Vortex polarity in 2-D magnetic dots by Langevin dynamics simulations

Ph. Depondt\textsuperscript{a,}\textsuperscript{*}, J.-C.S. Lévy\textsuperscript{b}, F.G. Mertens\textsuperscript{c}

\textsuperscript{a} Institut des NanoSciences de Paris, Université Pierre et Marie Curie, UMR 7588 CNRS, 75252 Paris Cedex 05, France
\textsuperscript{b} Matériaux et Phénomènes Quantiques, Université Denis Diderot, UMR 7162 CNRS, 75013 Paris, France
\textsuperscript{c} Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

\textsuperscript{*} Corresponding author.
E-mail addresses: depondt@insp.jussieu.fr (Ph. Depondt), jean-claude.levy@univ-paris-diderot.fr (J.-C.S. Lévy), franz.mertens@uni-bayreuth.de (F.G. Mertens).

1. Introduction and model

Vortices and other topological defects have been suggested by theory [1], Monte Carlo [2–5] simulations, micromagnetic simulations [6] and also experimentally observed in magnetic two-dimensional dots [7–9]. Analytical work based on Taylor expansions [10] again shows that dipolar interactions generate magnetic topological defects. The issue of data storage is clearly essential in such interest and, specifically, the polarity of vortices i.e. the out-of-plane spin component associated with a vortex (e.g. [11]) can be manipulated. This, however, assumes the presence of such polarity.

We present Langevin spin dynamics simulations [12] with dipolar interaction competing with nearest neighbour exchange which enable to study both spin structures, and, when present, vortex polarity, for various dipolar strengths and several dot sizes.

We solve the usual Landau–Lifshitz spin-dynamics equation:

\[
\dot{\mathbf{s}}_\ell = -\mathbf{s}_\ell \times \mathbf{H}_\ell - \mathbf{H}_{\text{dd}}(\ell) + \mathbf{H}_{\text{dt}}(\ell),
\]

where \(\mathbf{s}_\ell\) is the vector associated with spin \(\ell\) and \(\mathbf{H}_\ell\) the local field which is caused by all the other spins. The local field is the sum of two terms, where the first is a nearest-neighbour Heisenberg or exchange interaction, the second the dipole–dipole interaction; thus:

\[
\mathbf{H}_{\text{dt}}(\ell) = J \sum_{(\text{neighbour } \ell')} \mathbf{s}_{\ell'}
\]

\[
\mathbf{H}_{\text{dd}}(\ell) = d \sum_{(\ell' \neq \ell)} \frac{3 \mathbf{s}_{\ell'} \cdot \mathbf{r}_{\ell\ell'} (\mathbf{r}_{\ell\ell'} - \mathbf{s}_{\ell'})}{|\mathbf{r}_{\ell\ell'}|^3}
\]

\(J\) being, in this case, the identity matrix for the isotropic Heisenberg model. The strength of the dipole–dipole interaction is \(d\) and \(\mathbf{r}_{\ell\ell'}\) is the vector connecting spins \(\ell\) and \(\ell'\).

The simulated samples are square monolayers of identical spins on a rigid square lattice, (32 × 32), (64 × 64) or (128 × 128), in the \(xOy\) plane. The spins are free to rotate with \(|\mathbf{s}_\ell(t)| = 1\), \forall \ell, \forall t. The integration procedure is the same as in Ref. [12]: for every timestep, each spin explicitly precesses around the local field via a rotation matrix which conserves \(|\mathbf{s}_\ell(t)|\), and a Langevin dynamics allows to introduce temperature. The dipole–dipole interaction is dealt with using the convolution theorem and Fast Fourier Transforms: this introduces no additional approximation through zero-padding and the discrete character of the sample (see [12] and references therein).

These methods were checked in [12] for a X-Y Heisenberg model \((J_x = J_y = J_z = 1)\) without dipolar interaction \((d = 0)\) and with \(d = 0.2\) with varying temperatures: a variety of in-plane structures with or without vortices and vortex–antivortex pairs were observed, along with the associated dynamics.

We deal here with the isotropic Heisenberg model \((J_x = J_y = J_z = 1)\), low temperature \(T = 0.001\) in reduced units (in these units, the Kosterlitz–Thouless transition for the X-Y Heisenberg model \([13,14]\) takes place for \(T \simeq 0.7\), and varying dipole–dipole interactions \([6]\) and also experimentally observed in magnetic two-dimensional dots \([7–9]\). Analytical work based on Taylor expansions \([10]\) again shows that dipolar interactions generate magnetic topological defects. The issue of data storage is clearly essential in such interest and, specifically, the polarity of vortices i.e. the out-of-plane spin component associated with a vortex (e.g. [11]) can be manipulated. This, however, assumes the presence of such polarity.

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therefore decreases as actions lead to anisotropy: the overall out-of-plane contribution in\[10\], using a Taylor series expansion, that dipole–dipole inter-

motions can occur even at very low temperatures. It was shown

2. Instantaneous configurations

2.1. Instantaneous configurations

Typical configurations are shown on Figs. 1 and 2 for (128 ×

Fig. 1. Instantaneous 128 × 128 configurations, d = 0.006, 0.01, 0.02, and 0.06, T =

magnetizing field. In-plane configurations define, at the edges a

strength: 0.001 ≤ d ≤ 0.9, a way to change the ratio d/J or ex-

change length \(\sqrt{J/d}\). The choice of a low but finite temperature is a

compromise: we want to limit thermal fluctuations so that sig-

nificant features are not blurred beyond detection, but on the other hand, we wish to let the system explore available phase space in

order to avoid getting trapped in some metastable state. These re-

quirements are far from trivial as will be seen in Section 2.

All simulations, unless otherwise specified, were done in the

following manner: an initial, highly disordered configuration was

chosen and a first relaxation run with strong damping was car-

ried out; a second relaxation run was then performed with small

(0.0005) damping and a final production run was done with the

same small damping.

2. Configurations

2.2. Are these ground states?

For large d (approx. for \(d ≥ 0.08\)) convergence is rapid and

no inconsistency was detected. However, the snapshot shown for

d = 0.06 (Fig. 1, bottom right), at least, is clearly not a ground

state: the vortex is not in the middle of the sample where symme-

try would require it to be. It is known\[15\] that a non-central vor-

tex migrates toward the center via a gyrotropic motion: for small

dipolar interaction, this motion is very slow, and, in this instance, not completed. Thus the question of whether our configurations

can be considered to represent ground states should be addressed:

several tests were therefore done with different initial conditions, namely (1) a uniform in which all spins are parallel

in-plane and (2) with a single central vortex. These configurations

were left to relax in the usual manner, in order to let, for instance,
an out-of-plane component emerge. Despite attempts with varying relaxation times and dampings, it turns out that in none of these simulations would the system spontaneously switch from one structure to another: the uniform samples all remained devoid of vortices after relaxation, while the single vortex samples all ended up as single vortex final states, even for small $32 \times 32$ samples. It can, of course, be argued that the durations accessible to our simulations are too short; however, the system energies can be monitored (after relaxation) in both situations, compared in order to decide which structure has lowest energy and declare it is likely to be the ground state. The result of this procedure is given on Table 1 where quantity $\delta$ is the difference between the energy of the central vortex state and the energy of the uniform state.

For $128 \times 128$ samples, the value of $d$ for which the most stable structure changes from uniform to single vortex is 0.032: this means that on Fig. 1, the snapshot for $d = 0.02$ does not show a ground state as the uniform configuration has lower energy, while for $d = 0.06$, the vortex will simply proceed slowly towards the center to a ground state. It should be noted that the energy differences between the two structures remain small although above thermal fluctuations at this temperature.

### 2.3. Vortex polarity

The out-of-plane vortex-core contributions thus appear in the intermediate $d$ range and were fitted when present (Fig. 3) with a Gaussian function: the height remains constant and slightly less than 1 for $d < 0.08$ while the width decreases roughly as $1/\sqrt{d}$, meaning that the integrated intensity of the out-of-plane vortex components decreases roughly as $1/d$.

### 2.4. The effect of size

No major difference between the three samples of different sizes is to be observed. However the appearance of a vortex for increasing $d$ occurs for smaller $d$ in the larger samples (I to II in Fig. 4): the critical size roughly varies as $d \sim N_0^2$ following the results of Table 1. The $d$-range for which several vortices are present in the sample with non-zero polarity is narrow (Figs. 1 and 2); for these sample sizes, data storage via multi-vortex polarity might turn out to be uneasy, larger samples would be necessary.

### 3. Analysis and conclusion

We thus summarize our results in the following way. The equilibrium configurations are, as usual, obtained through the competition between the exchange (or Heisenberg) field $H_{\text{He}}$ and the dipolar field $H_{\text{d}}$ in Eq. (1): the exchange field tends to have all spins parallel while the dipolar field favors loops which can only reside in-plane in a 2-D system. When there is no dipolar field, the exchange term of course wins: spins are all parallel, but in any direction (in-plane, out-of-plane, or whatever) in the isotropic case. When the dipolar field is strong enough to overcome exchange, we obtain in-plane vortices [16].

For very small values of $d$ ($d \approx 0.002$), the spins escape in the third dimension, nearly freely. When $d$ is increased, this escape is restricted to the vicinity of the vortex core and is more and more reduced. Indeed, the interesting case resides in the intermediate range when one or several vortices appear: whenever a vortex is present, the exchange part will tend to reduce the nearest neighbour spin–spin angles, so it makes the spins stick out-of-plane. This of course costs energy because we cannot have out-of-plane loops (in 2-D) to satisfy the dipolar term (this is why the dipolar term produces an effective anisotropy [17], as it will tend to pull all spins back in-plane). We can try roughly to evaluate the relevant quantities that monitor this competition in a single-vortex configuration.

The out-of-plane exchange field component will be, for a spin within the area with an out-of-plane component surrounding a vortex, the sum of the $z$-components of its four neighbour spins,

$$H_{\text{He},z} = J_z \sum_{\ell} s_{z,\ell}$$

Since nearest neighbours will have reasonably similar orientations, this is roughly proportional to $s_{z,\ell}$, its own out-of-plane component:

$$H_{\text{He},z} \approx J_z C_{\ell} s_{z,\ell}$$

where $C_{\ell}$ is a constant.

Now, the out-of-plane component of the dipolar field is not reduced to nearest neighbours, but is a sum of all the contributions of the spins surrounding a vortex, within the area where they have out-of-plane components:
Fig. 3. Results of fitting a Gaussian function to the out-of-plane contribution to magnetization at vortex cores for system sizes \((32 \times 32), (64 \times 64)\) and \((128 \times 128)\). Top: fit example for \(d = 0.08\) (red: \(s_z\), green: Gaussian); middle: height of the Gaussian; bottom: width of the Gaussian and function \(f(d) = ad^{-b}\). \(a = 0.29 \pm 0.03, b = 0.52 \pm 0.022\) (logarithmic scales). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this Letter.)
The out-of-plane component of vortices only occurs in an intermediate range of dipolar interactions. The lower boundary is given by the limit when vortices can appear: this limit decreases to smaller values of $d$ with the size of the simulated sample as the effects of dipolar interactions add up on the whole sample, while the exchange term is local. The upper boundary occurs when the dipole–dipole interaction is locally strong enough to force spins in-plane: this limit does not appear to depend on size, as it is local. The $d$-range of co-existence of out-of-plane polarity and a multivortex configuration seems to be rather narrow for the sample sizes studied here.

The issue of whether we are dealing here with ground states, as we should if we are claiming to provide a phase diagram, was addressed. Several symptoms are to be pointed out: firstly the configuration for $d = 0.06$ in Fig. 1 cannot be a ground state because of symmetry since the vortex is not central and, secondly, the energy (Table 1) shows little sensitivity to configuration changes. This infers that many “ground states” with the same energy, or almost the same energy, exist, as in spin glasses in which a large number of nearly degenerate states are separated by energy barriers. Such frustration is general in dipolar systems, even without random interactions, be it magnetic systems (e.g. [19]), or liquid crystals (e.g. [20]). This creates a technical problem as we can never be quite sure we are studying the ground state: the obvious compromise is to work at finite temperature in order to allow the system to explore, at least partially, the available phase space, but low enough to avoid too large fluctuations that would blur significant features. The relaxation procedure from a highly disordered initial state mentioned at the end of Section 1, is a form of annealing which also is classic in dealing with frustration, however it requires cautious handling.

References