta > 0$), with the easy axis $\vec{e}_y$ perpendicular to the system plane. Here $\vec{e}_{x,y,z}$ are unit vectors along coordinate axis.

One can expect that the absence or presence of a vortex core will depend on the effective anisotropy of the system. It is important to note that the total magnetic anisotropy of the array results from the uniaxial anisotropy of separate particles and from the easy-plane anisotropy of the array induced by the demagnetization field of a planar set of magnetic moments (similar to the shape anisotropy in the thin films). Competition of these two contributions determines a complex character of the distribution of magnetization in the array.

If the easy-plane anisotropy induced by the demagnetization field is sufficiently large, that leads to a suppression of the vortex core. One can expect that the effective anisotropy can be changed by using magnetic particles possessing their own intrinsic easy-axis anisotropy. For the core to emerge, the effective anisotropy should be reduced, which takes place for particles with the easy axis perpendicular to the array plane. For arrays of particles made of soft magnetic materials, such situation is realized in case of elongated particles oriented perpendicular to the array plane, see Fig. Such a geometry
To analyze this problem, we have employed two methods: numerical minimization of the energy using the standard Gauss-Seidel algorithm, as in [41] and Monte Carlo analysis using the simulated annealing technique. The energy minimization has been performed as follows: we start with \( \beta = 0 \), choose a simple in-plane vortex as an initial condition, and numerically minimize the energy then the value of \( \beta \) is increased step by step. This method is working pretty fast and gives a good description of the structure for continuous transitions, see below, while the Monte Carlo method is important for the analysis of points where the magnetic structure of the system is changing discontinuously, with a coexistence of (metastable) states close to the transition point.

Numerical calculations have been carried out for comparatively small clusters shaped in the form of a regular hexagonal fragment of the lattice consisting of 19, 37, 61, 91, and 127 nanoparticles. For all studied systems, we have found an in-plane vortex in the ground state at \( \beta = 0 \). The structure of the vortex changes considerably as \( \beta \) increases and passes through two critical values \( \beta_1 \) and \( \beta_2 \), see Fig. 2 and the detailed discussion below. Further, we have found a prominent transition at some value \( \beta = \beta_t > \beta_{1,2} \) from the vortex state to the state with a fragment of the antiferromagnetic structure, and close to \( \beta = \beta_t \) we have observed a noticeable region of coexistence of vortex and antiferromagnetic states, see Fig. 3. The behavior of the energy as a function of the anisotropy constant \( \beta \) near this transition is similar to that for a thermodynamic potential as a function of temperature near first-order phase transition. On the other hand, the dependence of the energy on \( \beta \) did not exhibit visible peculiarities at \( \beta = \beta_{1,2} \), where a change of the vortex structure has been detected.

To analyze the structure and symmetry of the vortex core, after completing the energy minimization for each value of \( \beta \), we have been calculating the value of the out-of-plane component \( M_z \) of the total magnetic moment, as well as the length of the planar component \( M_{pl} = \sqrt{M_x^2 + M_y^2} \). It turns out that just these parameters are most sensitive to the vortex structure and allow observing peculiarities of the vortex core behavior, see Fig. 4.

The behavior of the total magnetic moment of a particle array with a vortex is rather complicated. At small anisotropy, the picture remains the same as for isotropic particles and a vortex with purely planar distribution of magnetic moments is realized. In this case, accordingly, the total \( z \)-projection of the magnetic moment vanishes, but the planar component of the total magnetic moment \( M_{pl} \) is non-zero. With increasing \( \beta \), a nonzero value of \( M_z \) emerges at some critical anisotropy \( \beta = \beta_1 \). The fact that \( M_z \neq 0 \) means that an out-of-plane core appears. However, with the appearance of nonzero \( M_z \), the planar component of the total moment does not vanish immediately, i.e. within some finite interval \( \beta_1 < \beta < \beta_2 \) both in-plane and out-of-plane components of the moment are nonzero, see Fig. 4. The planar component van-
shades for $\beta > \beta_2$, whereupon the vortex state structure becomes more symmetric than that observed at $\beta < \beta_2$, see Fig. 2. Such a symmetric vortex structure is observed within a wide range of $\beta$, $\beta_2 < \beta < \beta_1$ and the magnetic moment $M_z$ changes considerably while $M_{pl}$ remains zero. With the further increase of the anisotropy, the vortex structure becomes an antiferromagnetic structure similar to that which is found for strong perpendicular anisotropy. The presence of boundaries leads to the emergence of three different domains of such structure, as dictated by the system symmetry.

Note that the behavior of $M_z$ and $M_{pl}$ is similar to that of order parameters near second-order phase transitions. This observation can be used to perform a symmetry analysis of the transitions between the different vortex states. It is important to obtain analytical results, due to the limited accuracy of numerical data, but also because the numerical analysis is hindered near transition points $\beta = \beta_{1,2}$ because of the “critical slowing down” of relaxation similar to that found near a second-order phase transition, which manifests itself in a substantial increase in the numerical calculation time. Therefore, we should study the possibilities of existence of such transitions in our system from the viewpoint of symmetry.

III. SYMMETRY ANALYSIS

To describe the complex character of changing the vortex core structure let us use symmetry arguments in line with the phase transition theory of Landau. For both observed critical values of anisotropy, the symmetry of state changes essentially. At $\beta \geq \beta_1$, when out-of-plane core emerges for the first time, the sign of $M_z$ can be arbitrary, i.e., there is a spontaneous breaking of $Z_2$ symmetry with respect to $M_z$ at $\beta = \beta_1$. In contrast to that, the symmetry of the planar distribution of magnetic moments does not change at this transition point: within the range $\beta_1 < \beta < \beta_2$ it remains the same as for $\beta < \beta_1$. At the other transition point $\beta = \beta_2$ the situation is different: the dependence of the out-of-plane component $M_z(\beta)$ does not have any visible peculiarities, while the planar component $M_{pl}$ vanishes at $\beta = \beta_2$ and remains zero for $\beta_2 \geq \beta < \beta_1$, i.e., up to the point of destruction of the vortex state at $\beta = \beta_1$, see the detailed graph in Fig. 4.

For the ground state in the interval $\beta_2 \leq \beta \leq \beta_1$, we observe a higher symmetry of the moment distribution than the vortex states with $M_{pl} \neq 0$ at $\beta < \beta_2$ (specifically, within the numerical accuracy of our simulations, we observe the $C_5$ symmetry; it would be worth finding out whether this symmetry is exact). Rather low symmetry of the vortex ground state at $\beta < \beta_2$ is caused by the presence of nonzero $M_{pl}$, which can be traced down to the presence of a non-zero planar component of the central magnetic moment $\bar{\mu}_0$. Obviously, the emergence of non-zero $M_z$ at $\beta > \beta_1$ is caused by $\bar{\mu}_0$ coming out of plane. Writing down $\bar{\mu}_0$ as $\bar{\mu}_0 = \mu_0 (\sin \theta_0 \bar{e}_z + \cos \theta_0 \bar{e}_p)$, where $\bar{e}_p$ lies in plane of the system, we obtain that the transition at $\beta_1$ is connected to the appearance of non-zero $\theta_0$, with $\theta_0 = 0$ at $\beta \leq \beta_1$ and $\theta_0 \neq 0$ at $\beta \geq \beta_1$. As we pointed out, the symmetry of the state with $M_z \neq 0$ is lower than for a planar vortex, therefore the value of $\theta_0$ serves as the order parameter for the transition at $\beta = \beta_1$. In this case, one can expect that at $\beta \geq \beta_1$ the behavior of the “order parameter” close to the transition is given by $\theta_0 \propto \sqrt{\beta - \beta_1}$ and is characterized by singular behavior, $d\theta_0/d\beta \rightarrow \infty$ at $\beta \rightarrow \beta_1 + 0$. On the other hand, the
hexagonal symmetry in the spin distribution may appear only when the central moment is directed strictly perpendicular to the system plane, i.e. at \( \theta_0 = \pi/2 \). If at \( \beta = \beta_2 \) the symmetry increases up to the hexagonal one, the quantity \( \theta_0 = \pi/2 - \theta_0 \) should serve as the order parameter for this transition. We arrive at the conclusion that the behavior of the out-of-plane component of the central spin \( \mu_0 \), i.e. the dependence \( \theta_0(\beta) \), dictates the change of symmetry of the vortex state. The information about the full \( \theta_0(\beta) \) dependence can be obtained only numerically, but the presence of square-root singularities at \( \beta \to \beta_1 + 0 \) and \( \beta \to \beta_2 - 0 \) is rather easily verified, see Fig. 6.

The detailed analysis of the \( \theta_0(\beta) \) dependence allows one to present a closed phenomenological expression for the “thermodynamic potential” \( \Phi \) that defines the behavior of \( \theta_0(\beta) \) in a wide range of \( \beta \). Indeed, in line with the Landau theory, this potential can be constructed in the form of the expansion in powers of the order parameters, which are \( \theta_0 \) at \( \beta \approx \beta_1 \) or \( \theta_0 = \pi/2 - \theta_0 \) at \( \beta \approx \beta_2 \). Equivalently, \( \sin \theta_0 \) and \( \cos \theta_0 \) can be used instead of angles \( \theta_0 \) and \( \vartheta_0 \). As odd degrees of \( \mu_{0z} = \sin \theta_0 \) are forbidden by the condition of the time reversal invariance, and the simplest form of this energy is the following: \( \Phi = A \sin^2 \theta_0 + B \sin^4 \theta_0 \). It is easy to see that, up to an inessential overall factor, the correct behavior is provided by the expression

\[
\Phi = \frac{1}{2} (\beta_1 - \beta) \sin^2 \theta_0 + \frac{1}{4} (\beta_2 - \beta_1) \sin^4 \theta_0 , \quad (2)
\]

which leads to the simple result:

\[
\sin \theta_0 = \left( \frac{\beta - \beta_1}{\beta_2 - \beta_1} \right)^{1/2} , \quad \beta_1 \leq \beta \leq \beta_2 , \quad (3)
\]

while \( \theta_0 = 0 \) at \( \beta < \beta_1 \), and \( \theta_0 = \pi/2 \) at \( \beta > \beta_2 \).

Such simple dependence describes the numerical data fairly well, see Fig. 6. Deviation from the simple law given by (3) can be accounted for by adding the term \( (\beta/6) \sin^6 \theta_0 \) to the expansion (2). As seen from Fig. 6, it provides a perfect description of the numerical data at sufficiently small \( \beta \), typical values are \( \beta \leq 0.1 (\beta_2 - \beta_1) \).

The critical values of the anisotropy constant \( \beta_1 \) and \( \beta_2 \) grow with the increase of the cluster size \( N \), see Fig. 7, though for the studied values of \( N \) this dependence is rather slow. The numerical data for \( N \geq 37 \) can be well fitted by a logarithmic dependence of the form \( \beta_{1,2} = A_{1,2} + B_{1,2} \ln N \), where \( A_1 = 0.38397 \), \( B_1 = 0.08703 \); \( A_2 = 0.36236 \), \( B_2 = 0.10222 \).

The value of \( \theta_0 \) not only dictates the vortex core symmetry but it also quantitatively defines the important vortex characteristic, the total out-of-plane moment of the particle with the vortex. Singularities in the \( \theta_0 \) behavior at \( \beta = \beta_1 \) are reflected in the \( M_z(\beta) \) dependence, \( M_z \propto \sin \theta_0 \) near this point. It is worth noting that \( M_z \) plays a special role in the dynamic properties, namely, \( M_z \) serves as a proper collective variable describing the radial mode (with the azimuthal number \( m = 0 \)) of the magnetization oscillations in the particle with a vortex, i.e. the theory is in agreement with recent experiment. Therefore, the presence of singularities in \( M_z(\beta) \) should manifest itself in the behavior of an equivalent of this mode for the considered system.

In addition, the presence or absence of the vortex core is also important for the properties of azimuthal modes with \( m = \pm 1 \). For a purely planar vortex, the modes
with \( m = \pm 1 \) form degenerate doublets, while the emergence of the core leads to splitting of these doublets. Thus, one can expect a crucial impact of the vortex structure modification on the properties of eigenmodes of the vortex-state particle, although a detailed discussion of the dynamical properties of the particle with the vortex is beyond the scope of this work.

### IV. SUMMARY AND DISCUSSION

To conclude, we have shown that high-symmetry hexagonal fragments of a 2D closely-packed triangular lattice of magnetic particles contain a vortex in the ground state, even for a small fragment size. The vortex structure is very sensitive to the intrinsic anisotropy \( \beta \) of the particle. At small anisotropy, there is a purely planar vortex. With the increase of \( \beta \), the symmetry of the vortex ground state lowers initially at some critical value \( \beta = \beta_1 \), and then increases to a high sixfold axial symmetry above another critical value \( \beta = \beta_2 > \beta_1 \). It is worth to note that those two transformations bear a similarity to second-order phase transitions. Both transitions take place at sufficiently weak anisotropy, the dimensionless parameters \( \beta_{1,2} \) do not exceed one. This value is essentially smaller than the easy-plane anisotropy of a planar array induced by the demagnetization field with the characteristic value \( \beta_{\text{array}} \sim 10 \), see Ref. 36. Actually, this anisotropy is smaller than it is necessary to create the perpendicular magnetization of a cylindrical magnetic dot.

An important challenge in the physics of magnetic vortices is to find ultra-small (smaller than 100 nm) systems with vortices in the ground state, this problem is of great interest for both fundamental physics and applications. In addition to lithographic magnetic materials, where the particle size is of the order of tens of nanometers, the proposed theory is applicable to other 2D systems with anisotropic particles having magnetic or electrical dipole moment. One could expect that if an array can be composed from small enough particles, having finite magnetic or electric dipole moment, the vortex state will be present for arrays 10-20 times larger than the particle size. Such systems can be realized for composite magnetic materials, for example, for granular magnets with the content of the magnetic component less than the percolation threshold, where the exchange interaction between nanometer-sized grains is anomalously small. Another example is the inhomogeneous state arising in the vicinity of the metal–insulator transition in doped manganites, which involves small particles of the ferromagnetic (metallic) phase distributed over a nonmagnetic host; their physical properties are determined to a large extent by the dipolar interactions between these particles. The experimental implementation of the artificial crystals, in which particles with magnetic moments of the order of \( 10^3 \) Bohr magnetons form an ordered lattices, has been reported recently. As one more example, it is instructive to mention a new class of materials, namely, molecular crystals formed by high-spin molecules. The total magnetic moment of such a molecule can be as high as dozens of Bohr magnetons, but the exchange interaction between magnetic moments of different molecules is almost negligible. Note also so-called dense phases formed by nanometer-sized magnetic particles moving freely in a liquid (that is the standard situation for a ferrofluids). For all these systems with a particle size of the order of nanometers the vortices described here can be present for objects as small as dozen of nanometers; those are, to the best of our knowledge, the smallest vortex-bearing systems discussed in the literature.

It is worth noting that the presence of a vortex ground state for such small systems and the transitions with the vortex core reconstruction is a consequence of the high (hexagonal) symmetry of the array. For square or rectangular arrays the vortex state appears for large enough arrays only. As we found, for an array shaped as a regular triangle, the vortex state could be present for small arrays, but with the increase of the anisotropy the vortex remain coreless all the way till the transition to antiferromagnetic state. The two-dimensional nature of an array is also quite important. Thus, two-dimensional closely-packed arrays of magnetic particles represent vortex-bearing systems with potentially small sizes and offer a unique possibility for manipulating the symmetry and structure of the vortex core.

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