Critical anisotropies of two-dimensional magnetic vortices

G. M. Wysin [1]

Departamento de Física, ICEx, Universidade Federal de Minas Gerais, Belo Horizonte, CEP 30161, MG, Brazil

Abstract

Critical easy-plane anisotropies where in-plane magnetic vortices in two-dimensional Heisenberg models are stabilized are determined precisely on square, hexagonal and triangular lattices, by finding the anisotropy that leads to a zero frequency mode.

Key words: Two-dimensional magnets; Easy-plane magnets; Magnetic vortices.

Introduction— It is known from simulations[1–3] and analytic calculations[4] that magnetic vortices in two-dimensional(2D) Heisenberg models with easy-plane anisotropy exhibit an instability that depends on the anisotropy strength. Here we discuss a method to compute very precisely the critical anisotropy that is necessary to stabilize a vortex to have purely in-plane (xy) spin components, for square, hexagonal and triangular lattices. This calculation relies on making an exact summation over spin degrees of freedom on a lattice, and analyzing when the in-plane vortex has a zero frequency mode that leads to evolution of nonzero spin components out of the easy plane (out-of-plane vortex). Rough estimates of only the critical *exchange* anisotropy were obtained earlier[4] by analyzing the spins within a small-radius core of the vortex. Similar to a calculation of vortex energy by Zaspel et al.[5], we now make the required summations to any desired radius, obtaining *both* the exchange and single-ion critical anisotropies in the infinite sized limit.

The Model— We consider 2D lattice models with easy-plane (XY) anisotropy of exchange type (dimensionless parameter $\delta \geq 0$) and of single-ion type (dimensionless parameter $d \geq 0$), with Hamiltonian:

$$H = J \sum_{\mathbf{n}} \Big\{ \mp \tfrac{1}{2} \sum_{\mathbf{a}} \Big[\vec{S}_{\mathbf{n}} \cdot \vec{S}_{\mathbf{n+a}} - \delta S^z_{\mathbf{n}} S^z_{\mathbf{n+a}} \Big] + d (S^z_{\mathbf{n}})^2 \Big\}, \tag{1}$$

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

where $J>0$, subscript $\mathbf{n}$ labels the lattice sites and subscript $\mathbf{a}$ labels the set of displacements to the nearest neighbors. Upper and lower signs correspond to ferromagnetic (FM) and antiferromagnetic (AFM) models, respectively. In terms of in-plane angle ϕ and out-of-plane component $m = S^z/S$, $\vec{S}_\mathbf{n} = S(\sqrt{1-m_\mathbf{n}^2}\cos\phi_\mathbf{n}, \sqrt{1-m_\mathbf{n}^2}\sin\phi_\mathbf{n}, m_\mathbf{n})$. Then for an in-plane FM vortex with vorticity $q = \pm 1$ located at the origin, $S^z_\mathbf{n} = 0$ and $\phi^o_\mathbf{n} = \Phi^v_\mathbf{n}$, where the static vortex angles $\Phi^v_\mathbf{n}$ satisfy the discrete lattice Laplace-like equation,

$$\sum_\mathbf{a} \sin(\Phi^v_\mathbf{n} - \Phi^v_{\mathbf{n}+\mathbf{a}}) = 0. \tag{2}$$

We solved this equation by first setting the angles to their continuum vortex values, $\Phi^v_\mathbf{n} = q\tan^{-1} y/x$, and then iteratively setting each spin's xy-components to point along the direction of the effective field due to its neighbors. This results in small differences of the discrete solution from the continuum result that is usually used, especially near the vortex core. For AFM vortices, $\phi^o_\mathbf{n}$ is modulated according to the sublattice l that site $\mathbf{n}$ lives in. Letting $\Phi_l = 2\pi l/L$, where L is the number of sublattices ($L = 2$ for square and hexagonal lattices, $L = 3$ for triangular lattice), and $l = 0, 1, ...(L-1)$, the AFM vortex has in-plane component $\phi^o_\mathbf{n} = \Phi^v_\mathbf{n} + \Phi_{l_\mathbf{n}}$. The $l_\mathbf{n}$ are assigned such that that no neighboring sites have identical values. However, frustration makes consideration of out-of-plane vortex structure and calculation of critical anisotropy impossible for the triangular lattice. Thus the AFM model is considered only on square and hexagonal lattices.

Now we consider simple ways in which the spins in the vortex structure perform small-amplitude oscillations φ and m,

$$\phi_\mathbf{n} = \phi^o_\mathbf{n} + \varphi_\mathbf{n}, \qquad S^z_\mathbf{n} = S m_\mathbf{n}. \tag{3}$$

and seek any mode of vibration whose frequency drops to zero, signalling an instability of the original vortex structure. The Hamiltonian in terms of these perturbations is

$$H = JS^2 \sum_\mathbf{n} \Big\{ \mp\tfrac{1}{2} \sum_\mathbf{a} \Big[\sqrt{1-m^2_\mathbf{n}}\sqrt{1-m^2_{\mathbf{n}+\mathbf{a}}}\cos(\phi^o_\mathbf{n} - \phi^o_{\mathbf{n}+\mathbf{a}})\cos(\varphi_\mathbf{n} - \varphi_{\mathbf{n}+\mathbf{a}}) + \lambda m_\mathbf{n} m_{\mathbf{n}+\mathbf{a}} \Big] + d m^2_\mathbf{n} \Big\}, \tag{4}$$

where $\lambda \equiv 1 - \delta$ is the relative coupling of the S^z components.

The simplest motion to consider is one where the perturbations φ and m depend only on the radius $r_\mathbf{n}$ of site $\mathbf{n}$ from the vortex center, with no explicit dependence on the angular position of the sites. It is this kind of motion that has already been seen in the mode responsible for the vortex instability[6,7].

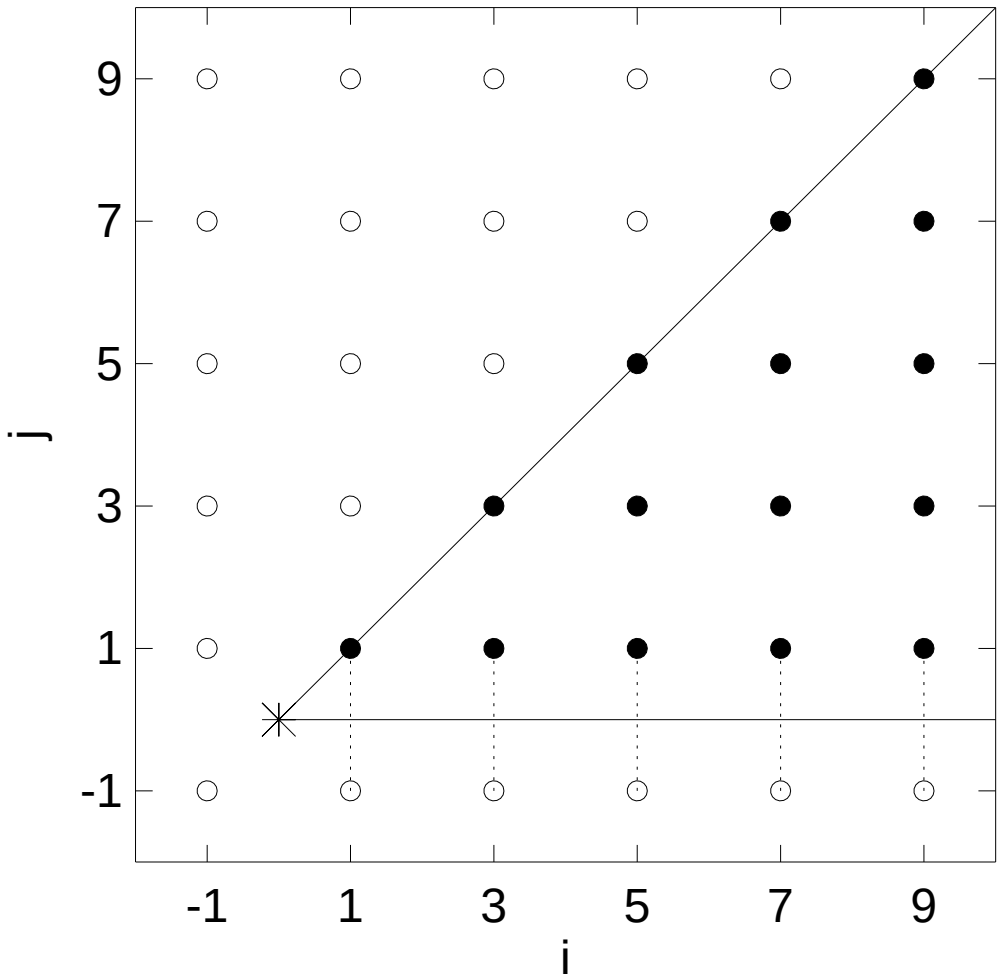

Fig. 1. Ring coordinates (i, j) for square lattice. The vortex center is denoted by *. Solid circles indicate the sites needed to identify the rings, with other sites of a ring obtained by appropriate reflections and rotations. Rings on the solid lines have half as many sites as other rings. Dotted lines indicate ring (exchange) self-interaction.

Instead of supposing that φ and m depend on the radius r, we make the Ansatz that they depend on what we will call here shells or "rings", where the sites belonging to a given ring are all at the same radius, and in addition to this, they can be mapped into each other by symmetry operations which depend on the lattice. The FM Ansatz is to assume that all sites on a given ring have the *same* perturbations φ_α and m_α, completely in phase. For the AFM Ansatz on square and hexagonal lattices, it is assumed that sites on the same sublattice on a ring move in phase, with the same φ_α and m_α, while the other sublattice is exactly out of phase with this, having perturbations $-\varphi_\alpha$ and $-m_\alpha$. To further define what we mean by these rings, it is necessary to consider square, hexagonal, and triangular lattices separately.

Square Lattice—With the vortex placed at the origin (0,0), lying at the center of a unit cell, the sites of the lattice have coordinates $(x, y) = (\frac{a}{2}i, \frac{a}{2}j)$, where a is the lattice constant and i and j are *odd* integers (Fig. 1). When $i = j$

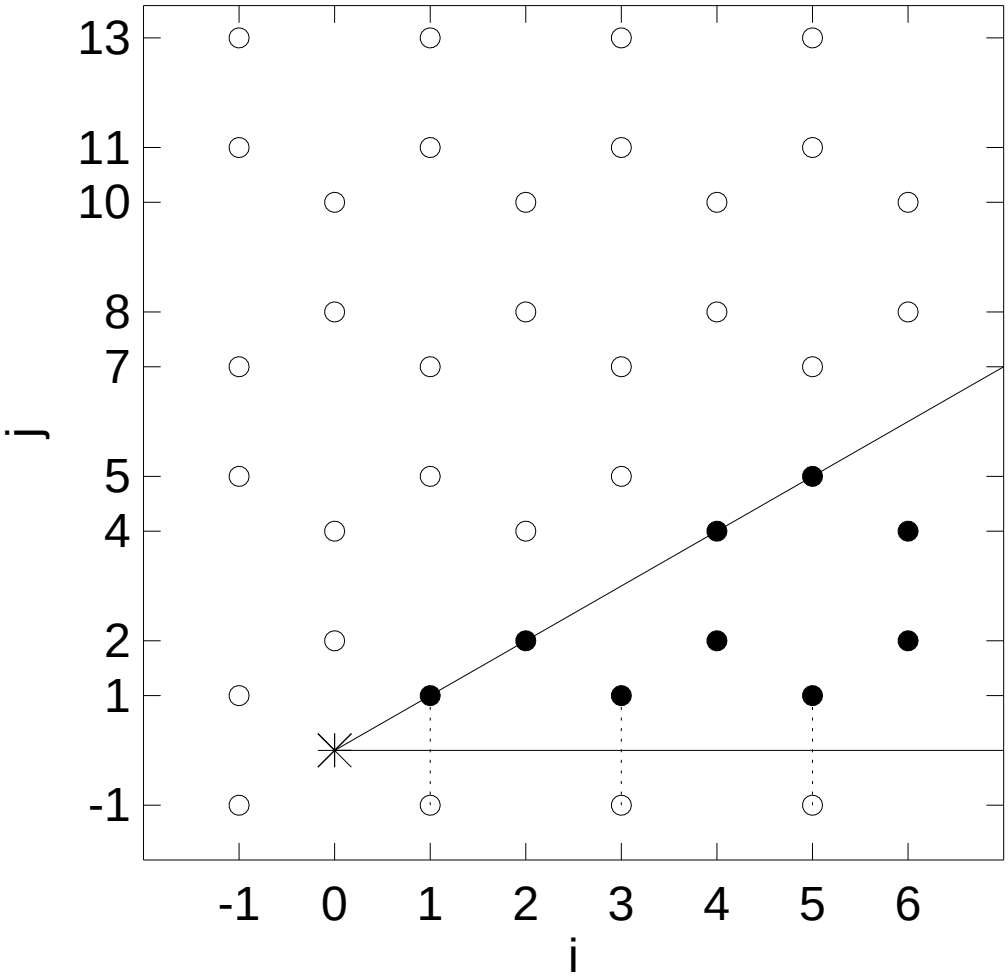

Fig. 2. Ring coordinates (i, j) for hexagonal lattice, notation as in Fig. 1.

(on solid line in Fig. 1), then the four sites $(x, y) = \frac{a}{2}(\pm i, \pm i)$, related by reflection operations through the x and y axes, comprise the ring (i, i). When $i \neq j$, then the eight sites, $(x, y) = \frac{a}{2}(\pm i, \pm j), \frac{a}{2}(\pm j, \pm i)$ related by reflections through the x,y axes and through the (11) directions, comprise the ring (i, j). In general, a given ring α can be uniquely denoted by the pair $\alpha_{(i,j)} \equiv (i, j)$, with $i > 0$, $j > 0$, and $i \geq j$. Different rings may have identical radii, such as rings $(5, 5)$ and $(7, 1)$, but we still consider them as independent variables. In this way there is actually some angular dependence that can occur in the normal mode, since the sites in equal radii rings lie in different directions. All defined rings either have four or eight sites, and we denote the number of sites in a ring by $\mu_{(i,j)} = 8 - 4\delta_{i,j}$. For expressing the perturbed energy of the vortex in terms of the ring variables, we also define a variable, $c_{\alpha,\alpha'}$, which is the number of bonds between the rings α and α'. For the square lattice, $c_{\alpha,\alpha'} = 8$ between any two neigboring rings and zero otherwise. Also, rings with $j = 1$ always have 4 internal bonds (ring self-interaction, dashed lines in the Fig. 1).

Hexagonal lattice— Using appropriate orthogonal x and y axes (Fig. 2), the

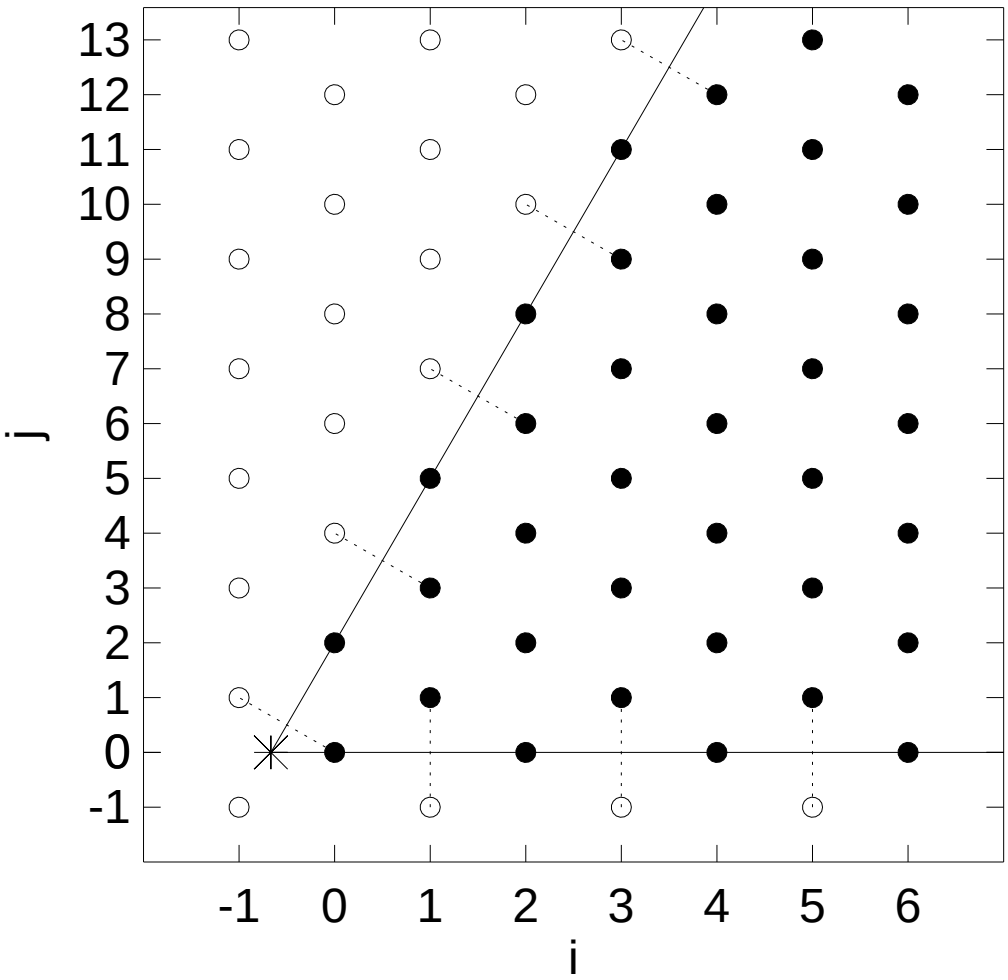

Fig. 3. Ring coordinates (i, j) for triangular lattice, notation as in Fig. 1.

hexagonal lattice sites are located at $(x, y) = (\sqrt{\frac{3}{2}}i, \frac{1}{2}j)a$, where i and j are integers such that $(i + j)$ is even and j is not equal to zero nor equal to any multiple of 3. When $i = j$ (on solid line in Fig. 2), there are six sites at the same radius, all related to each other by 60^o rotations, comprising a ring. When $i \neq j$, there are twelve sites at the same radius, related to each other by 60^o rotations together with reflections through the line $i = j$, and these sites also comprise a ring. So in general a pair $\alpha = (i, j)$ under the above constraints together with $i > 0$, $j > 0$, $i \geq j$ always falls in the first 1/12 of the full circle, and can be used to denote a ring. The number of members of each ring is $\mu_{(i,j)} = 12 - 6\delta_{i,j}$, and the number of bonds between neighboring rings is $c_{\alpha,\alpha'} = \max[\mu_\alpha, \mu_{\alpha'}]$. As in the square lattice, rings with $j = 1$ have 6 internal bonds or self-interactions.

Triangular lattice— Again with orthogonal coordinate axes as in Fig. 3, the triangular lattice sites are located at $(x, y) = (\frac{1}{\sqrt{3}} + \frac{\sqrt{3}}{2}i, \frac{1}{2}j)a$, where i and j are integers such that $(i+j)$ is even. Starting with any site, the other members of its ring are obtained through 120^o rotations together with reflection across

the x-axis. So a pair $\alpha = (i, j)$ under the above constraints together with $i \geq 0$, $j \geq 0$, giving $y \leq \sqrt{3}x$, always falls in the first 1/6 of the full circle, and can be used to denote a ring. The rings with $j = 0$ and those with $j = 3i + 2$ ($y = \sqrt{3}x$) (on solid lines in Fig. 3) have number of sites $\mu_\alpha = 3$ (these rings lie on the boundaries of the first 1/6 of the full circle); all other rings have $\mu_\alpha = 6$. The number of bonds between neighboring rings is $c_{\alpha,\alpha'} = \max[\mu_\alpha, \mu_{\alpha'}]$, except when α or α' is the smallest ring, in which case $c_{\alpha,\alpha'} = 6$. Rings with $j = 1$ *and* rings with $j = 3i$ have 3 internal bonds.

The dynamics— The Hamiltonian is expressed in terms of the ring variables by considering how the rings interact with each other. For example, in the square lattice, a ring $\alpha_{(i,j)}$ interacts with the rings containing the sites $(i \pm 2, j \pm 2)$; there are similar simple neighbor relations for the other lattices. We use n_α to represent the rings that are neighbors of ring α. As noted above, certain rings also have a number n of internal interactions, where $n = 4, 6$, and 3 for square, hexagonal and triangular lattices, respectively. Therefore we define $s_\alpha \equiv 1$ for rings with self-interaction bonds and $s_\alpha \equiv 0$ for those rings without self-interaction bonds. Assuming that sites on a given ring all move either in-phase (FM model) or in-phase for each sublattice, and out-of-phase between sublattices (AFM model, square and hexagonal lattice only), then the Hamiltonian can be rewritten as $H = H_{\rm int} + H_{\rm self}$, where the terms corresponding to interactions between rings, and self-interactions within rings are

$$H_{\rm int} = -\tfrac{1}{2}JS^2 \sum_\alpha \sum_{\alpha,n_\alpha} c_{\alpha,n_\alpha} \Big[\sqrt{1-m_\alpha^2}\sqrt{1-m_{n_\alpha}^2}\cos(\Phi_\alpha^v - \Phi_{n_\alpha}^v) \times \cos(\varphi_\alpha \mp \varphi_{n_\alpha}) + \lambda m_\alpha m_{n_\alpha} \Big], \tag{5}$$

$$H_{\rm self} = -JS^2 \Big\{ \sum_\alpha n\ s_\alpha \Big[(1-m_\alpha^2)\cos 2\tilde{\Phi}_\alpha^v \cos(\varphi_\alpha \mp \varphi_\alpha) + \lambda m_\alpha^2 \Big] - d\ \sum_\alpha \mu_\alpha m_\alpha^2 \Big\}. \tag{6}$$

The Φ_α^v indicate Φ^v at the site defined by $\alpha = (i, j)$; the unperturbed vortex angles at the other sites in the ring are obtained by appropriate rotations. The related angles needed for the ring self-interactions, $\tilde{\Phi}_\alpha^v$, are identical to Φ_α^v except for the triangular lattice rings with $j = 3i$, where $\tilde{\Phi}_\alpha^v \equiv \Phi_\alpha^v + 2\pi/3$. To obtain $H_{\rm self}$ we used the fact that at the lattice sites such as $(i, 1)$ and $(i, -1)$ in the square lattice, for instance, which is a bond within one ring, the values of Φ^v differ in sign while φ values are either equal (FM Ansatz, upper signs) or exactly opposite (AFM Ansatz, lower signs). This argument is modified for the $j = 3i$ triangular lattice rings because the bond involved in this interaction that crosses the x axis is only obtained from a $2\pi/3$ rotation

of the site (i, j).

We obtain the dynamics from the Lagrangian in terms of the ring variables,

$$L = S\sum_{\mathbf{n}} \dot{\phi}_{\mathbf{n}} m_{\mathbf{n}} - H = S\sum_{\alpha} \mu_\alpha \dot{\varphi}_\alpha m_\alpha - H. \tag{7}$$

Euler-Lagrange variation with respect to the ring variables followed by linearization in φ and m leads to equations of motion:

$$S\mu_\alpha \dot{m}_\alpha = -\frac{\partial H}{\partial \varphi_\alpha} \approx -JS^2\Big\{ \sum_{n_\alpha} c_{\alpha,n_\alpha} \cos(\Phi^v_\alpha - \Phi^v_{n_\alpha})\ (\varphi_\alpha \mp \varphi_{n_\alpha}) \\ +2ns_\alpha \cos 2\tilde{\Phi}^v_\alpha\ (\varphi_\alpha \mp \varphi_\alpha)\Big\}, \tag{8}$$

$$S\mu_\alpha \dot{\varphi}_\alpha = \frac{\partial H}{\partial m_\alpha} \approx JS^2\Big\{ \sum_{n_\alpha} c_{\alpha,n_\alpha}\Big[\cos(\Phi^v_\alpha - \Phi^v_{n_\alpha})\ m_\alpha - \lambda m_{n_\alpha}\Big] \\ +2ns_\alpha[\cos 2\tilde{\Phi}^v_\alpha - \lambda]m_\alpha + 2d\ \mu_\alpha m^2_\alpha\Big\}. \tag{9}$$

Only the equation for $\dot{\varphi}_\alpha$ depends on the anisotropies, and it is only that equation (9) that is needed to determine the critical values. As Eq. (9) is the same for FM and AFM models on square and hexagonal lattices, their critical anisotropies are the same. These equations could be re-expressed in a matrix form,

$$\dot{\varphi}_\alpha = \sum_{\alpha'} \mathcal{F}_{\alpha,\alpha'} m_{\alpha'}, \qquad \dot{m}_\alpha = \sum_{\alpha'} \mathcal{M}_{\alpha,\alpha'} \varphi_{\alpha'}. \tag{10}$$

Combining these, it is clear that there exist solutions with $e^{i\omega t}$ time dependence, whose frequencies are given by the square roots of eigenvalues of the product matrix, $\mathcal{F}\cdot\mathcal{M}$. A soft mode therefore will occur if either of these matrices has a zero determinant. Thus, locating where the determinant of matrix $\mathcal{F}$ becomes zero gives the critical anisotropies. This was done by using the secant method to adjust either δ or d in order to zero the determinant, with the other anisotropy parameter held fixed.

Numerical results— We found the critical value of exchange anisotropy δ_c for $d = 0$, and the critical value of single-ion anisotropy d_c for $\delta = 0$, as shown in Tables I–III, for systems using N rings, with radius R. For these lattices with a large number of rings $N \approx 1000$, the critical anisotropies converge to asymptotic limits with precisions of more than 10 digits. These values agree with ones found by applying an iterative relaxation scheme[6,7] to the xyz

Table 1
Square lattice critical anisotropies for N rings.

N	R/a	δ_c	d_c
1	0.7071	0.10557280900	0.10557280900
2	1.5811	0.27446539019	0.38843887462
3	2.1213	0.28643238165	0.42478912981
10	4.5277	0.29656481620	0.46833961304
50	10.700	0.29659060442	0.46896265300
200	22.102	0.29659050706	0.46896252233
800	44.637	0.29659050565	0.46896252034
1200	54.777	0.29659050564	0.46896252032

Table 2
Hexagonal lattice critical anisotropies.

N	R/a	δ_c	d_c
1	1.0	0.0	0.0
2	2.0	0.1307376318148	0.1561467541400
3	2.6457	0.1601968462747	0.2057106580230
5	4.0	0.1656106696448	0.2172002774585
10	6.0828	0.1670109518547	0.2210532692993
50	14.731	0.1670441181236	0.2212091262411
100	21.517	0.1670441181407	0.2212091266671
200	30.610	0.1670441181409	0.2212091266675
400	43.589	0.1670441181409	0.2212091266675

spin components of the vortex, similar to that used to solve Eq. (2). For anisotropy strengths less than these values, Eqs. (10) possess an imaginary frequency eigenmode and the assumed planar vortex structure is unstable towards formation of an out-of-plane vortex. For anisotropy strengths larger than the critical values there are only real frequency eigenmodes and the planar vortex structure is stable. Generally, within the above Ansatz, we can determine exactly the structure and frequency of the mode associated with the vortex instability. For the square lattice model, with anisotropy greater than critical value, the wavefunction described by this Ansatz agrees exactly with that found by numerical diagonalization for planar vortices on small lattices, showing that the Ansatz and critical anisotropies are exact; details will be reported in a future work.

Table 3
Triangular lattice critical anisotropies.

N	R/a	δ_c	d_c
1	0.5773	0.055088817003	0.055088817003
2	1.1547	0.284806466706	0.431315777709
3	1.5275	0.371940464706	0.721444433674
10	3.5119	0.387061576109	0.835881781969
50	8.5049	0.387143616872	0.839118755870
200	17.673	0.387143586629	0.839118869127
800	35.921	0.387143586190	0.839118868570
1200	44.061	0.387143586186	0.839118868564

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