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

M. E. Gouvêa, G. M. Wysin,* and A. S. T. Pires
Departamento de Física, ICEx, Universidade Federal de Minas Gerais, Belo Horizonte, CEP 30161, MG, Brazil
(Received 2 December 1996)

Many physical systems of interest can be mapped into the planar rotator and *XY* magnetic models with a magnetic field applied within the easy plane. In this work we study how the shape and energy of a vortex-antivortex pair depends on the applied field and on the pair separation. Our results show a new feature: the energy related to the vortex-antivortex pair has a coefficient which depends strongly on the applied field. For large separation of the pair, the energy increases roughly with the square root of the field and linearly with the pair separation. [S0163-1829(97)03522-4]

The two-dimensional *XY* model has been the subject of very intense experimental and theoretical research in the last two decades.[1] This model is known to support topological excitations and, although no long range order is established at any finite temperature, it shows a phase transition related to the unbinding of vortex-antivortex pairs. In particular, the *XY* model has been extensively used in the study of high temperature superconductors[2–5] since it is believed that the most important fluctuations in the order parameter describing the superconducting condensate are phase fluctuations.

When a magnetic field is applied along the easy plane the properties and behavior of the system change considerably: no phase transition is expected then. The field modifies the vortex-vortex interaction; instead of an interaction which grows logarithmically with distance, the vortex interaction becomes linear for large distances[2,5] due to the applied field. Although this system has been treated in several previous works,[6–9] a complete understanding of the *XY* model with an in-plane field ($2DXY+H$, from now on) is still missing and questions about how vortex pairs and domain walls contribute to the properties of the system have not yet been satisfactorily answered. Nevertheless, the investigation of the properties of the $2DXY+H$ model is very appealing not only for the model itself but also because this model is related to more realistic systems in which at least a small three dimensional interaction exists and may influence the overall behavior. It has been shown[8] that the anisotropic 3D*XY* model with *weak* coupling between the planes can be mapped into the $2DXY+H$ model with the in-plane field accounting for, in a mean field approach, the interplanar interaction.

Our aim in this work is to analyze the modifications due to the applied magnetic field on the vortex pair shape and energy. We start by writing the Hamiltonian for the 2D*XY* model with in-plane magnetic field $h=g\mu_B H$ applied along the x-axis and easy-plane anisotropy parameter $\delta>0$:

$$H=-\frac{J}{2}\sum_{m,n}\left[\mathbf{S}_{m,n}\cdot\mathbf{g}_{m,n}-\delta S^z_{m,n}g^z_{m,n}\right]-h\sum_{m,n}S^x_{m,n}, \quad (1)$$

where the sums are performed over all the (m,n) sites of a two-dimensional square lattice, J is the ferromagnetic exchange interaction, $g^\alpha_{m,n}$ corresponds to the sum over the four nearest neighbors of each spin.

Parametrizing the spin at site (m,n) in terms of spherical coordinates,

$$\mathbf{S}_{m,n}=S\{\cos\phi_{m,n}\cos\theta_{m,n};\sin\phi_{m,n}\cos\theta_{m,n};\sin\theta_{m,n}\}, \quad (2)$$

we obtain, in the continuum limit, equations of motion corresponding to the Hamiltonian (1):

$$-\dot{\theta}/JS=-\cos\theta\nabla^2\phi+2\sin\theta\nabla\theta\cdot\nabla\phi+b\sin\phi,$$

$$\cos\theta\,\dot{\phi}/JS=2\delta\sin 2\theta-\nabla^2\theta-\tfrac{1}{2}\sin 2\theta(\nabla\phi)^2+b\sin\theta\cos\phi. \quad (3)$$

Above we defined the reduced field $b=g\mu_B H/JS$.

When δ is greater than a critical value[10] (approximately 0.3 for the square lattice) the spins of the static vortex solutions are restricted to the *XY* plane, that is, $\theta=0$. In this case, or, for the planar (two-component spins) model, Eqs. (3) reduce to $\dot{\phi}=0$ and to the 2D sine-Gordon equation:

$$\nabla^2\phi=b\sin\phi. \quad (4)$$

The expression for the energy relative to the ground state becomes

$$E=JS^2\int d^2r\left\{\frac{1}{2}(\nabla\phi)^2+b(1-\cos\phi)\right\}. \quad (5)$$

For zero magnetic field, $b=0$, Eq. (4) leads to the well-known vortex pair solution given by

$$\Phi(x,y)=\tan^{-1}[2ay/(x^2+y^2-a^2)] \quad (6)$$

for a pair formed by a vortex at $(a,0)$ and an antivortex at $(-a,0)$, with separation $2a$. For $b\neq 0$, Eq. (6) does not correspond to an *exact* solution to the problem. However, we will consider here that, for small applied fields, the vortex-antivortex pair solution given by Eq. (6) is still meaningful in the sense that the effect of the field will be to *deform* it. In this reasoning, we will write the solution to Eq. (4) as being given by

$$\phi(x,y)=\Phi(x,y)+\xi(x,y), \quad (7)$$

where $\xi(x,y)$ describes the deformation due to the field. The function $\Phi(x,y)$ enforces the desired positions of the vortex and antivortex.

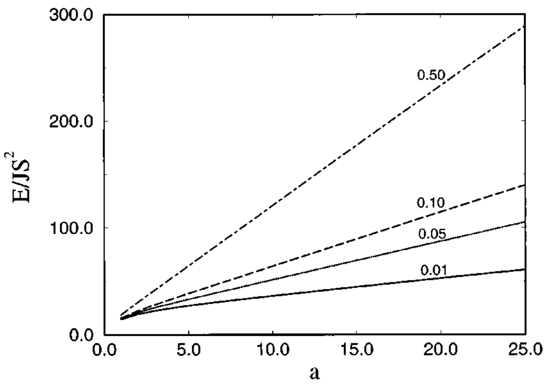

FIG. 1. Total vortex-antivortex pair energy [Eq. (9)] vs half-separation a, for the indicated applied field values b.

Inserting ansatz (7) into Eq. (4), we obtain a nonlinear Schrödinger-like equation for the deformation ξ:

$$\nabla^2\xi = b\sin(\Phi+\xi) = b\sin\Phi\cos\xi + b\cos\Phi\sin\xi. \tag{8}$$

In the linearized limit ($\xi \ll 1$), $b\cos\Phi$ is an effective potential term and $-b\sin\Phi$ is an effective driving field in Eq. (8), when viewed as a Schrödinger equation. For the energy, we have

$$E = E_0 + JS^2\int d^2r\left[\tfrac{1}{2}(\nabla\xi)^2 + \nabla\Phi\cdot\nabla\xi + b\sin\Phi\sin\xi + b\cos\Phi(1-\cos\xi)\right], \tag{9}$$

where

$$E_0 = JS^2\int d^2r\left\{\frac{1}{2}(\nabla\Phi)^2 + b(1-\cos\Phi)\right\}. \tag{10}$$

The term E_0 is due to the presence of a nondeformed vortex-antivortex pair in the field, and the remaining terms represent the energy associated with the field-induced deformation of the pair.

We solved Eq. (8) numerically for ξ with b ranging from 0.01 to 0.5 and $1.0 \leq a \leq 25.0$ by using an iterative nonlinear Gauss-Seidel method applied to a circular square lattice system of radius $R=200$. The idea is to rewrite the Laplacian term in Eq. (8) in its simplest finite difference form for the square lattice,

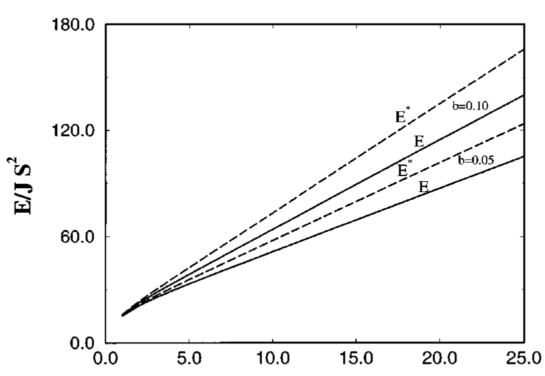

FIG. 2. Comparison of the full nonlinear (solid lines) and linearized (dashed lines) calculations of the vortex-antivortex pair total energy vs half-separation a, for indicated applied fields.

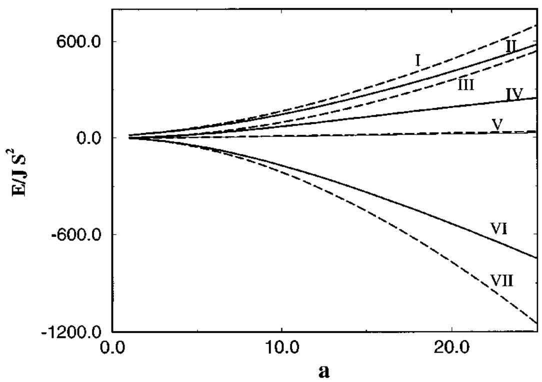

FIG. 3. Particular contributions to the vortex-antivortex pair energy vs half-separation a, for $b=0.05$. Solid lines refer to the full nonlinear calculation (this work), dashed lines are the linearized calculation as in Ref. 2. The various curves correspond to (I) E_0^*, (II) E_0, (III) $b\zeta^2/2$, (IV) $b\cos\Phi(1-\cos\xi)$, (V) $(\nabla\zeta)^2$ and $(\nabla\xi)^2$, (VI) $b\sin\Phi\sin\xi$, (VII) $b\Phi\zeta$.

$$\nabla^2\xi = -4\xi_{m,n} + \sum_{i=\pm1}\sum_{j=\pm1}\xi_{m+i,n+j} \tag{11}$$

and then "solve" Eq. (8) for the new value of $\xi_{n,m}$ at the next iteration:

$$\xi'_{m,n} = \frac{1}{4}\left[\sum_{i=\pm1}\sum_{j=\pm1}\xi_{m+i,n+j} - b\sin\Phi_{m,n}\cos\xi_{m,n} - b\cos\Phi_{m,n}\sin\xi_{m,n}\right]. \tag{12}$$

Iterating this procedure leads to a minimum energy state. We would like to stress that no linearization of the problem has been used, and a numerically exact solution of the original Hamiltonian (1) was obtained. A free boundary condition was applied by cutting off the system at a chosen radius ($R=200$), and then any sites on the boundary of the system have less than four nearest neighbors. For those boundary sites, the factor of $\frac{1}{4}$ in Eq. (12) is replaced by $1/z_{m,n}$, where $z_{m,n}$ is the number of neighbors of that site. Our results are shown in Figs. 1–5: we will discuss these results after describing, briefly, some previous results available in the literature.

A problem similar to this one was considered by Cataudella and Minnhagen[2] some years ago and, since then, their results — which are summarized below — have been used to account for the energy of a vortex pair in the presence of a field.[3,4] It is important to notice that, in fact, their work was directed to the *XY layered* superconductor model and not to the $2DXY+H$ model. However, for small interplanar coupling, the layered XY model can be represented by the $2DXY+H$ model. This fact has been stated very clearly by Ito[8] who used the following Hamiltonian to describe the XY-layered model:

$$\mathcal{H} = -\sum_i\sum_{m,n}\left[J\mathbf{S}_{m,n,i}\cdot\mathbf{g}_{m,n,i} + J'\mathbf{S}_{m,n,i}\cdot\mathbf{S}_{m,n,i+1}\right], \tag{13}$$

where the summation in i runs over the layers, J' is the interlayer coupling, and the spin $\mathbf{S}$ has only two components ($S^z=0$ or $\theta=0$). Obviously, the system described by Eq.

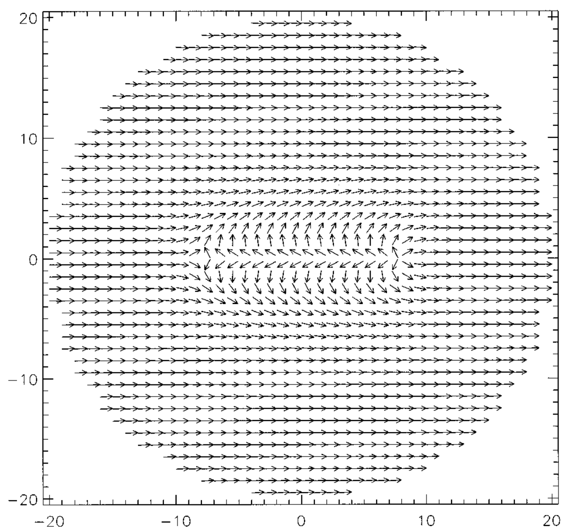

FIG. 4. The total spin field $\phi=\Phi+\xi$ for system radius $R=20$, half-separation $a=8$, field $b=0.25$.

(13) shows conventional long-range order, $\langle \mathbf{S}\rangle \neq 0$, and exhibits a second-order phase transition. Assuming $J' \ll J$, we can say that the system will have a *quasi*-two-dimensional behavior for $T \gg J'$ and, then, take account of the interlayer interaction by an effective field. This corresponds to rewriting Eq. (13) as

$$\overline{\mathcal{H}}=\sum_i \overline{H_i}, \quad \overline{H_i}=-\sum_{m,n}[J\mathbf{S}_{m,n,i}\cdot\mathbf{g}_{m,n,i}+2J'mS^x_{m,n,i}], \tag{14}$$

where $m=\langle \mathbf{S}\rangle$ is the magnetization. The Hamiltonian (14) is identical to our Hamiltonian (1) (for $S^z=0$) if we define the effective field as $h_{\mathrm{eff}}=2J'm$. The continuum version for Eq. (14) will be identical to Eq. (4). In the following, we will compare the equations and approximations done by Cataudella and Minnhagen[2] — keeping in mind that they were treating a layered model — to the equations we used and solved in this work.

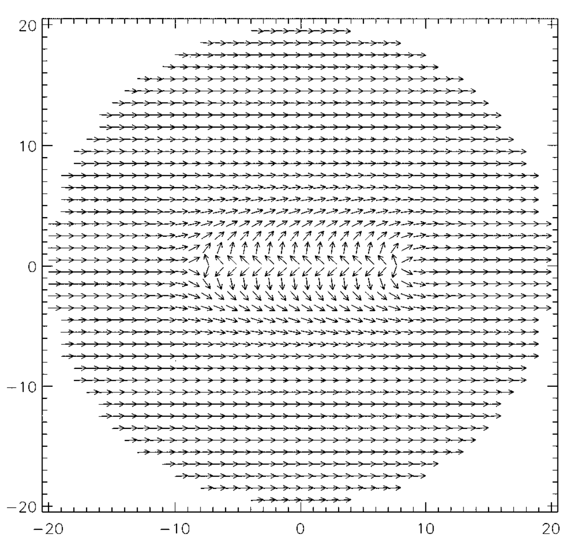

FIG. 5. The total spin field $\phi=\Phi+\zeta$, for radius $R=20$, $a=8$, $b=0.25$, from the linearized calculation.

As we said before, in layered superconductors, it is accepted that the important fluctuations are described by the fluctuations of the phase ϕ_i in the ith plane. The Hamiltonian used by Cataudella and Minnhagen to describe the layered superconductor is

$$H^*=\frac{1}{2}J\sum_i \int d^2r[(\nabla\phi_i)^2+b(\phi_i-\phi_{i+1})^2], \tag{15}$$

where b is the parameter controling the coupling between planes. Note clearly that the interplane interaction is taken as purely quadratic in the phase difference, in strong contrast to the more physical trigonometric form as seen in the $2\mathrm{D}XY+H$ model, Eq. (5). A quadratic coupling is reasonable for small interplane phase differences, however, we see below that relatively large phase differences between planes are possible. In the case of large phase differences, we would expect that a coupling term of the form $b[1-\cos(\phi_i-\phi_{i+1})]$ is necessary.[12]

In order to estimate the effect of adjacent planes on a vortex pair, Cataudella and Minnhagen looked for a minimum energy configuration for a pair on a particular plane i by solving the Euler equation with the constraint $\phi=\Phi_i+\zeta$ for that plane. This treatment corresponds to assuming that vortex pairs can be created in one layer independently of pairs in adjacent layers.[13,14] In the approach used in Ref. 2, Φ is the vortex pair expression (6) and ζ is the deformation (fluctuation) of that configuration — as is ξ in our ansatz (7). We use ζ here to distinguish this solution from the solution of the $2\mathrm{D}XY+H$ problem, Eq. (8). In order to simplify the calculation, those authors assumed that the phases in the planes adjacent to the one supporting the vortex pair are zero, that is, $\phi_{i+1}=\phi_{i-1}=0$. With these approximations, the equation to be solved for ζ is *linear* [in contrast to Eq. (8) for ξ]:

$$\nabla^2\zeta=b(\Phi+\zeta), \tag{16}$$

while the energy in terms of ζ becomes

$$E^*=\frac{1}{2}J\int d^2r[(\nabla\Phi)^2+b\Phi(\Phi+2\zeta)+2\nabla\Phi\cdot\nabla\zeta+(\nabla\zeta)^2+b\zeta^2]. \tag{17}$$

They solved Eq. (16) numerically for zero temperature, finding that the energy of a vortex-antivortex pair of size $2a$ can be parametrized as[2,5]

$$E^*(a)=\frac{1}{2}J\left[\pi^2+2\pi\ln\left(\frac{2a}{a_0}\right)+2\pi^2\sqrt{b}\left(\frac{2a}{a_0}-1\right)\right], \tag{18}$$

where the first term corresponds to the vortex pair creation energy, the second one gives the logarithmic dependence expected for a pair even in the absence of a field, and the term depending linearly on the pair size corresponds to the energy of a domain wall.[11] In this equation, a_0 is the diameter of the vortex core.

Comparing Eqs. (8) to Eq. (16) and Eq. (9) to Eq. (17) we conclude that our equations reduce to the ones obtained by Cataudella and Minnhagen if one considers both Φ and ξ to be small and expand the sine and cosine functions of them. However, it must be pointed out that this assumption is not obvious and that, at least in the region surrounding the vortex and antivortex centers, the Φ field, the ξ field, and their variations are not small.

In Fig. 1 we show the result we obtained for the total energy of the pair Eq. (9) for some values of the applied field, $b=0.01$, 0.05, 0.1, and 0.5, by solving Eq. (8). We also solved Eq. (16), which corresponds to the linearized version of Eq. (8), by using the linear version of the Gauss-Seidel iteration described in this paper, and evaluated the corresponding energy E^* of Eq. (17). Figure 2 shows the energies E [solid lines, from Eqs. (8) and (9)] and E^* [dashed lines, from Eqs. (16) and (17)] for $b=0.05, 0.10$. For small pair separation $(a<5)$, the agreement between the two results is surprisingly good, considering the approximations leading to Eqs. (16) and (17). For larger pair separations, we obtain $E^*>E$, as could be expected. In Fig. 3 we show the separate contributions due to each term of Eqs. (9) and (17). In both calculations, the $\nabla\xi\cdot\nabla\Phi$ or $\nabla\zeta\cdot\nabla\Phi$ contribution is negligible and is not shown. It is interesting to notice that the combinations of errors made in the various terms contributing to E^* nearly cancel, leaving a small net difference between E and E^*.

The total field $\phi=\Phi+\xi$ for $a=8$, $b=0.25$, calculated for a circular system with radius $R=20$, is shown in Fig. 4. It is seen that the field confines the vortex-antivortex pair to a small region of the system composed basically by a vortex and an antivortex — whose radii decrease with the field b — linked to each other by a kind of domain wall whose width also decreases with increasing b. For comparison, the total field $\phi=\Phi+\zeta$ from the linearized calculation with the same parameters is shown in Fig. 5. In the field far from the pair, it is difficult to distinguish any significant differences between the two results. The largest differences are seen along the line connecting the pair, where the spins tend to point more against the applied field in the full nonlinear calculation, compared to the linearized calculation. In this domain wall region, this results in a lower exchange energy density at the expense of a higher magnetic field energy density. In an intermediate region a few lattice constants above and below this domain wall, ξ (and also ζ, not shown here) can approach the value $\pi/2$, where the linearization approximation starts to fail. This occurs also for smaller b, although apparently a fortuitous cancellation of errors in the linearized calculation (see Fig. 3) results in a relatively small error in the total energy.

We fitted our results for the energy for $0.01\leqslant b\leqslant 0.5$ and $a_{\rm min}=1.0\leqslant a\leqslant a_{\rm max}=10.0$ to the following expression:

$$E=c_1+c_2\ln(2a)+c_3 a. \tag{19}$$

Notice that we chose $a_{\rm max}\leqslant 200$ in order to guarantee that our results would not be strongly influenced by the finite size of our lattice. This equation is formally equivalent to Eq. (18) because both assume that the energy must somehow depend logarithmically on the pair distance since the vortex and antivortex particles are kept there and depend linearly on the pair distance because, as can be seen in Fig. 4, the region connecting the vortex to the antivortex resembles a 2π domain wall of length $2a$ and width decreasing as b increases. According to Eq. (18), the c_2 coefficient in Eq. (19) should be a constant while $c_1=A-2J\pi^2\sqrt{b}$ $[A=J\pi^2+2\pi J\ln(2/a_0)]$ and $c_3=2J\pi^2\sqrt{b}/a_0$ should both vary with $\sqrt{b}$. We made a rough evaluation of the vortex core a_0 by fitting the vortex pair energy for $b=0$ to the expression $E_p=2\pi J\ln(2a/a_0)$ obtaining $a_0=0.20$ which agrees with previous estimates[10] for a_0. The fitting obtained for each of the coefficients c_1, c_2, and c_3 gave $c_1=15.5-10.1b^{0.36}$, $c_2=0.19-1.12\ln b$, and $c_3=-0.69+16.5b^{0.49}$. In fact, the term linear in a is the important one for large a and the dependence on $\sqrt{b}$ of its coefficient is the expected one for a 2π domain wall in a $2DXY+H$ system. We do not have any theoretical prediction to which we could compare the obtained dependence of c_2 with b. However, it seems reasonable that this coefficient decreases with increasing b because the effect of the field is to reduce the effective *area* affected by the pair.

The linear dependence of the energy on the distance a suggests that the pair may become unstable, and the domain wall connecting them may break and form new smaller pairs: a mechanism which resembles particle creation. This possibility will be investigated in a future work.

This work was supported by NSF/CNPq International Grant No. INT-9502781. G.M.W. also gratefully acknowledges the support of NSF Grant No. DMR-9412300 and a FAPEMIG Grant for Visiting Researchers. M.E.G. gratefully acknowledges the support of a FAPEMIG grant for computing equipment used in this calculation.

*Permanent address: Department of Physics, Kansas State University, Manhattan, KS 66506-2601 [electronic address: wysin@phys.ksu.edu].

[1] P. Minnhagen, Rev. Mod. Phys. **59**, 1001 (1987).
[2] V. Cataudella and P. Minnhagen, Physica C **166**, 442 (1990).
[3] H. Weber and H.J. Jensen, Phys. Rev. B **44**, 454 (1991).
[4] H.J. Jensen and H. Weber, Phys. Rev. B **45**, 10 468 (1992).
[5] P. Minnhagen and P. Olsson, Phys. Rev. B **44**, 4503 (1991).
[6] V.L. Pokrovskii and G.V. Uimin, Sov. Phys. JETP **38**, 847 (1974).
[7] V.L. Berezinskii and A.Ya. Blank, Sov. Phys. JETP **37**, 369 (1973).
[8] M. Ito, Prog. Theor. Phys. **66**, 1129 (1981).
[9] L.I. Glazmann and A.E. Koshelev, Zh. Eksp. Teor. Fiz. **97**, 1371 (1990) [Sov. Phys. JETP **70**, 774 (1990)].
[10] G.M. Wysin, Phys. Rev. B **49**, 8780 (1994).
[11] S. Tang and S. D. Mahanti, Phys. Rev. B **33**, 3419 (1986).
[12] One expects that the Hamiltonian interaction should be written in a fundamental way in terms of the local superconducting wave function, rather than the phases, which are derived from the wave function. A coupling of complex wave functions Ψ_i and Ψ_{i+1} with equal magnitudes $\sqrt{\rho}$ but different phases ϕ_i and ϕ_{i+1} in a quadratic form $|\Psi_i-\Psi_{i+1}|^2$ is exactly equal to $2\rho[1-\cos(\phi_i-\phi_{i+1})]$. The linearization of this result leads to the interplane interaction used in Eq. (15).
[13] S. Hikami and T. Tsuneto, Prog. Theor. Phys. **63**, 387 (1980).
[14] I. Nakayama and T. Tsuneto, Prog. Theor. Phys. **65**, 1246 (1981).