Instability of In-Plane Vortices in Two-Dimensional Easy-Plane Ferromagnets

G. M. Wysin
Department of Physics
Kansas State University
Manhattan, KS 66506-2601
(November 9, 1993)

An analysis of the core region of an in-plane vortex in the two-dimensional Heisenberg model with easy-plane anisotropy $\lambda = J_z/J_{xy}$ leads to a clear understanding of the instability towards transformation into an out-of-plane vortex as a function of anisotropy. The anisotropy parameter λ_c at which the in-plane vortex becomes unstable and develops into an out-of-plane vortex is determined with an accuracy comparable to computer simulations for square, hexagonal, and triangular lattices. For $\lambda < \lambda_c$, the in-plane vortex is stable but exhibits a normal mode whose frequency goes to zero as $\omega \propto (\lambda_c - \lambda)^{1/2}$ as λ approaches λ_c. For $\lambda > \lambda_c$, the static nonzero out-of-plane spin components grow as $(\lambda - \lambda_c)^{1/2}$. The lattice dependence of λ_c is determined strongly by the number of spins in the core plaquette, is fundamentally a discreteness effect, and cannot be obtained in a continuum theory.

PACS numbers 75.10.Hk, 75.40.Gb

I. Introduction: In-Plane Vortex Instability

The easy-plane anistropic Heisenberg ferromagnet on a two-dimensional lattice has been studied for many years, for its relation to the Kosterlitz-Thouless vortex unbinding transition[1]. More recently the model is still studied, especially for the dynamics of individual and pairs of vortices[2], and their contributions to dynamic correlation functions[3]. It has been known for some time that the classical model supports two distinct types of vortices, termed "in-plane" and "out-of-plane", depending on the absence or presence respectively of nonzero out-of-easy-plane spin components in the static vortex[4,5]. The interest here concerns the question of why are there two types of vortices possible, and what determines the stability of these excitations. Because the type of stable vortex is determined by the anisotropy strength[6,7], which may cover a wide range in available materials[8], this discussion is relevant for the interpretation of dynamic correlation measurements, such as neutron scattering experiments. Especially the vortex contributions to dynamic correlation functions for the out-of-plane spin components may be influenced by the type of vortices present in the system.

This discussion of instability also is analogous to the similar problem of normal modes and instabilities in solitons in one-dimensional magnets[9,10]. Instabilities of one-dimensional magnetic solitons have been found using continuum theory, for ferromagnets[9] and for antiferromagnets[10]. However, generally, solitons can be well-described by a continuum field, except perhaps for certain parameter ranges. This is not true for vortices on a lattice, in the sense that the region close to the vortex center cannot be described very well by a continuum field, for any parameter ranges. This is because the spins near the vortex "core" vary rapidly over small distances, which is represented by a singularity in a continuum theory. On the other hand, there is usually no such singularity at the center of a soliton. The calculations here will avoid the problem of how to deal with the singularity at the vortex core by treating the discrete degrees of freedom in the core region exactly on a lattice, without any continuum approximations.

Specifically in this paper we consider the following easy-plane Hamiltonian for classical spin variables $\vec{S}_{\mathbf{n}}$:

$$H = -J \sum (S_n^x S_m^x + S_n^y S_m^y + \lambda S_n^z S_m^z) \tag{1}$$

where $0 \leq \lambda < 1$ determines the degree of easy-plane anisotropy, and the spins $\vec{S}_{\mathbf{n}}$ are located on sites of a lattice in two dimensions, such as square, hexagonal or triangular. It will be convenient to describe each classical spin variable by an angle in the xy plane, ϕ, and the canonically conjugate out-of-easy-plane spin component, S^z. In Eq. (1) the coupling of x and y spin components will be refered to as "in-plane exchange," and the coupling of the z components as "out-of-plane exchange." The static vortices have an in-plane angle given by

$$\phi = q \tan^{-1}(y/x), \tag{2}$$

where q is an integer charge.

The two different vortex types correspond to two separate solutions of a nonlinear equation of motion for the out-of-plane component[7]. However, the stability of these solutions has only been determined via computer simulations by placing the solutions on a discrete lattice. It has been found that the in-plane vortex is numerically stable provided $\lambda < \lambda_c$, where λ_c is a critical anisotropy that depends on the lattice[6,7]. For the square lattice, $\lambda_c \approx 0.72$, similarly $\lambda_c \approx 0.86$ for the hexagonal lattice and $\lambda_c \approx 0.62$ for the triangular lattice. Conversely, when $\lambda > \lambda_c$, the in-plane vortex becomes unstable, and develops into an out-of-plane vortex, whereas the out-of-plane vortex becomes the only stable vortex solution. For a particular choice of easy-plane anisotropy parameter λ, only one type is found to be stable. The dependence of these critical values on the lattice was not understood.

There have been some attempts to describe the vortex stabilty and make a normal mode analysis in a continuum limit. For example, Costa et al.[11] considered a linear stability analysis of vortices in the XY model ($\lambda = 0$). This type of calculation determines the normal modes of the spin field about the static vortex structure, but in the process it must make certain assumptions about the structure of the vortex core. This is difficult because the vortex core is a singularity in a continuum limit. Usually this means that a short distance cutoff must be applied ad hoc to integrals over the spin field, but the cutoff radius itself is not well-known. In addition to this any inherent effects of the particular lattice must be lost in the continuum limit. For this magnetic vortex problem, and correspondingly for any other vortex problems on lattices, it is found that the vortex structure is strongly affected by the discreteness of the lattice, especially near the core. Since the vortex core is the region where the energy density of the vortex is highest, it is essential to take these discrete effects accurately into account. Any continuum limit will breakdown at small distance near the core, and be incapable of correctly describing these important discrete effects.

The philosophy of the present calculation is to try to take the core region of the vortex more precisely into account, at the expense of treating the far field only approximately. The deviations away from the static in-plane vortex will be assumed to be small so that linearization is possible, and included only for a finite set of spins near the core. We know from simulations that a vortex on a discrete lattice energetically prefers to be centered within a unit cell. This adds considerable symmetry to simplify the calculation. Also the deviations are assumed to depend only on the radial coordinate away from the vortex center.

In the first part of this paper, the static vortex structure is considered, by allowing perturbations away from the structure of the static in-plane vortex. The energy of a set of spins near the core is minimized, with a boundary condition that spins outside this core region are held in the easy plane, but the spins in the core region can tilt out-of-plane. The minimization directly leads to a critical value of anisotropy λ, below which the minimum energy configuration lies purely in the easy plane, and above which the minimum energy configuration has nonzero out-of-plane spin components. This behavior can be seen in different levels of approximation using different numbers of core spins that are allowed to move. Using a larger core region with more spins being allowed to move out of plane leads to successively lower estimates of λ_c, which converge to a limit. For two digit accuracy in λ, about 12 spins near the core are needed, regardless of whether the lattice is square, hexagonal or triangular.

In the second part of the paper, the dynamics of the instability of the in-plane vortex is considered, for $\lambda < \lambda_c$. Once again, a continuum theory is inadequate. On the other hand, a complete description of the spin wave normal modes about the static in-plane vortex structure on a lattice is intractable. However, A. Volkel[2,12] has made preliminary numerical studies on small lattices of the discrete normal modes on a square lattice. These suggest that as a function of increasing λ, there is one mode in particular whose frequency goes to zero at a specific value of λ, i.e., at the critical anisotropy or unstable point of the in-plane vortex[2]. This special instability mode is seen to have a circular symmetry around the vortex center (see below). Thus it makes sense to use this fact in a model of the spin motions near the vortex core.

A Lagrangian will be constructed for the core region under the assumption of a circularly symmetric normal mode, where the spin deviations depend only on the radial distance from the vortex center, which itself is held fixed in position. In this constrained Lagrangian the normal mode frequency is obtained as a function of λ. The basic result is only weakly dependent on the lattice or on the number of spins allowed to participate in the core. The frequency of this mode is found to approach zero as $\omega = A\sqrt{\lambda_c - \lambda}$, with A and λ_c lattice- dependent. The spatial structure of the mode's out-of-plane component bears a strong resemblance to that of the static out-of-plane vortex for $\lambda > \lambda_c$.

II. Core Model for Square Lattice, Static Energy Functional

The vortex structure on a square lattice is considered first. We assume that the vortex is centered in a unit cell, at the origin of a coordinate system, and the in-plane angles are given by the usual in-plane vortex, Eq. (2). In the most crude approximation of the core region's out-of-plane spin components, we assume that only the first four spins nearest to the vortex center have nonzero out-of-plane components, as indicated in Fig. 1. By symmetry these four lattice sites are equidistant from the vortex center, at radius $r_1 = 1/\sqrt{2}$, and they all have the same S^z, taken to be $S^z = Sm_1$. All other sites have $S^z = 0$ by assumption.

Then by using Hamiltonian (1), and only including the m_1 degree of freedom, leads to the following core energy functional due to the 12 bonds nearest to the vortex center:

$$E_{core} = -4JS^2 \left[\lambda m_1^2 + \frac{4}{\sqrt{5}} \sqrt{1-m_1^2} - 3 \right] \tag{3}$$

The first term is the out-of-plane exchange energy, the second term is the in-plane exchange energy, and the constant ground state (in-plane exchange) energy $-12JS^2$ has been subtracted out. The factor $\sqrt{1-m_1^2}$ reflects the fact that as the out-of-plane components increase, the in-plane components are reduced, an important effect controlling the competition between in-plane and out-of-plane exchange energies. For small m_1, an expansion leads to

$$E_{core} \approx -4JS^2 \left[\frac{4}{\sqrt{5}} - 3 + (\lambda - \frac{2}{\sqrt{5}}) m_1^2 + O(m_1^4) \right] \tag{4}$$

It is clear that the energy can be reduced by creating an out-of-plane component provided $\lambda > 2/\sqrt{5}$, defining the critical anistropy, $\lambda_c = 2/\sqrt{5} \approx 0.894$ in this approximation.

More generally, for arbitrary $m_1 < 1$, the extrema of the core energy are determined by a nonlinear equation:

$$\frac{\partial E_{core}}{\partial m_1} = -8JS^2 m_1 \left[\lambda - \frac{2}{\sqrt{5}} \frac{1}{\sqrt{1-m_1^2}} \right] = 0 \tag{5}$$

The equation always has two solutions, either $m_1 = 0$, which is the in-plane vortex solution, or

$$m_1 = \sqrt{1 - (\lambda_c/\lambda)^2}, \tag{6}$$

which is the out-of-plane vortex solution. The in-plane solution exists for any λ, and has fixed energy $E_{ip} = -8JS^2\lambda_c$. The out-of-plane solution exists only for $\lambda > \lambda_c$, and has core energy $E_{op} = -4JS^2(\lambda + \lambda_c^2/\lambda)$, which is lower than E_{ip}. Thus we see that at $\lambda = \lambda_c$, the in-plane vortex becomes unstable, and must grow into an out-of-plane vortex. The numerical value for λ_c is rather high compared to the computer experiments' value[6,7] of $\lambda_c = 0.72$, but this is a result of the crude approximation, not allowing more spins to participate in the energy function. However, the results of this crudest approximation do not differ in substantial details from the more accurate approximations involving more core spins.

It is interesting to re-write the out-of-plane component just above the critical anisotropy, where approximately,

$$m_1 \approx \sqrt{\frac{2}{\lambda_c}(\lambda - \lambda_c)} \tag{7}$$

This square root dependence on the deviation from the critical anisotropy is also seen in the hexagonal and triangular lattice.

In the next order of approximation, the next set of eight spins all equidistant at radius $r_2 = \sqrt{10}/2$ from the vortex center are included in the core energy, as in Fig. 1. This will include a total of 32 bonds. When the first set of four spins has $S^z = Sm_1$, and the next set of eight spins has $S^z = Sm_2$, the core energy with the ground state energy $-32JS^2$ subtracted out is

$$E_{core} = -4JS^2[\lambda(m_1+m_2)^2 + \frac{4}{\sqrt{5}}\sqrt{1-m_1^2}\sqrt{1-m_2^2}$$

$$+\frac{4}{\sqrt{5}}(1+\frac{4}{\sqrt{13}})\sqrt{1-m_2^2} + \frac{4}{5}(1-m_2^2) - 8] \tag{8}$$

The term proportional to λ is the out-of-plane exchange energy, other terms are in-plane exchange. Minimization with respect to m_1 and m_2 simultaneously leads to coupled nonlinear equations, as follows:

$$-2\lambda(m_1+m_2) + \frac{4}{\sqrt{5}}\frac{m_1}{\sqrt{1-m_1^2}}\sqrt{1-m_2^2} = 0 \tag{9a}$$

$$-2\lambda(m_1+m_2) + \frac{4}{\sqrt{5}}\frac{m_2}{\sqrt{1-m_2^2}}\left[\sqrt{1-m_1^2} + (1+\frac{4}{\sqrt{13}})\right] + \frac{8}{5}m_2 = 0 \tag{9b}$$

Again, there is the trivial solution, $m_1 = m_2 = 0$, which is the in-plane vortex, with energy independent of λ. For λ large enough, there is also a nontrivial solution, that can be estimated numerically, for example, by solving Eqs. (9) using a two-dimensional Newton-Raphson method. One finds that m_1 and m_2 grow proportional to $\sqrt{\lambda - \lambda_c}$ just about the critical anisotropy (not shown here). Naturally, the approximation limits the out-of-plane motion strongly compared to the results where a larger set of spins can have out-of-plane motion, but this effect is not too large provided λ is not too far above λ_c.

The critical value of λ can be obtained accurately by supposing that λ is slightly higher than λ_c, in which case m_1 and m_2 are small but nonzero. Then Eqs. (9) can be linearized, and produce a nontrivial solution only when the determinant of the coefficient matrix vanishes. This linearization is valid only in the limit $\lambda \to \lambda_c$ from above, and the determinant vanishes only at the critical anisotropy. Doing so, we obtain the linearized system,

$$(A_s - \lambda)m_1 - \lambda m_2 = 0, \tag{10a}$$

$$-\lambda m_1 + (B_s - \lambda)m_2 = 0. \tag{10b}$$

$$A_s \equiv \frac{2}{\sqrt{5}} \approx 0.89443, \quad B_s \equiv \frac{4}{\sqrt{5}}(1+\frac{1}{\sqrt{5}}+\frac{2}{\sqrt{13}}) \approx 3.58113 \tag{10c}$$

The critical anisostropy at which the determinant vanishes is

$$\lambda_c = \frac{A_s B_s}{(A_s + B_s)} \approx 0.716 \tag{11}$$

This agrees very well with the results of computer experiments, $\lambda_c \approx 0.72$. At the same point, the ratio of core out-of-plane spin components is

$$m_2/m_1 = A_s/B_s \approx 0.24976 \tag{12}$$

This ratio characterizes the initial growth of the out-of-plane components just above the critical point.

One can continue to carry this calculation to higher orders, for instance, the next step is to include an additional set of four more spins, all equidistant from the vortex center, at radius $r_3 = 3/\sqrt{2}$, as in Fig. 1. The energy functional is given in the Appendix. The critical value of λ is determined by the zero of a 3 x 3 determinant. The result is $\lambda_c = 0.7044$, a value somewhat lower than the numerical experiments.

Some results for that model are shown in Fig. 2 for the development of the out-of-plane components for $\lambda > \lambda_c$. These results also are compared with a new simulation of the out-of-plane vortex structure on a 50 x 50 lattice with free boundaries. In the simulation, the system was allowed to relax to a local energy mimimum through the use of Landau-Gilbert damping[13], starting from an in-plane vortex initial configuraton, but with the four spins closest to the vortex center given $S^z = 0.5$. That is, an out-of-plane bias was included in the initial condition, and then the time evolution was followed to see whether the stable vortex would be an in-plane or out-of-plane vortex. Previous simulations[6,7] relied on computer roundoff errors to initiate the transformation from in-plane to out-of-plane vortex, thereby overestimating λ_c. This new simulation shows that the critical anisotropy is actually less than 0.7044, which is to be expected, since the boundary condition used in the model of Fig. 1 overly restricts out-of-plane motions.

The competetion between in-plane and out-of-plane exchange energies is also shown in Fig. 2. Although there are large changes in the in-plane and out-of-plane exchange energies, the total core energy of the out-of-plane vortex is only slightly below the core energy of the in-plane vortex.

III. Core Model for Hexagonal Lattice

It is very instructive to consider how the instability depends on the underlying lattice, and to see why the in-plane vortex apparently is more stable on a hexagonal lattice for a given λ than on a square lattice for the same λ. That is, why is λ_c largest on the hexagonal lattice and smallest on the triangular lattice? Clearly this must be due to the difference in the coordination number of the lattice, but a further explanation is needed.

In the lowest approximation for a vortex on a hexagonal lattice, with coordination number 3, only the first 6 spins (at radius $r_1 = 1$) nearest the vortex center are allowed to move out-of-plane, with $S^z = Sm_1$ (See Fig. 3). All in-plane angles are given by the static in-plane vortex, Eq. (2). Then the core energy associated with the out-of-plane motion (12 bonds total) is

$$E_{core} = -6JS^2 \left[\lambda m_1^2 + \frac{1}{2}(1 - m_1^2) + \sqrt{1 - m_1^2} - 2 \right] \tag{13}$$

At this level of approximation, an expansion for small m_1 leads to

$$E_{core} \approx -6JS^2 \left[-\frac{1}{2} + (\lambda - 1)m_1^2 + O(m_1^4) \right] \tag{14}$$

This results in the estimate, $\lambda_c = 1$.

To a better approximation, an additional set of 6 more spins, at radius $r_2 = 2$, are also allowed to move out-of-plane, with $S^z = Sm_2$ (See Fig. 3). Then the core energy (24 bonds) is

$$E_{core} =$$

$$-6JS^2 \left[\lambda(m_1^2 + m_1 m_2) + \frac{1}{2}(1 - m_1^2) + \sqrt{1 - m_1^2}\sqrt{1 - m_2^2} + \frac{5}{\sqrt{7}}\sqrt{1 - m_2^2} - 4 \right] \tag{15}$$

The energy extrema are determined by the nonlinear equations,

$$\left(1 - 2\lambda + \sqrt{\frac{1 - m_2^2}{1 - m_1^2}} \right) m_1 - \lambda m_2 = 0 \tag{16a}$$

$$-\lambda m_1 + \left(\frac{5}{\sqrt{7}} + \sqrt{1-m_1^2}\right)\frac{m_2}{\sqrt{1-m_2^2}} = 0 \tag{16b}$$

Letting $A_h \equiv (1+5/\sqrt{7}) \approx 2.88982$, the determinant of the linearized system goes to zero at $\lambda_c = -A_h + \sqrt{A_h^2 + 2A_h} \approx 0.869$, in good agreement with the numberical results of 0.86 . If an additional set of 12 more spins at radius $r_3 = \sqrt{7}$ are allowed to have out-of-plane components, the critical anisotropy is found to be $\lambda_c \approx 0.8395$, slightly lower than the numerical results. The core energy function is given in the Appendix. The growth of the out-of-plane components with λ is shown in Fig. 4, with results similar to the square lattice.

IV. Core Model for Triangular Lattice

Finally we turn to the triangular lattice, with coordination number 6. The spins in the core plaquette of an in-plane vortex have 120^o angles between them, or, they are starting to be more antiparallel than parallel. This has a strong effect on the in-plane vs. out-of-plane exchange energy balance.

Starting as before, the lowest approximation is to allow only three spins nearest the vortex center, at radius $r_1 = 1/\sqrt{3}$, to tilt out of the easy plane, with $S^z = Sm_1$, as shown in Fig. 5. The in-plane angles are given by Eq. (2). Then taking the geometry into account, the core energy (15 bonds) is

$$E_{core} = -3JS^2[\lambda m_1^2 - \frac{1}{2}(1-m_1^2) + (1+\frac{5}{\sqrt{7}})\sqrt{1-m_1^2} - 5] \tag{17}$$

An expansion for small m_1 gives the first estimate, $\lambda_c = 5/\sqrt{28} \approx 0.94$, high compared to the numerical experiment value of 0.62.

Next we can allow another set of three more spins at radius $r_2 = 2/\sqrt{3}$ to have out-of-plane components, $S^z = Sm_2$. The core energy (27 bonds) is modified to

$$E_{core} = -3JS^2[\lambda(m_1^2 + 2m_1m_2) - \frac{1}{2}(1-m_1^2) + \frac{5}{\sqrt{7}}\sqrt{1-m_1^2}$$

$$+\sqrt{1-m_1^2}\sqrt{1-m_2^2} + \left(\frac{4}{\sqrt{7}} + \frac{7}{\sqrt{13}}\right)\sqrt{1-m_2^2} - 9] \tag{18}$$

When this system is linearized, the determinant goes to zero at $\lambda_c = -A_t + \sqrt{A_t^2 + 5A_t/\sqrt{7}} \approx 0.715$, where $A_t \equiv \frac{1}{4}(1 + 4/\sqrt{7} + 7/\sqrt{13}) \approx 1.1133$. This is still rather high compared to the numerical experiments, suggesting that another layer of spins around the vortex center must be allowed to move out-of-plane. When an additional set of 6 more spins at radius $r_3 = \sqrt{7/3}$ are allowed to have out-of-plane components $S^z = Sm_3$, a more tedious calculation (E_{core} given in the Appendix) gives $\lambda_c = 0.6278$. In this latter model, the out-of-plane spin components grow with λ above λ_c as indicated in Fig. 6. Of course, even here the out-of-plane components are being underestimated because of the restriction that the next set of spins further out from the vortex center are held fixed in the xy-plane.

By now it is clear what is causing the instability of the in-plane vortex with increasing λ, which corresponds physically to decreasing the strength of the easy-plane anisotropy, or, approaching the isotropic limit. The spins near the vortex core have in-plane exchange energy above the ground state energy due to the fact that they are not close to being parallel. At the same time, they have zero out-of-plane exchange energy. If there is strong easy-plane anisotropy

(λ near zero), then out-of-plane spin components would cost too much additional total energy, so they don't occur. However, as the easy-plane anisotropy strength is reduced (increasing λ), at a certain point these core spins can favorably tilt up out of the easy-plane. In fact, when the out-of-plane components grow, the out-of-plane exchange energy E_{out} *decreases*, while the in-plane exchange energy E_{in} *increases*, such that the total energy change comes out negative. Of course, this can occur only if λ is large enough, such that the decrease in the out-of-plane exchange energy dominates over the increase in in-plane exchange energy (which itself does not depend on λ). These energy changes have been indicated in Figs. 2, 4 and 6, which show how the two energy components vary with λ. The instability is driven mostly by the first set of core spins nearest the vortex center (3 for the triangular lattice, 4 for the square lattice, 6 for the hexagonal lattice). It is interesting to note that even though the changes in E_{in} and E_{out} with λ are rather large, the total vortex core energy decreases very slowly for $\lambda > \lambda_c$. In this sense the out-of-plane vortex is only slightly energetically prefered over the in-plane vortex.

The dependence of λ_c on the lattice is also clear, and again is determined primarily by the first set of core spins. Consider an in-plane vortex on a triangular lattice, where the first three core spins are starting to be antiparallel (120^o angles between them), creating a large in-plane exchange energy in the core. However, normally the easy-plane anisotropy prevents these from tilting up out of plane. But it is clear that they will have a much stronger tendency to come out of plane to avoid pointing against each other, than for the core spins of a vortex on the square or hexagonal lattices, which are already closer to being parallel even when staying in-plane. Essentially the core spins come out of plane to try to align ferromagnetically, provided they can do so against the easy-plane anisotropy forces. They must come out of the easy plane at a lower value of λ on the triangular lattice because they pay a small cost in additional in-plane exchange energy (because the in-plane energy is already large) but get in the deal a larger reduction in out-of-plane exchange energy. Conversly, the hexagonal lattice has the largest critical λ, since the core spins do not have a large in-plane exchange energy (only a 60^o angle between them in-plane) and they stay in the xy-plane until the anisotropy comes much closer to isotropic.

V. Time-Dependent Symmetric Normal Mode of a Vortex

The dynamics of this instability can be understood to a certain extent, by looking for time-dependent normal modes of the in-plane vortex. For example, previous calculations for the XY model using a continuum limits[11] considered the normal modes about the in-plane vortex. However, it is clear from the calculations here that a continuum limit cannot capture the essential features of how the core drives the instability. We want to stress that this is a discrete lattice instability, the strongest evidence of this being the dependence of λ_c on the lattice.

To do a complete stability analysis of the in-plane vortex on a lattice requires a numerical calculation of the eigenmodes for a finite system. Völkel[12] has made a preliminary calculation on a 10 x 10 square lattice, which showed that there is one mode in particular whose frequency goes to zero as λ is increased towards λ_c , and is apparently closely related to the instability[2]. The spatial structure of the mode involves a radially symmetric out-of-plane amplitude about the vortex center, combined with a radially symmetric in-plane spin rotation. Indeed, this is reasonably the simplest symmetrical mode of the in-plane vortex. If there are time-dependent out-of-plane components then there must necessarily be time-dependent in-plane motions with the same kind of symmetry, since S^z is the momentum that is conjugate to the in-plane angle ϕ. In this mode, the time-dependent deviations in S^z and ϕ depend primarily on the radial distance from the vortex center, which itself does not move. We can use this information to make a very reasonable Ansatz for the mode, concentrating on the motion of the most important spins near the core, in the same spirit as the calculations giving λ_c.

So we proceed to consider only the properties of this one particular symmetric mode that is responsible for the in-plane vortex instability. The Ansatz for the mode, on a square lattice, is as follows. The first set of spins nearest to the vortex center, at radius $r_1 = 1/\sqrt{2}$, have out-of-plane component $S^z = Sm_1$, and equal deviations ϕ_1 from the static in-plane angles. This means they all are rotated counterclockwise through ϕ_1 relative to the static in-plane structure, Eq. (2). Similarly, the next set of 8 spins at radius $r_2 = \sqrt{5/2}$, have equal out-of-plane components Sm_2, and equal in-plane deviations ϕ_2. All other spins further out from the vortex core are assumed to lie in the xy plane, with in-plane angles being those of the static in-plane vortex. Then by its design the Ansatz assumes a well-organized radially symmetric motion, with only radial dependence of S^z and ϕ.

A Lagrangian is constructed for the system, by using the fact that S^z is the momentum conjugate to ϕ, and modifying the core energy functional found above to include the in-plane degrees of freedom, ϕ_1 and ϕ_2. The Lagrangian is

$$L = \sum_{\mathbf{n}} \dot{\phi}_{\mathbf{n}} S^z_{\mathbf{n}} \quad - \quad E_{core} \tag{19}$$

where the sum is over the lattice sites in the core region participating in the motion. Making the appropriate changes to the energy to include the ϕ_1 and ϕ_2 degrees of freedom, we have,

$$L = 4S\left(m_1\dot{\phi}_1 + 2m_2\dot{\phi}_2\right)$$

$$+4JS^2[\lambda(m_1+m_2)^2 + \frac{4}{5}(1-m_2^2) + \frac{4}{\sqrt{5}}\sqrt{1-m_1^2}\sqrt{1-m_2^2}\cos(\phi_1-\phi_2)$$

$$+\frac{4}{\sqrt{5}}(1+\frac{4}{\sqrt{13}})\sqrt{1-m_2^2}\cos\phi_2] \tag{20}$$

The equations of motion follow from the usual Euler-Lagrange variation. In particular, the linearized equations of motion are found to be:

$$\frac{1}{JS}\dot{\phi}_1 = 2(A_s-\lambda)m_1 - 2\lambda m_2,$$

$$\frac{1}{JS}\dot{\phi}_2 = -\lambda m_1 + (B_s-\lambda)m_2,$$

$$\frac{1}{JS}\dot{m}_1 = -2A_s\phi_1 + 2A_s\phi_2,$$

$$\frac{1}{JS}\dot{m}_2 = A_s\phi_1 - 2A_s(1+C_s)\phi_2, \tag{21a}$$

$$C_s \equiv \frac{2}{\sqrt{13}}. \tag{21b}$$

A_s and B_s were defined in Eq. (10c). These equations have a solution with time dependence $e^{i\omega t}$. The frequency is determined from the zero of a 2 x 2 determinant, leading to a quadratic equation in ω^2,

$$\omega^4 + 2A_s[(1+C_s)(\lambda-B_s) - 2A_s]\omega^2 + 4A_s^2(2C_s+1)[A_sB_s - (A_s+B_s)\lambda] = 0. \tag{22}$$

From this equation we see first of all, that the eigenfrequency becomes zero when the constant coefficient vanishes, which occurs when $\lambda = \lambda_c = A_s B_s/(A_s + B_s)$, a result previously obtained in the discussion of the static structure. For other values of $\lambda < \lambda_c$, the desired solution to the quadratic that recovers $\omega \to 0$ as $\lambda \to \lambda_c$ from below, is

$$\omega^2 = D_0(D_1 - \lambda)\left[1 - \sqrt{1 - D_2(\lambda_c - \lambda)/(D_1 - \lambda)^2}\right], \tag{23a}$$

where the new numerical constants are

$$D_0 = A_s(1 + C_s) \approx 1.39057,$$

$$D_1 = B_s + 2A_s/(1 + C_s) \approx 4.73174,$$

$$D_2 = 4(A_s + B_s)(2C_s + 1)/(1 + C_s)^2 \approx 15.62331 \tag{23b}$$

But now since D_1 is rather large compared to λ, and because we are most interested in the region near the critical point, an expansion of the square root can be made that is quite accurate, even when λ is near zero. Doing so gives, to a very good approximation,

$$\omega \approx \sqrt{\frac{D_0 D_2}{2(D_1 - \lambda_c)}}\sqrt{\lambda_c - \lambda} \approx 1.645\sqrt{\lambda_c - \lambda} \tag{24}$$

In fact, even for $\lambda = 0$, the difference between Eq. (24) and Eq. (23a) is much less than 1 %. We should note that the pre-factor, 1.645, is determined primarily by the number of spins allowed to move in the core region, and should not be taken as definitive. For comparison, when only the m_1 and ϕ_1 degrees of freedom are allowed, then a short calculation gives eigenfrequencies $\omega = 2\sqrt{A_s}\sqrt{\lambda_c - \lambda} \approx 1.8915\sqrt{\lambda_c - \lambda}$. On the other hand, including 3 sets of spins, out to radius r_3, a numerical fit to the solution of the eigenfrequency problem gives the result, $\omega \approx 1.5281\sqrt{\lambda_c - \lambda}$ (See Fig. 7). So it is clear that the prefactor will decrease as a greater number of core spins' motions are included, while the functional form for $\omega(\lambda)$ remains unchanged. The prefactor is expected to be slightly less than 1.52 for the infinite sized system. Note that λ_c in these formulas means the value found for the approximation under question, i.e., λ_c= 0.894, 0.716, 0.7044, for including one, two, or three sets of spins, respectively.

VI. Time Dependent Symmetric Mode in Hexagonal and Triangular Lattices

Next the dynamics of the instability is investigated on the hexagonal and triangular lattices, to see whether the lattice has any strong influence on the unstable mode's frequency. The principal modifications from the square lattice calculation require using the appropriate core energies in the Lagrangian.

On the hexagonal lattice, with two sets of spins allowed to participate in the dynamics, the effective Lagrangian is

$$L = 6S(m_1\dot{\phi}_1 + m_2\dot{\phi}_2) + 6JS^2[\frac{1}{2}(1 - m_1^2) + \lambda(m_1^2 + m_1 m_2)$$
$$+\sqrt{1 - m_1^2}\sqrt{1 - m_2^2}\cos(\phi_1 - \phi_2) + \frac{5}{\sqrt{7}}\sqrt{1 - m_2^2}\cos\phi_2] \tag{25}$$

The linearized equations that result are

$$\frac{1}{JS}\dot{\phi}_1 = 2(1 - \lambda)m_1 - \lambda m_2,$$

$$\frac{1}{JS}\dot{\phi}_2 = -\lambda m_1 + A_h m_2,$$
$$\frac{1}{JS}\dot{m}_1 = -\phi_1 + \phi_2,$$
$$\frac{1}{JS}\dot{m}_2 = \phi_1 - A_h\phi_2, \qquad (26a)$$

where
$$A_h \equiv 1 + \frac{5}{\sqrt{7}} \approx 2.88982. \qquad (26b)$$

The eigenfrequencies for this system are easily found to be determined by the quadratic equation,

$$\omega^4 - (2 + A_h^2)\omega^2 - (A_h - 1)(\lambda^2 + 2A_h\lambda - 2A_h) = 0. \qquad (27)$$

We see once again that $\omega \to 0$ when the last coefficient vanishes, which reproduces $\lambda_c = -A_h + \sqrt{A_h^2 + 2A_h} \approx 0.869$. The root for ω that approaches zero for $\lambda \to \lambda_c$ can be approximated quite accurately in a way similar to that for the square lattice calculation,

$$\omega \approx \sqrt{\frac{(A_h - 1)(B_h + \lambda)}{(A_h^2 + 2)}}\sqrt{\lambda_c - \lambda} \approx 1.172\sqrt{\lambda_c - \lambda} \qquad (28)$$

where $B_h = A_h + \sqrt{A_h^2 + 2A_h}$. Thus, this level of approximation gives results very similar to that found for the square lattice, but naturally with a different energy scale. (Due essentially to the coordination number and size of the unit cell of the lattice.) The calculation of ω can be repeated in the approximation that three sets of spins out to radius $r_3 = \sqrt{7}$ participate in the motion. In that case, a fit to a numerical solution leads to the result, $\omega \approx 0.9373\sqrt{\lambda_c - \lambda}$, with $\lambda_c = 0.8395$ (See Fig. 7).

Similar calculations can be made for the triangular lattice. Using three sets of spins, out to radius $r_3 = \sqrt{7/3}$, the eigenfrequency of the linearized equations was found numerically. The core energy is given in the Appendix. The numerical solution for ω is shown in Fig. 7, and is well-approximated by the function, $\omega \approx 2.40\sqrt{\lambda_c - \lambda}$, using $\lambda_c = 0.6278$. Again, it is likely that the prefactor may be slightly overestimated from the value that would be appropriate for an infinite system. Also, the relatively larger coefficient compared to hexagonal and square lattices is to be expected, due to the smaller unit cell and higher coordination number, making the system "stiffer."

VII. Summary

The above calculations allow for a complete explanation of the instability of the in-plane vortices in the easy-plane ferromagnet. They have concentrated on the degrees of freedom near the core, where the energy density is highest, where spatial gradients of the spin field are largest, and therefore where continuum theories would have the most difficulties. The instability has been explained as being a consequence of the competition between in-plane and out-of-plane exchange forces. When the easy-plane anisotropy becomes too weak, (λ increasing towards 1), the spins near the vortex core must come out of the easy-plane to attempt to become more parallel and reduce their total exchange energy. This means they reduce their out-of-plane exchange energy while increasing their in-plane exchange energy. This must happen at a lower value of λ for the triangular lattice than for the square or hexagonal lattice, because the spins near the vortex core start out being far from parallel and thus possessing a large in-plane exchange energy. If they come out of the xy-plane, they can become more parallel, they increase their in-plane exchange energy, but at the same time reduce their out-of-plane exchange energy and also their total energy, provided λ is large enough.

While the spins nearest to the core are primarily responsible for driving the instability, it is important to allow for a large enough number of spins to participate in the out-of-plane motion in order to get an accurate estimate of the critical anisotropy, especially for the triangular lattice. This discrete calculation of the in-plane vortex stability limit, using three sets of core spins, must overestimate the critical anisotropies λ_c, because it restricts out-of-plane spin motion compared to that that would occur in the inifinite system. The critical anisotropies obtained are $\lambda_c \approx 0.8395, 0.7044$, and 0.6278 for hexagonal, square, and triangular lattices, respectively.

The instability is closely related to a dynamic mode of the in-plane vortex, for $\lambda < \lambda_c$. This mode involves a symmetrical oscillatory out-of-plane motion coupled to an in-plane rotational motion, all with circular symmetry about the vortex center. For λ slightly below λ_c, this mode consists mostly of out-of-plane motions, with weaker in-plane motions. The in-plane motions get stronger for λ farther away from λ_c (i.e., λ near zero). The frequency of this mode goes to zero at the critical anisotropy as $\omega \propto \sqrt{\lambda_c - \lambda}$, signalling the growth of large out-of-plane spin components becoming energetically favorable for $\lambda > \lambda_c$. We can also speculate that a similar analysis of the out-of-plane vortex for $\lambda > \lambda_c$ will reveal a corresponding normal mode whose frequency also goes to zero as λ approaches λ_c from above.

Acknowledgements

Discussions with A.R. Völkel, A.R. Bishop and F.G. Mertens are greatly appreciated. This work was partially supported by The University of Bayreuth, Germany, Los Alamos National Laboratory, and by NATO (Collaborative Research Grant No. 0013/89).

Appendix: Core Energies for Three Sets of Spins

For completeness we give here the core energy functions when three sets of spins out to radius r_3 are included. The three sets of spins have out-of-plane components m_1, m_2, and m_3, and for the time-dependent calculation, in-plane deviations from the static in-plane vortex of ϕ_1, ϕ_2, and ϕ_3.

For a vortex on a square lattice, evaluation of Hamiltonian (1) in the core region for Fig. 1 (40 bonds) gives,

$$E_{core} = -4JS^2\{\lambda(m_1^2 + m_2^2 + 2m_1m_2 + 2m_2m_3) + \frac{4}{5}(1-m_2^2)$$
$$+\frac{4}{\sqrt{5}}\sqrt{1-m_2^2}[\sqrt{1-m_1^2}\cos(\phi_1-\phi_2) + \sqrt{1-m_3^2}\cos(\phi_2-\phi_3) + \frac{4}{\sqrt{13}}\cos\phi_2]$$
$$+\frac{8}{\sqrt{17}}\sqrt{1-m_3^2}\cos\phi_3 - 10\} \qquad (A1)$$

Various terms involve either interactions between the levels of spins or within a given level. This includes interactions of level 3 with spins further out that are held fixed in the xy-plane. For the static stability analysis, the in-plane deviations can be set to zero.

For a vortex on the hexagonal lattice, the core energy (42 bonds) is evaluated as

$$E_{core} = -6JS^2\{\lambda(m_1^2 + m_1m_2 + 2m_2m_3 + m_3^2) + \sqrt{1-m_1^2}\sqrt{1-m_2^2}\cos(\phi_1-\phi_2)$$

$$+\frac{5}{\sqrt{7}}\sqrt{1-m_2^2}\sqrt{1-m_3^2}\cos(\phi_2-\phi_3)+\frac{19}{\sqrt{7\cdot 13}}\sqrt{1-m_3^2}\cos\phi_3+\frac{13}{14}(1-m_3^2)-7\}. \qquad (A2)$$

For the triangular lattice, it was necessary to use at least three sets of spins to get an accurate result for λ_c. In this case the core energy (48 bonds) is

$$E_{core}=-3JS^2\{\lambda[m_1^2+2(m_1m_2+m_1m_3+m_2m_3)+m_3^2]-\frac{1}{2}(1-m_1^2)+\frac{25}{28}(1-m_3^2)$$

$$+\sqrt{1-m_1^2}\sqrt{1-m_2^2}\cos(\phi_1-\phi_2)+\frac{5}{\sqrt{7}}\sqrt{1-m_1^2}\sqrt{1-m_3^2}\cos(\phi_1-\phi_3)$$

$$+\frac{4}{\sqrt{7}}\sqrt{1-m_2^2}\sqrt{1-m_3^2}\cos(\phi_2-\phi_3)$$

$$+\frac{7}{\sqrt{13}}\sqrt{1-m_2^2}\cos\phi_2+\frac{1}{\sqrt{7}}(5+\frac{23}{\sqrt{19}}+\frac{17}{\sqrt{13}})\sqrt{1-m_3^2}\cos\phi_3-16\}. \qquad (A3)$$

REFERENCES

1 J.M. Kosterlitz and D.J. Thouless, J. Phys. C**6**, 1181 (1973).

2 A.R. Völkel, F.G. Mertens, A.R. Bishop and G.M. Wysin, Phys. Rev. B**43**, 5992 (1991).

3 F.G. Mertens, A.R. Bishop, G.M. Wysin and C. Kawabata, Phys. Rev. Lett. **59**, 117 (1987); Phys. Rev. B**39**, 591 (1989).

4 S. Hikami and T. Tsuneto, Prog. Theor. Phys. **63**, 387 (1980).

5 S. Takeno and S. Homma, Prog. Theor. Phys. **64**, 1193 (1980); **65**, 172 (1980).

6 G. M. Wysin, M.E. Gouvêa, A.R. Bishop and F.G. Mertens, in *Computer Simulation Studies in Condensed Matter Physics*, D.P Landau, K.K. Mon and H.-B. Schüttler, eds., Springer-Verlag, Berlin (1988).

7 M.E. Gouvêa, G.M. Wysin, A.R. Bishop and F.G. Mertens, Phys. Rev. B**39**, 11840 (1989).

8 For example, L.P. Regnault and J. Rossat-Mignod, J. Magn. Magn. Mater. **14**, 194 (1974); L.P. Regnault et al., Physica B+C, **136B**, 329 (1986).

9 E. Magyari and H. Thomas, J. Phys. C: Solid St. Phys. **16**, L535 (1983); P. Kumar, Phys. Rev. B**25**, 483 (1982).

10 G.M. Wysin, A.R. Bishop and J. Oitmaa, J. Phys. C: Solid St. Phys. **19**, 221 (1986).

11 B.V. Costa, M.E. Gouvêa and A.S.T. Pires, Phys. Lett. A **165**, 179 (1992).

12 A.R. Völkel, private communication.

13 L.D. Landau and E.M. Lifshitz, Phys. Z. Sowjet **8**, 153 (1935); F.H. de Leeuw, R. van den Poel and U. Enz, Rep. Prog. Phys. **43**, 44 (1980).

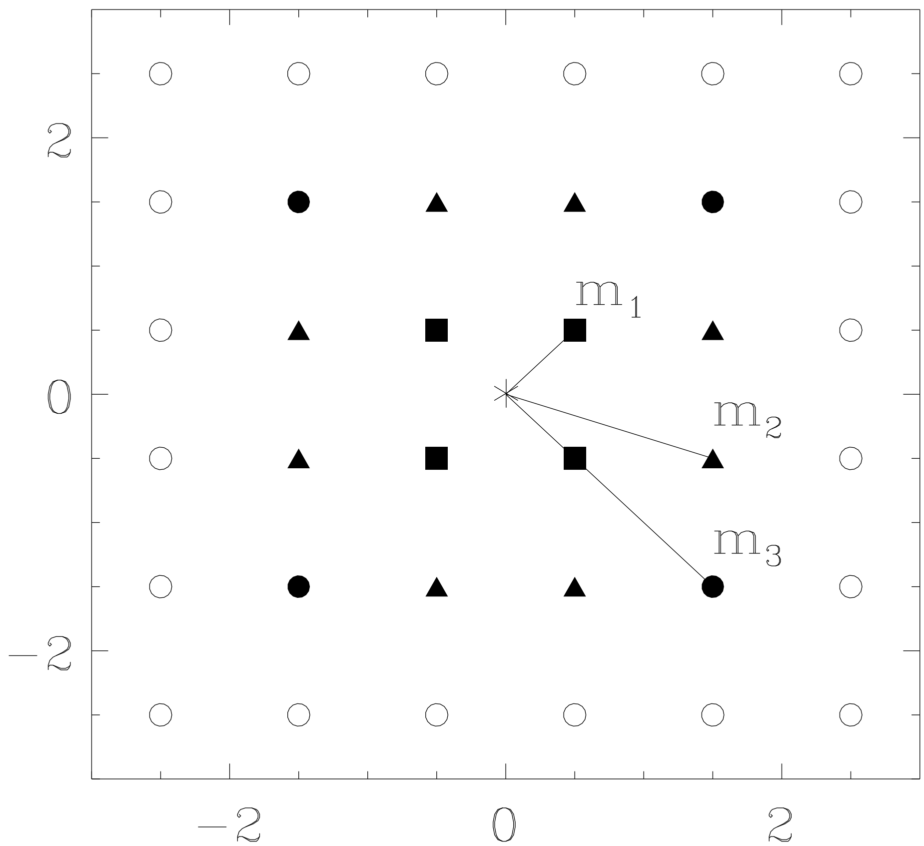
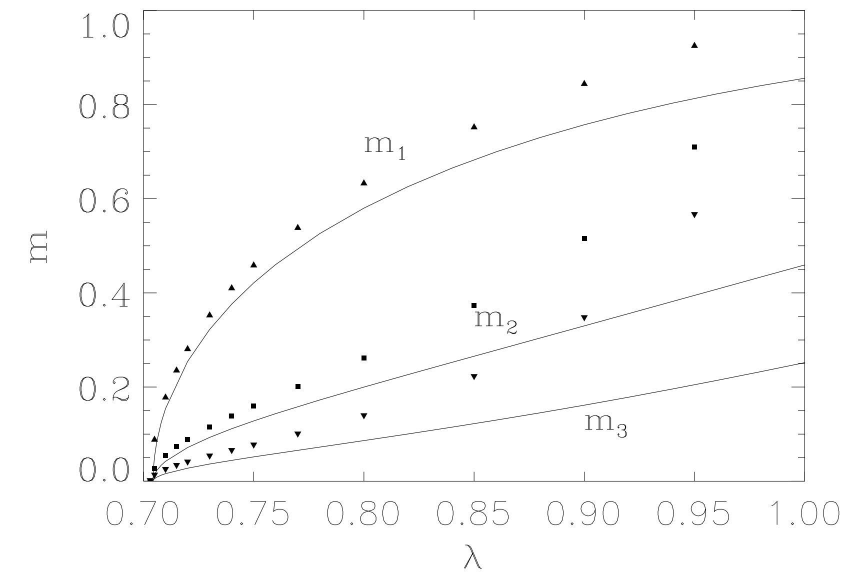
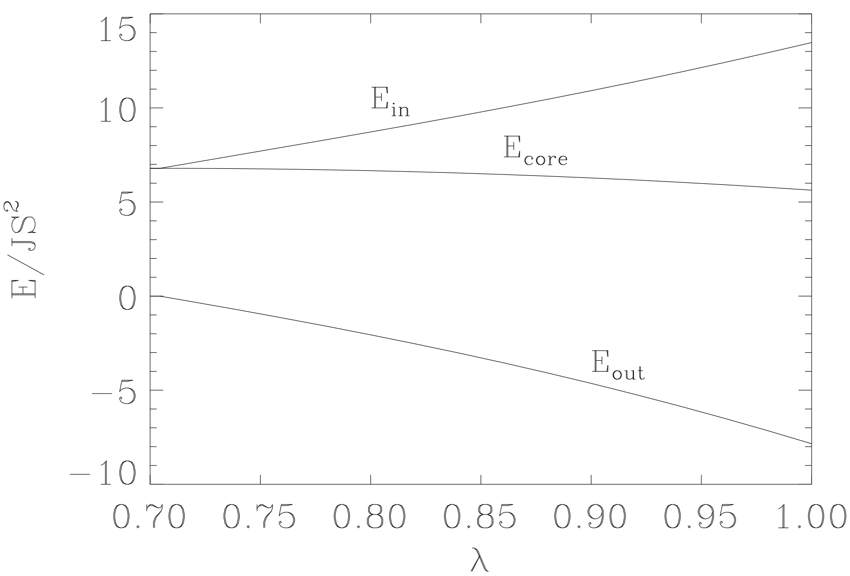


Fig. 1 Notation for the square lattice calculations. The vortex center is at (0,0), and there are 4 sites at radius $r_1 = 1/\sqrt{2}$ with $S^z/S = m_1$ (solid squares), 8 sites at radius $r_2 = \sqrt{10}/2$ with $S^z/S = m_2$ (solid triangles), and 4 sites at radius $r_3 = 3/\sqrt{2}$ with $S^z/S = m_3$ (solid circles). The other sites are held fixed in the xy plane (open circles).



(a)



(b)

Fig. 2 Static vortex structure on the square lattice in the the m_1, m_2, m_3 approximation. (a) Growth of out-of-plane components in the core region. The symbols are the new 50×50 simulation results. (b) Variation of the in-plane and out-of-plane exchange energies and total core energy with anisotropy. The critical anisotropy is $\lambda_c = 0.7044$.

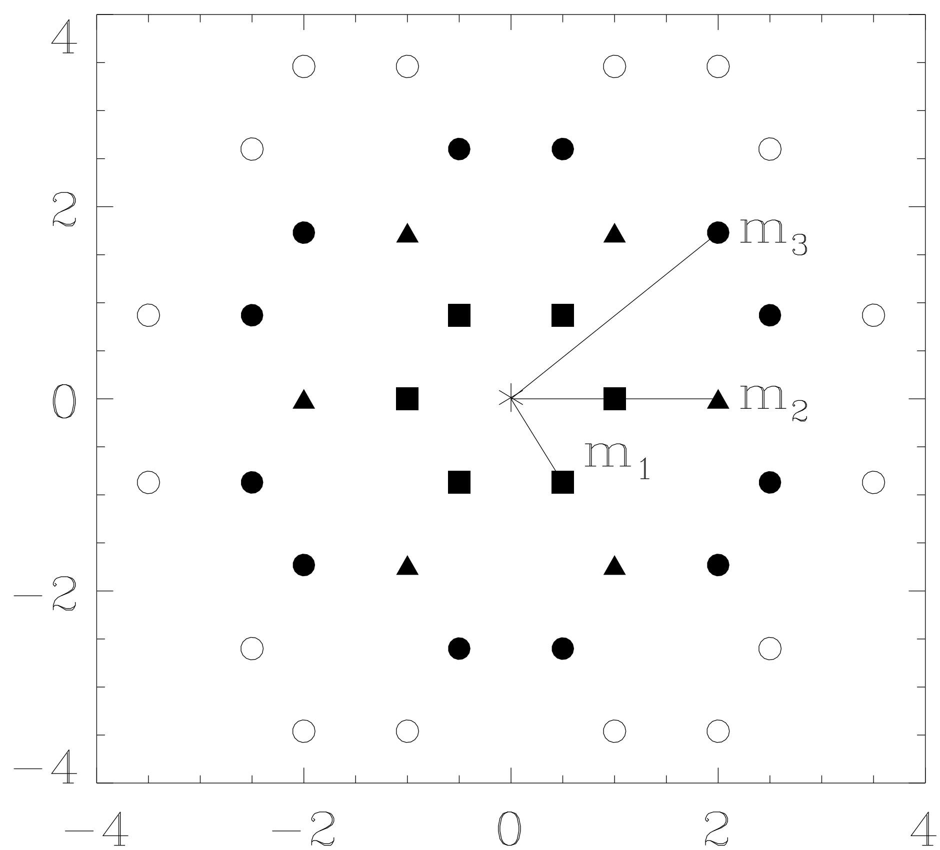
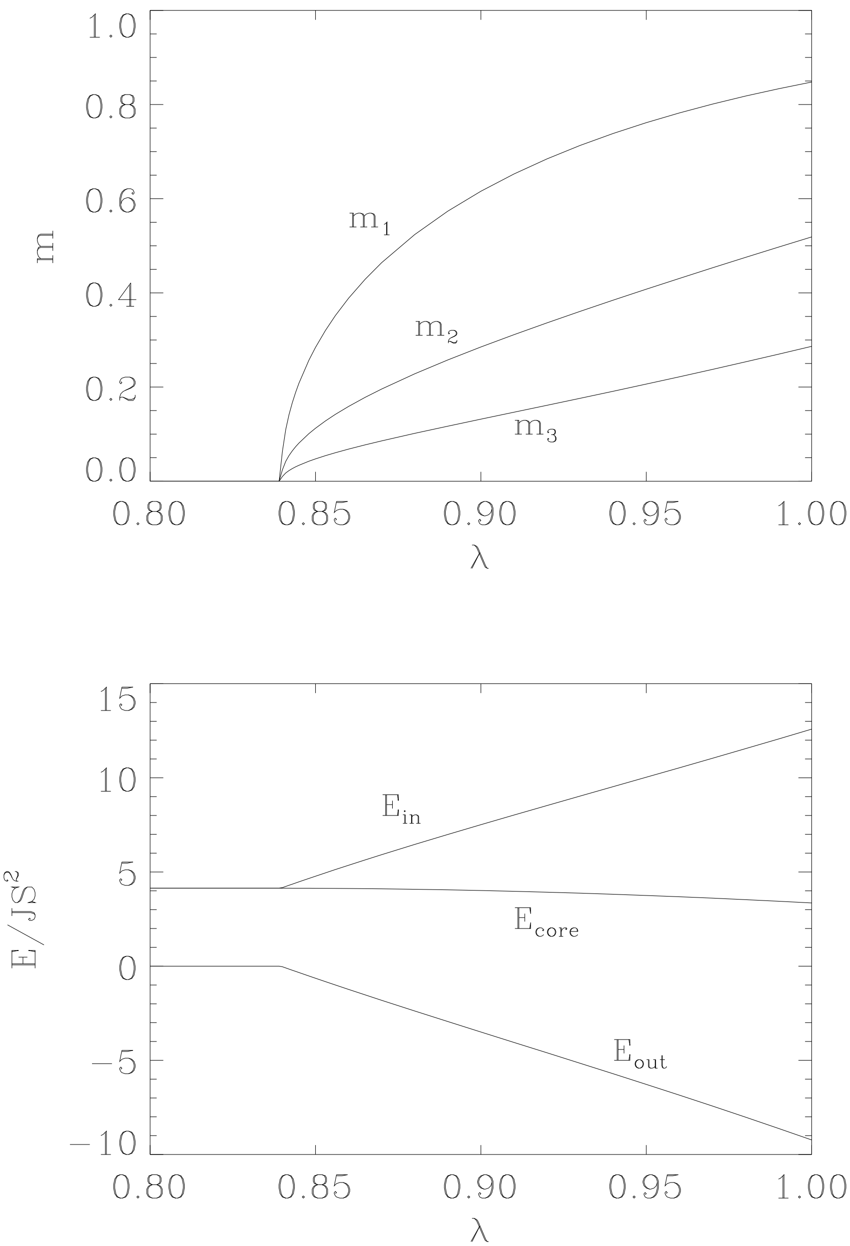


Fig. 3 Notation for the hexagonal lattice calculations. The vortex center is at (0,0), and there are 6 sites at radius $r_1 = 1$ with $S^z/S = m_1$ (solid squares), 6 sites at radius $r_2 = 2$ with $S^z/S = m_2$ (solid triangles), and 12 sites at radius $r_3 = \sqrt{7}$ with $S^z/S = m_3$ (solid circles). The other sites are held fixed in the xy plane (open circles).



(a)

(b)

Fig. 4 Static vortex structure on the hexagonal lattice in the the m_1, m_2, m_3 approximation. (a) Growth of out-of-plane components in the core region; (b) Variation of the in-plane and out-of-plane exchange energies and total core energy with anisotropy. The critical anisotropy is $\lambda_c = 0.8395$.

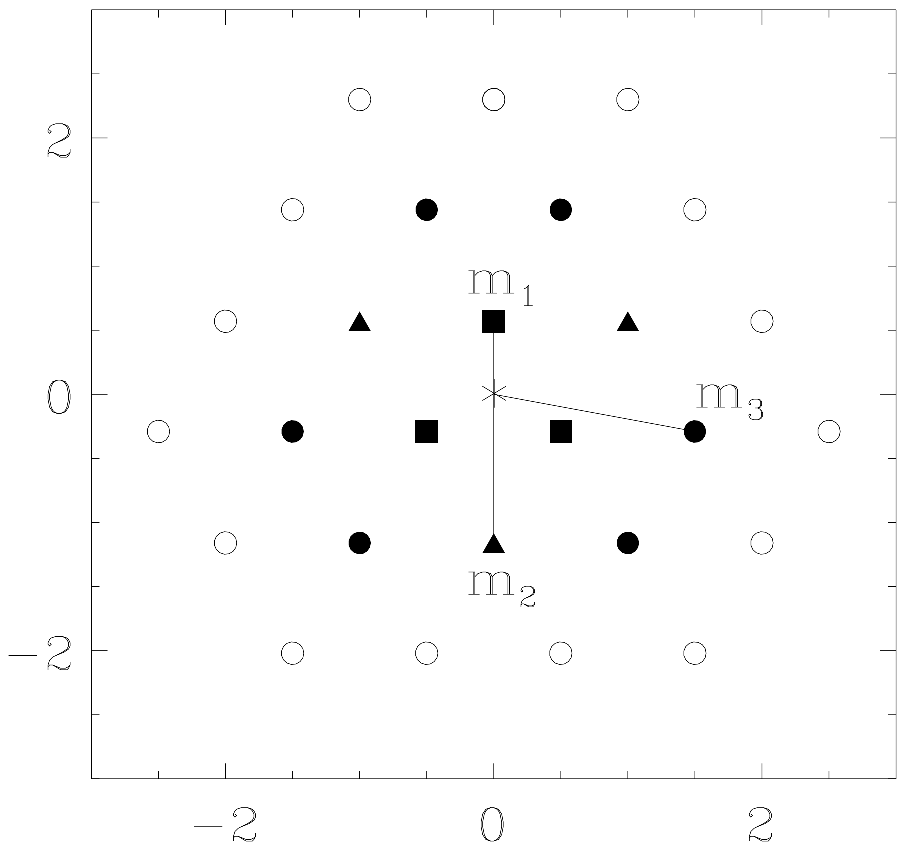


Fig. 5 Notation for the triangular lattice calculations. The vortex center is at (0,0), and there are 3 sites at radius $r_1 = 1/\sqrt{3}$ with $S^z/S = m_1$ (solid squares), 3 sites at radius $r_2 = 2/\sqrt{3}$ with $S^z/S = m_2$ (solid triangles), and 6 sites at radius $r_3 = \sqrt{7/3}$ with $S^z/S = m_3$ (solid circles). The other sites are held fixed in the xy plane (open circles).

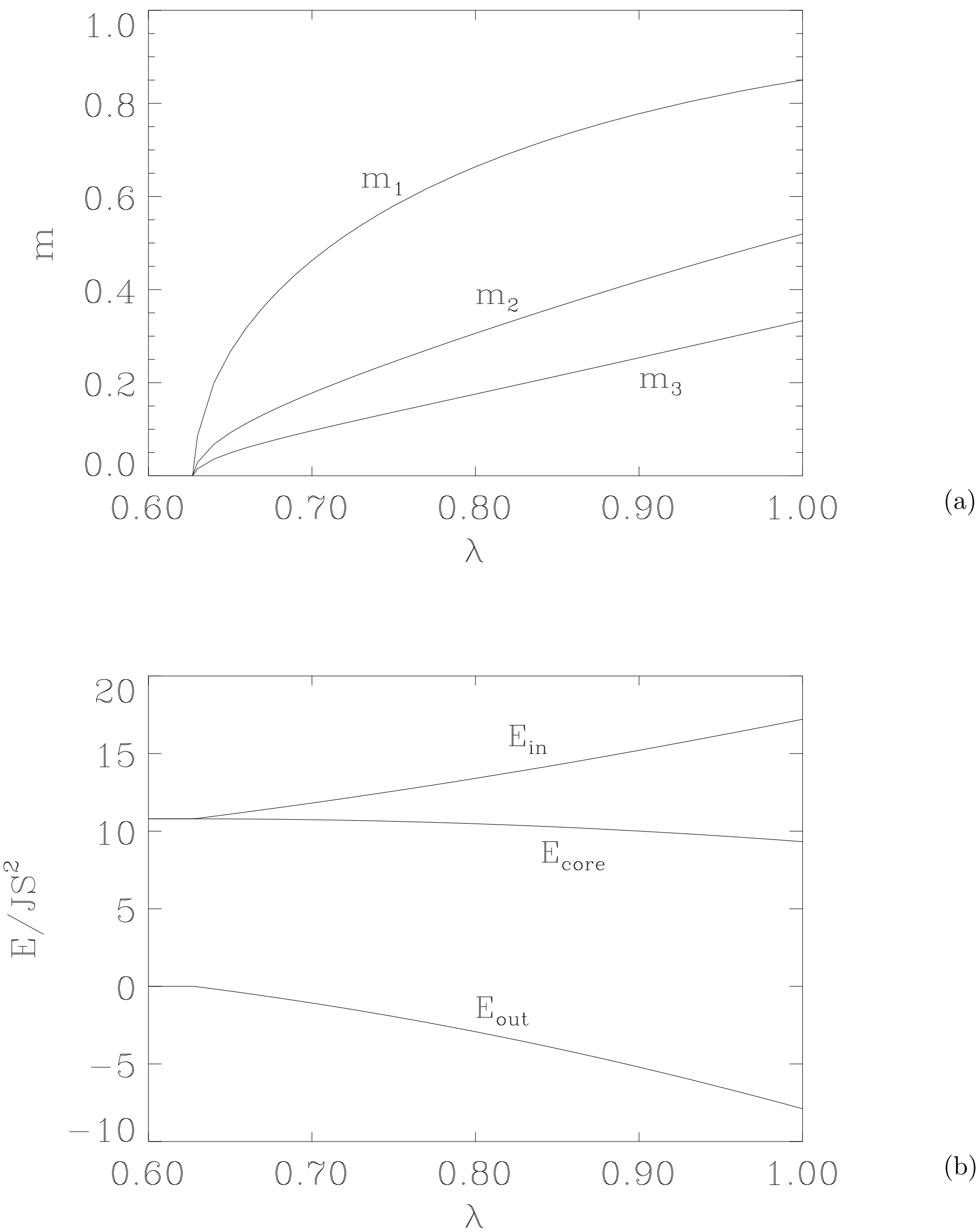
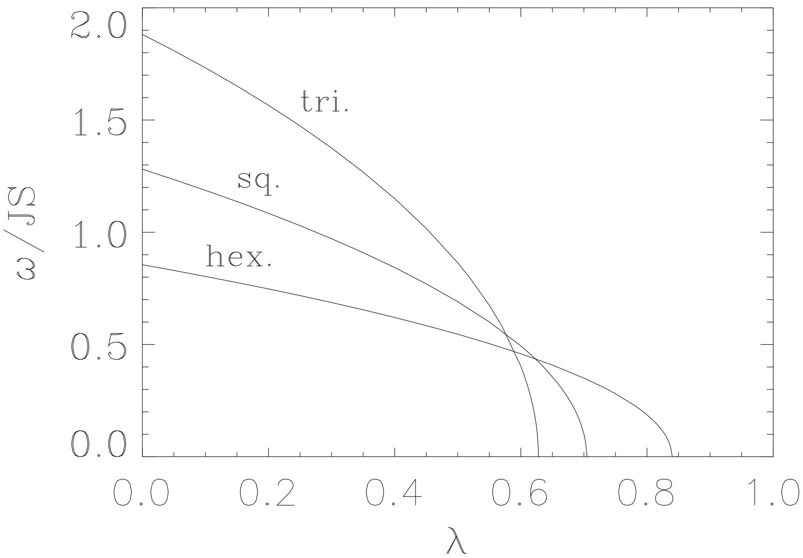
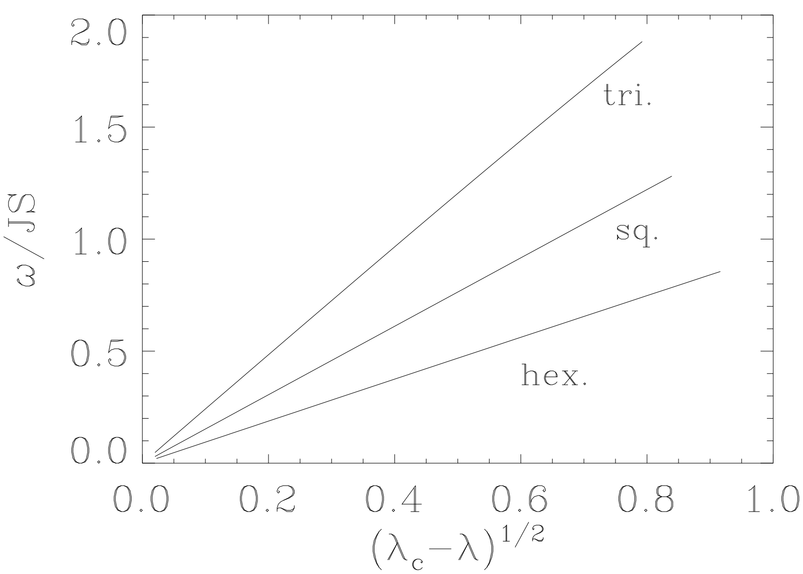


Fig. 6 Static vortex structure on the triangular lattice in the the m_1, m_2, m_3 approximation. (a) Growth of out-of-plane components in the core region; (b) Variation of the in-plane and out-of-plane exchange energies and total core energy with anisotropy. The critical anisotropy is $\lambda_c = 0.6278$.



(a)



(b)

Fig. 7 (a) The frequencies of the unstable symmetric mode vs. λ in the m_1, m_2, m_3 approximation, for the three different lattices. In part (b), the same results re-plotted vs. $\sqrt{\lambda_c - \lambda}$, using the critical values $\lambda_c = 0.6278$, 0.7044, and 0.8395, for the triangular, square, and hexagonal lattices respectively.