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Numerical study of spirals in a two-dimensional XY model with in-plane magnetic field

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Abstract

The behaviour of topological defects of the spiral type is studied numerically within a two-dimensional XY model with an applied in-plane magnetic field. The energy dependence of the 'spiral–antispiral' pair on the field value and direction is investigated. It turns out to be linear when the field is directed along the pair axis and exhibits a combined linear–logarithmic behaviour for the perpendicular orientation.

The two-dimensional (2D) XY model is one of the most intensively studied in solid-state physics, mainly due to its wide use in low-dimensional magnetism and the Josephson effect theory [1, 2]. The model also has a specific interest because it allows us to study non-linear excitations such as Kosterlitz–Thouless vortices and an associated phase transition which occurs due to unbinding of the vortex–antivortex pairs. An inclusion of an in-plane magnetic field essentially changes the system behaviour and gives no topological transition. The 2D XY model with the in-plane field is widely used in superconductivity and magnetism [3] and leads to the well known sine–Gordon equation

$$\Delta\Phi = \sin p\Phi \tag{1}$$

where p is an integer, which has been a subject of intensive investigations by both analytical and numerical methods [4, 5]. Recently it has been shown that two-dimensional domain structures found in Monte Carlo simulations could be obtained from the multisoliton solution of the sine–Gordon equation [6]. The model resulting from this equation belongs to the class of scalar models with the real order parameter Φ. Most of the interest in a study of these models is the structures with non-trivial topological properties. In the two-dimensional case these reveal themselves through singular points in a solution. Existence of the singularities is associated with the appearance of topological defects in the medium.

The vortex-like singularities with $\Phi \sim k\tan^{-1}(y/x)$ have been treated in detail in numerous studies. The exact solutions with the $k = \pm 4$ have been obtained in [7–9]; later, a

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wider class of similar multi-vortex solutions was found by Hirota's method [10]. As a result of intensive investigations of equation (1) the solutions with another vorticity $k = \pm 1, \pm 2, \pm 3$ have been found [4, 11].

The situation with the nodal singularities having radially symmetric asymptotic $\Phi \sim \alpha \log(\sqrt{x^2 + y^2})$ is less clear. It has been shown that these solutions are closely related to the solution of the third type Painleve equation with the same logarithmic asymptotic [12, 13]. The detailed consideration of topological defects of this type can be found in [14, 15]. The interest in these solutions arises in the theory of Josephson junctions [16] and Heisenberg [17] and non-Abelian field models [18].

A numerical study of the changes made to the two-vortex solution in the presence of magnetic field has been carried out in the work [5], where they discussed the dependence of the shape and energy of the vortex–antivortex pair on pair separation distance and the applied field. Earlier the same problem was considered in [4]. The authors investigated vortex-like structures described by equation (1) where $p = 1, 2, 4$ corresponds to the preferred direction imposed by magnetic field and crystallographic magnetic anisotropy, respectively.

The purpose of this work is to study numerically features of the spiral-like pairs with a finite energy in the external in-plane magnetic field on the base of the numerical procedure developed in [5]. In particular, we focus on the pair energy dependence on the direction and the value of the in-plane magnetic field. We find the energy as a function of the half-separation between the defects and compare the results obtained with the vortex-like singular magnetization distributions found in [4].

The model Hamiltonian is

$$H = -J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j) - h \sum_i \cos \phi_i \tag{2}$$

where $\phi_i \in [0, 2\pi]$ is the spin $\vec{S}$ polar angle at the ith site. The summation $\langle i, j \rangle$ goes over the nearest neighbours. J is the ferromagnetic coupling integral and h is the in-plane magnetic field parallel to the Ox axis. In the continuum limit, the static in-plane solutions are those provided by the two-dimensional sine–Gordon equation

$$\Delta\Phi = b \sin \Phi, \tag{3}$$

where $b = h/JS$. An exact vortex solution centred at (x_0, y_0) has been obtained by Hudak

$$\Phi = \pm 4 \tan^{-1} \left[\frac{\sinh \alpha (x - x_0)}{\sinh \alpha (y - y_0)} \right] \tag{4}$$

for the vorticity ± 4, where $\alpha = \sqrt{h/2J}$. The previous numerical study of the sine–Gordon equation used the following substitution [4]:

$$\Phi(r, \phi) = \Phi_0(\phi) + v(r, \phi), \tag{5}$$

where Φ_0 obeys the equation $\Delta\Phi_0 = 0$ and (r, ϕ) are the polar coordinates. This separation has been interpreted as a superposition of the vortex solution $\Phi_0 = q \tan^{-1}(y/x) = q\phi$ with the integral topological charge q and an addition v with a radial dependence obtained by a numerical method.

However, for the numerical study it is convenient to use the general form of the solution of the 2D Laplace equation:

$$\Phi_0(r, \phi) = q\phi + \alpha \log \frac{r}{R} \tag{6}$$

which describes spiral defects [4]. Here, q is an integer and α and R are the continuum parameters. The q value defines the degree of the spiral and α governs the spiral twist.

The case $\alpha = 0$ corresponds to the ordinary vortex solution. It is easy to obtain the energy of the isolated spiral which scales logarithmically with the size L of the system

$$E = 2\pi JS^2(q^2 + \alpha^2)\log L \tag{7}$$

assuming that L is measured in lattice units. The spiral defects have been observed distinctively in liquid crystals [19] and thin magnetic films [20].

Let us consider the spiral–antispiral pair solution

$$\Phi(x, y) = q\tan^{-1}\left(\frac{y - y_1}{x - x_1}\right) - q\tan^{-1}\left(\frac{y - y_2}{x - x_2}\right) + \alpha\log\frac{\sqrt{(y - y_1)^2 + (x - x_1)^2}}{\sqrt{(y - y_2)^2 + (x - x_2)^2}} \tag{8}$$

which is formed by a spiral (q, α) in (x_1, y_1) and anti-spiral $(-q, -\alpha)$ in (x_2, y_2) positions. These pairs act like a particles of an ideal gas. In full analogy with the case of a vortex–antivortex pair this formation has a finite energy

$$E = 2\pi JS^2(q^2 + \alpha^2)\log 2a, \tag{9}$$

where $a = \frac{1}{2}\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$ is the half-separation between the spiral centres. The size of the pair is an internal degree of freedom since the energy of the pair depends on the distance between the defects.

For the non-zero in-plane field expression (8) does not correspond to the exact solution of the sine–Gordon problem. However, in this case one can exploit the main idea used in [5]: we suppose that, in a case of small fields, the spiral–antispiral solution (8) is still meaningful and the effect of the field is in its deformation. This assumption allows us to write the solution of equation (3) in the same manner as in equation (5)

$$\Phi(x, y) = \Phi_0(x, y) + \xi(x, y), \tag{10}$$

where $\Phi_0(x, y)$ is the unmodified spiral–antispiral solution (8) and the addition $\xi(x, y)$ describes the deformation. Below we will show that this approach allows us to get structures which are similar to the vortex-like static solutions found by Borisov *et al* [4], in particular, the 2π domain wall of a finite length. The ansatz (10) has an essential advantage: one can study the dependence of the shape and energy of the spiral–antispiral pair on the angle between the axis of the pair and the applied field just by changing the position of the singularities (x_1, y_1), (x_2, y_2) in equation (8). Finally, we would like to note the different numerical realization in comparison with the previous consideration. Ansatz (10) allows us to use the simple iterative non-linear Gauss–Seidel scheme, whereas the non-linear addition v has been found in [4] by using the relaxation method reducing a solution to the Cauchy problem

$$-\frac{\partial v}{\partial t} + \Delta v = \sin\Phi_0(\phi) + v \tag{11}$$

with the starting value $v(t = 0) = 0$. Then, the stationary solution $v(x, y)$ is one that corresponds to $v(x, y, t \to \infty)$.

By using equations (10) and (3) one can easily obtain the equation for $\xi(x, y)$

$$\Delta\xi = b\sin(\Phi_0 + \xi). \tag{12}$$

As mentioned before, the solution of this equation may be found numerically using the non-linear Gauss–Seidel method. First, one should rewrite (12) in the finite-difference form

$$\xi_{i+1,j} + \xi_{i-1,j} + \xi_{i,j+1} + \xi_{i,j-1} - 4\xi_{i,j} - b\sin(\Phi_0(x_i, y_j) + \xi_{i,j}) = 0, \tag{13}$$

where x_i, y_j are discrete coordinates. It is convenient to enumerate $\xi_{i,j}$ in some way. After this, the loop should be made through all $\xi_{i,j}$ and they should be replaced with newly calculated values $\xi_{i,j}^{\mathrm{new}}$ as soon as $\xi_{i,j}^{\mathrm{new}}$ become available. The exact form of the Gauss–Seidel method depends on the chosen ordering. It is usually best to use the 'red–black ordering' making one

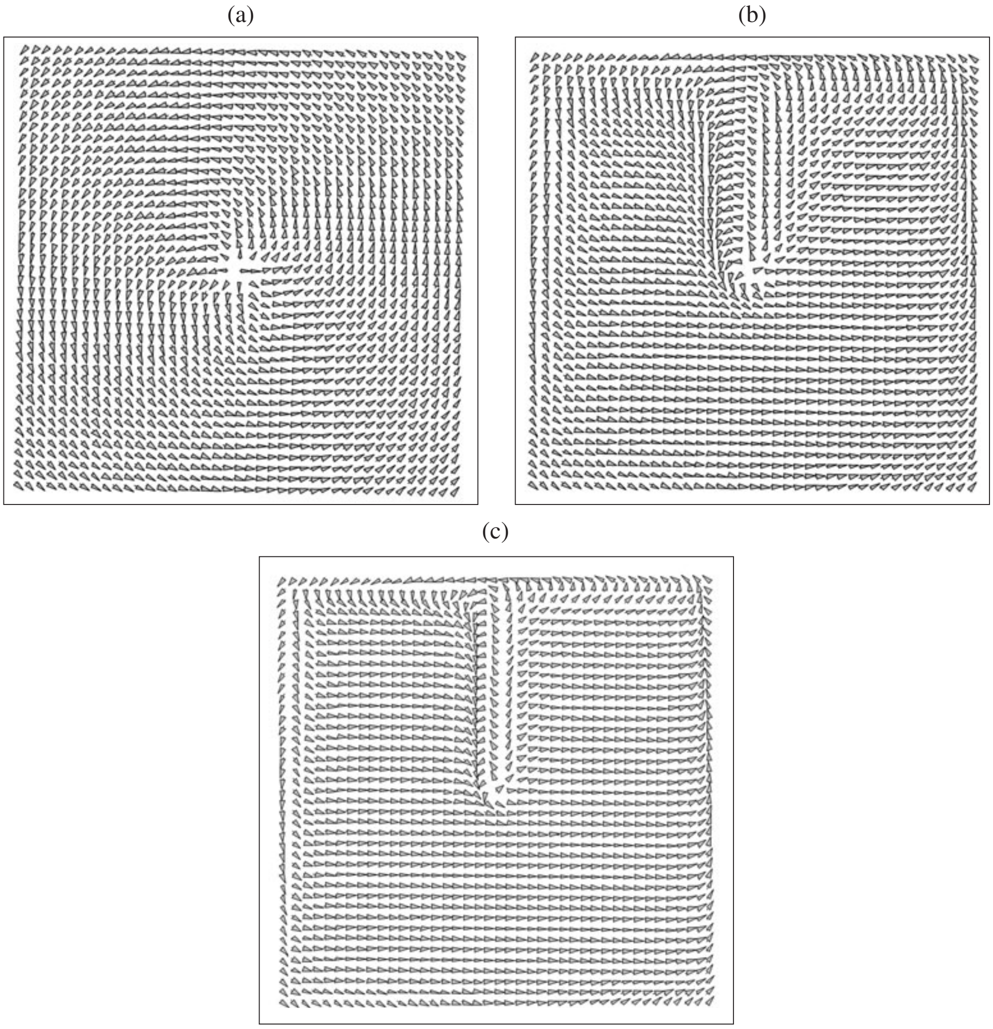

Figure 1. The single spiral $q = 1$, $\alpha = 1/2$ without the field (a) and with the in-plane magnetic field $b = 0.1$ (b), $b = 0.5$ (c).

pass to update points with even indices and another pass for odd ones. In this case $\xi_{i,j}^{\mathrm{new}}$ is defined by

$$\xi_{i,j}^{\mathrm{new}} = \xi_{i,j} - \frac{L(\xi_{i,j})}{\partial L(\xi_{i,j})/\partial \xi_{i,j}}, \tag{14}$$

where L is the non-linear differential operator $Lu = \Delta u - b\sin(\Phi_0 + u)$. By using equation (13) one can rewrite equation (14) as

$$\xi_{i,j}^{\mathrm{new}} = \xi_{i,j} + \frac{L(\xi_{i,j})}{4 + b\cos(\Phi_0(x_i, y_j) + \xi_{i,j})}. \tag{15}$$

This rule should be used iteratively until convergence is achieved. It should be noted that no linearization of the initial problem was used.

We implement this method to solve equation (12) numerically on the square lattice of radius $R = 200$ with the imposed fixed boundary conditions $\xi(x, y) = 0$. The half-separation

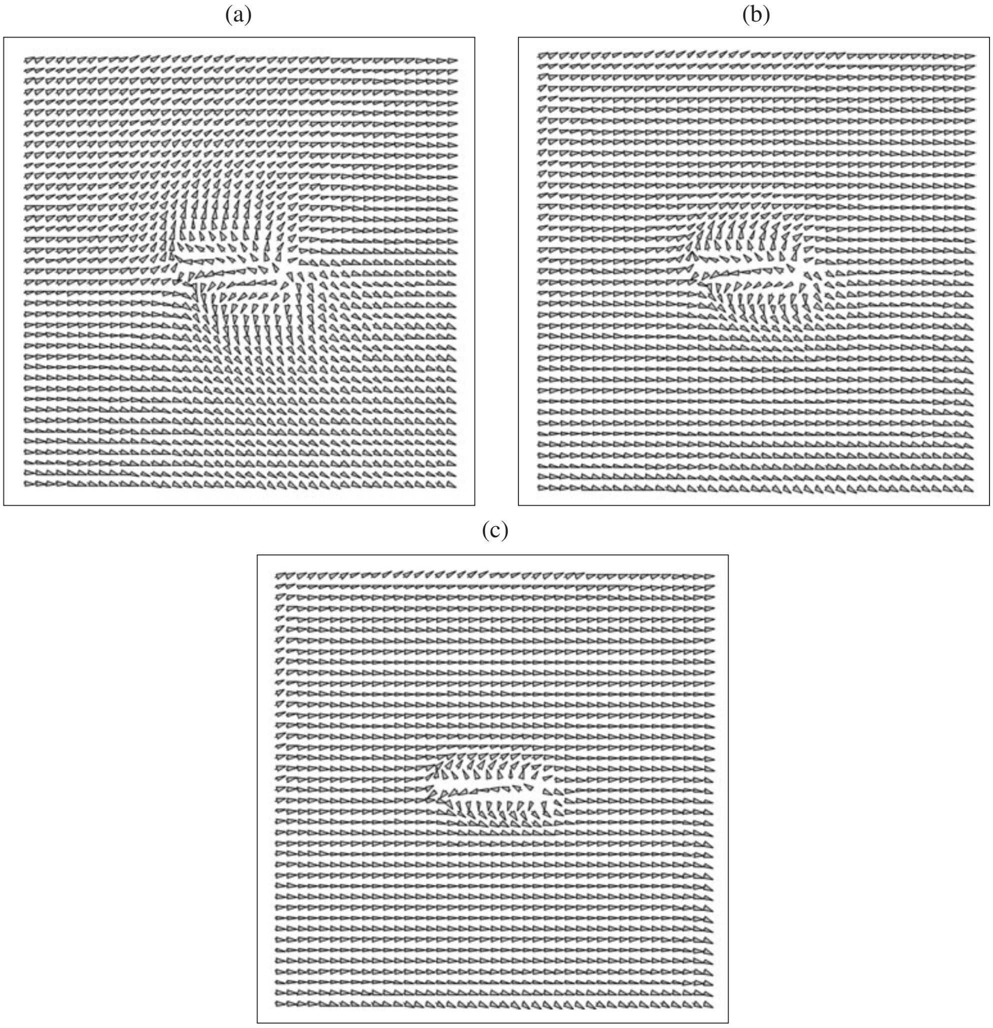

Figure 2. The spiral–antispiral pair $a = 5, q = 1, \alpha = 1/2$ in the longitudinal in-plane magnetic field $b = 0.01$ (a), $b = 0.10$ (b) and $b = 0.50$ (c).

a ranges from 5 up to 30 lattice units and the in-plane field b varies from 0.01 to 0.50 both for longitudinal, i.e. parallel to the axis of the pair, and transversal orientations. The spin configurations we obtained are presented in figures 1–3.

We estimate the energy of the pair in the external in-plane field which is given by the expression

$$E/JS^2 = 2\pi(q^2 + \alpha^2)\log 2a + \int \mathrm{d}x\,\mathrm{d}y\,[b(1 - \cos\Phi_0) + \nabla\Phi_0\nabla\xi + b\cos\Phi_0(1 - \cos\xi) + (\nabla\xi)^2 + b\sin\Phi_0\sin\xi], \tag{16}$$

where all field effects are included in the integral term. The total spiral–antispiral energy versus the half-separation a for the different field b values is shown in figure 4. The dependence turns out to be linear when the external magnetic field is parallel to the axis of the pair and non-linear

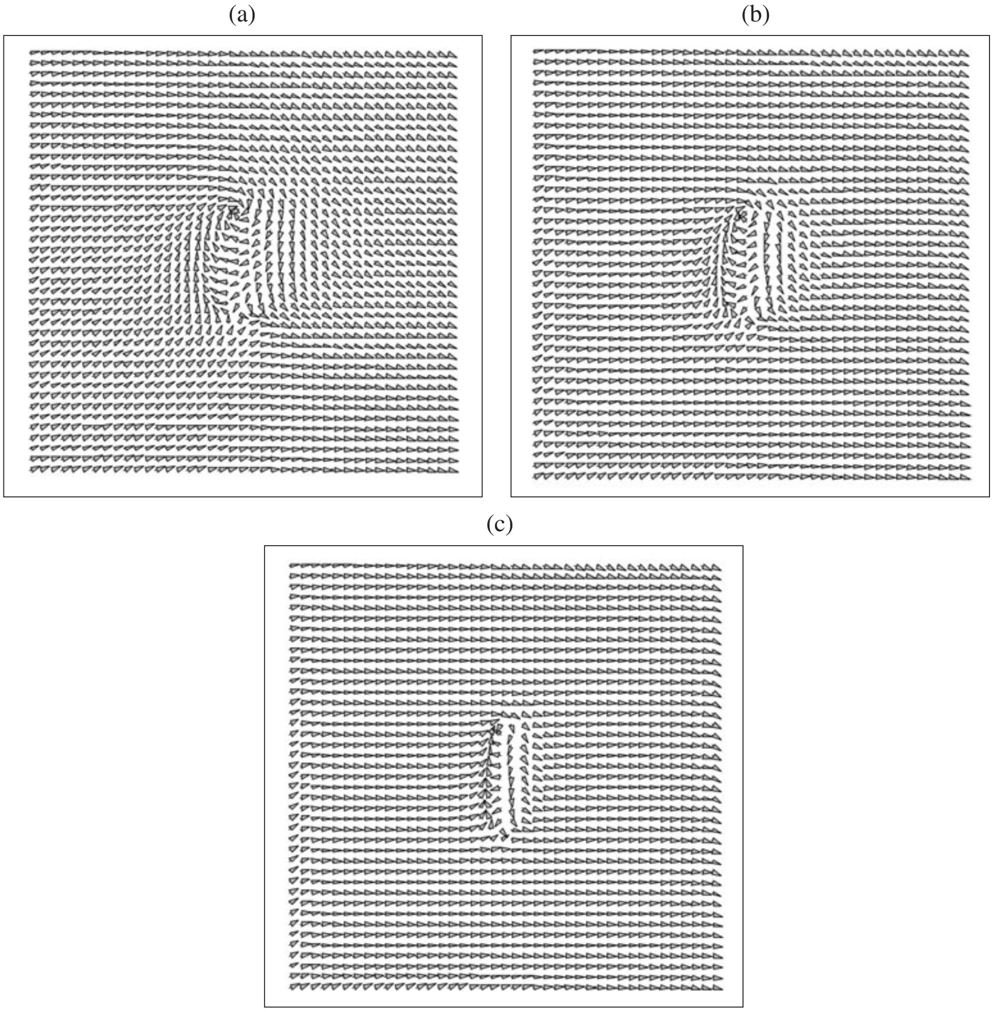

Figure 3. The spiral–antispiral pair $a = 5, q = 1, \alpha = 1/2$ in the transversal in-plane magnetic field $b = 0.01$ (a), $b = 0.10$ (b) and $b = 0.50$ (c).

when b is directed perpendicularly to it. The latter case is well fitted to the expression

$$E(a) = c_1 + c_2 \log(2a) + c_3 a \tag{17}$$

where c_1, c_2 and c_3 depend on the field value b. As can be seen from figure 4(b), the dependence is logarithmic when a is sufficiently small and becomes linear for large a.

The evolution of the single spiral in the external magnetic fields is shown in figure 1. The case in figure 1(a) corresponds to the pure spiral arrangement with no deformation caused by the field. The inclusion of the in-plane field results in the appearance of a single domain wall (figures 1(b), (c)). This effect has been observed in the previous numerical simulations [4]. The width of such a wall decreases with the field growth as long as the larger number of spins arranges along the field. As expected, an inclusion of the field does not change topological properties of this spin configuration. As can be seen from figures 1(b) and (c), the spin order parameter makes the full 2π rotation by passing along the boundary.

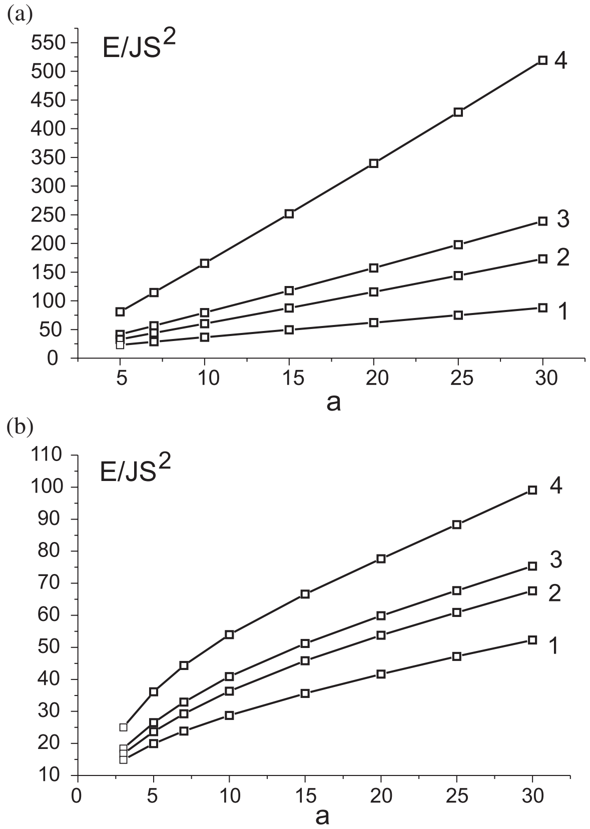

Figure 4. The total energy of the spiral–antispiral pair versus half-separation a for the longitudinal (a) and perpendicular (b) in-plane field $b = 0.01$ (1), $b = 0.05$ (2), $b = 0.10$ (3) and $b = 0.50$ (4).

The behaviour of the spiral–antispiral pair in the magnetic field directed along the pair axis (figure 2) is a full counterpart of the 'vortex–antivortex' case [5]. The main effect of the applied field is in the formation of the 2π domain wall of finite length. The growth of the field value results in the decrease of the wall width. A twist of the spiral spin arrangement keeps a linear dependence of the pair energy on the half-separation a, just giving some increase of the energy value (figure 4(a)).

The results for the fields directed perpendicularly to the pair axis are shown in figure 3. One can observe the formation of the 2π domain wall in the same range of the applied fields. However, smaller field values are required to reach a narrow domain wall (figure 4(b)).

The difference between the energy dependences in these two cases can be explained by the following arguments. In the first case the spins in the domain wall 'core' are initially directed antiparallel to the field, which forces them to rotate by π. In the last case the initial angle between the field and the domain wall is just $\pi/2$, thus, the inner spins must be rotated by an angle half the size.

In conclusion, the numerical analysis presented shows that there is no principal difference between the behaviour of the spiral–antispiral pair and the vortex–antivortex pair. As expected, the pair axis orientation with respect to the in-plane magnetic field is an essential factor for the energy value and its dependence on the pair size.

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References

[1] Pokrovskii V L and Uimin G V 1974 *JETP* **38** 847
[2] Minnhagen P 1987 *Rev. Mod. Phys.* **59** 1001
[3] Glazman L I and Koshelev A E 1990 *Zh. Eksp. Teor. Fiz.* **97** 1371
[4] Borisov A B, Tankeev A P and Shagalov A G 1989 *Fiz. Tverd. Tela (Leningrad)* **31** 141
[5] Gouvea M E, Wysin G M and Pires A S T 1997 *Phys. Rev.* B **55** 14144
[6] Cluri S T and Ryzhkov V N 1997 *Phys. Rev. Lett.* **78** 2224
[7] Khodenkov H E 1981 *Phys. Status Solidi* a **63** 461
[8] Hudak O 1982 *Phys. Lett.* A **89** 245
[9] Takeno S 1982 *Prog. Theor. Phys.* **68** 992
[10] Borisov A B 1990 *Phys. Lett.* A **143** 52
[11] Borisov A B, Tankeev A P, Shagalov A G and Bezmaternih G V 1985 *Phys. Lett.* A **111** 15
[12] Novockshonov V Yu 1985 *Dokl. Akad. Nauk USSR* **85** 1161
Its A R and Novokshenov V Yu 1986 *The Isomodromic Deformation Method in the Theory of Painleve Equation* (*Springer Lecture Notes in Mathematics* vol 1191) (Berlin: Springer)
[13] Novockshonov V Yu and Shagalov A G 1997 *Physica* D **106** 81
[14] Borisov A B, Ionov S N and Shagalov A G 1990 *Nonlinear World* ed V G Bar'yachtar *et al* (Singapore: World Scientific) p 65
[15] Shagalov A G 1992 *Phys. Lett.* A **165** 412
[16] Vabishev P N, Vasenko S A, Likharev K K and Semenov V K 1984 *Zh. Eksp. Teor. Fiz.* **86** 1132
[17] Bostrem I G and Ovchinnikov A S 2002 *JETP Lett.* **76** 716
[18] Patrascioiu A and Seiler E 1995 *Phys. Rev. Lett.* **74** 1920
[19] Pang J, Muzny C D and Clark N A 1992 *Phys. Rev. Lett.* **69** 2783
[20] Kandaurova G S 2002 *Phys.—Usp.* **45** 1051