Finite-size Kosterlitz-Thouless transition in a ferromagnetic ultrathin film with fourfold anisotropy: Determination of the exchange coupling, vortex density, anisotropy and magnetic susceptibility

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The renormalization group equations describing a finite 2DXY system with fourfold anisotropy are solved in two steps, in order to study the magnetic transition to paramagnetism in an ultrathin film. First, the equations are linearized near the critical coupling \( K = J/k_B T = 2\pi \). This allows integration constants to be evaluated at the fixed point, and the tuning of the constants to represent a ferromagnetic ultrathin film. An exact solution of the linearized equations confirms that a finite-size Kosterlitz-Thouless (KT) transition can occur in the presence of fourfold anisotropy, but the solution is not quantitatively reliable across the temperature range of the finite-size transition. In the second approach, the fourfold anisotropy is treated as a perturbation. The perturbative treatment provides a quantitative determination of the renormalized exchange coupling, vortex density, and anisotropy throughout the transition. In particular, the coupling has a point of inflection where vortex-antivortex pairs unbind (as opposed to a “universal jump”), and goes to zero asymptotically in the paramagnetic state. These results are used to calculate the magnetic susceptibility as the system moves from one dominated by spin waves to one dominated by a free vortex gas. The presence of anisotropy makes it necessary to include both the susceptibility \( \chi \) due to fluctuations of the magnitude of the magnetization, and \( \chi_\perp \) due to angular fluctuations of the magnetization about an easy axis. Comparison to recent measurements of the magnetic susceptibility of ultrathin Fe/W(001) films suggests that a detailed quantitative analysis of the measurements can provide information on vortex formation, the disappearance of anisotropy, and dissipative processes in the finite-size KT transition of a real system.

I. INTRODUCTION

Nearly half a century after Berezinskii, Kosterlitz and Thouless, and Kosterlitz, introduced the ideas underlying the transition of a spin system between phases supporting excitations of different topologies, there has been a resurgence of interest in topological spin textures in material systems. Topological spin textures of current interest include chiral “bubbles” in perpendicularly magnetized films, vortices bounded within a ferromagnetic microstructure, and skyrmiions in ferromagnetic and antiferromagnetic layers, 3D skyrmions in crystals, as well as the chiral domain wall spin textures in these systems. There is great interest in the phase diagrams and transitions between the topological phases, as well as non-equilibrium dynamics of the topological excitations. These investigations are driven both by fundamental questions in the larger area of topological materials, and by the prospect of potential applications in spintronics.

Within the context of this larger field of work, the simpler, archetypical 2DXY ferromagnetic system originally considered by Kosterlitz and Thouless, can provide insight into basic questions relevant to many of the systems that support topological spin textures. These include the effects of dissipation and relaxation towards equilibrium, finite-size effects, fluctuations near transitions and the influence of perturbations from an ideal symmetry as may be provided by, for example, defects and anisotropies.

Despite these opportunities, there is a relatively small literature reporting experimental studies of 2DXY ferromagnetic films focused on the Kosterlitz-Thouless (KT) transition and vortex dynamics. Experimental work has focused instead on superconductors and layered three dimensional antiferromagnets. For the most part, studies of ferromagnetic films consist of magnetization studies of ferromagnetic films grown on (001)-oriented metallic substrates, where a non-Ising magnetization exponent was reported and only later interpreted as the signature of a finite-size KT transition. Early indications that experimental measurements of the magnetic susceptibility displayed the characteristic form of a KT transition in such films were made quantitative only recently, using Fe/W(001) ultrathin films. This opens the path for further quantitative studies using the magnetic susceptibility, aimed at a better understanding of topological spin textures using this simple realization of a topological phase transition.

The first step is to make contact between the experimental thin film results and theoretical predictions through a quantitative determination of the exchange and anisotropy parameters in a 2DXY system. Kosterlitz and Thouless treated the infinite, isotropic system and introduced the KT transition. Bramwell, Holdsworth and coworkers investigated the finite, isotropic system and identified essential finite-size effects and the finite-size KT transition with separate characteristic temperatures for the formation of vortex-antivortex pairs and for unbinding of the pairs to form a free vortex gas. Jose et al. derived the renormalization group equations for the infinite, anisotropic system with an n-fold, in-plane...
axis. They showed that the system is Ising-like for \( n < 4 \), and has a KT transition when \( n > 4 \). A system with microscopic fourfold anisotropy flows to a second order transition to paramagnetism with non-universal critical exponents that depend upon the strength of the anisotropy. For large anisotropy, there is a cross-over to 2D Ising exponents.

The finite, anisotropic 2DXY model with fourfold anisotropy has not been investigated in detail. Taroni et al. have reported Monte Carlo simulations as a function of the strength of the fourfold anisotropy, and of system size. They find a competition between the finite size effects and anisotropy. For small anisotropy, finite size effects prevail and the value of the effective critical exponent of the magnetization indicates that a finite-size KT transition occurs. As the anisotropy increases, the effective critical exponent crosses over to the 2D Ising value. The present article concentrates instead on solutions of the RG equations to provide a detailed description of the behaviour of an ultrathin ferromagnetic film with fourfold anisotropy. This is accomplished in two stages. In the first stage, the RG equations are expanded to lowest order about the critical coupling, when \( K = J/k_B T = 2/\pi \), and solved exactly. This allows appropriate physical parameters to be set, and makes contact with the previous findings for the finite, isotropic system. These results validate a second approach, where the fourfold anisotropy is treated as a perturbation. This method yields quantitative results for the effective exchange coupling, vortex density and screened fourfold anisotropy as a function of temperature and system size throughout the full temperature range of the finite-size transition. It shows that the coupling has a point of inflection where vortex-antivortex pairs unbind (as opposed to a “universal jump”), and goes to zero asymptotically in the paramagnetic state. The fourfold anisotropy also goes to zero smoothly just above the temperature where the vortex pairs unbind.

These quantities are then used to find two components of the magnetic susceptibility: an improved calculation of the longitudinal susceptibility due to fluctuations in the magnitude of the magnetization and, in addition, the transverse susceptibility due to fluctuations of the magnetization direction about an easy axis in the fourfold system. The appropriate combination of these susceptibilities give an excellent qualitative account of the experimental measurements of Atchison et al. and suggest that a detailed quantitative comparison with the measurements can provide information on vortex formation, the disappearance of anisotropy, and domain processes in the finite-size KT transition of an experimental system.

II. RENORMALIZATION GROUP EQUATIONS UNDER GEOMETRIC SCALING

The 2DXY ferromagnetic spin model with a fourfold anisotropy is represented by the Hamiltonian

\[
H = J \sum_{i,j} [1 - \cos(\theta_i - \theta_j)] + \sum_i [1 - h_4 \cos(4\theta_i)],
\]

where \( J \) is the bare nearest neighbour exchange coupling, \( \theta_i \) is the angle the in-plane spin at lattice site \( i \) makes with a fixed in-plane “easy” magnetic axis, and \( h_4 \) is the microscopic anisotropy energy for a fourfold in-plane anisotropy. The sum over \( i,j \) is over nearest neighbours on a square lattice. The renormalization group (RG) equations under geometric scaling for this model have been derived by Jose et al.\textsuperscript{22,31} using an approximation due to Villain\textsuperscript{13} that is applicable for small anisotropy. After defining \( K = J/k_B T \) as the temperature-normalized exchange coupling, they find:

\[
\frac{dK^{-1}}{d\ell} = 4\pi^2 y_0^2 e^{-\pi^2 K} - 16\pi y_0^2 K^{-2} e^{-4K^{-1}},
\]

\[
\frac{dy_0}{d\ell} = (2 - \pi K)y_0,
\]

\[
\frac{dy_4}{d\ell} = (2 - \frac{4}{\pi} K^{-1})y_4.
\]

These equations are first order in the system variables \( y_0 \) and \( y_4 \) (see below), with corrections in the third order. \( \ell = \ln L \) is the scaling length, where the system size \( L \) is in units of the nearest neighbour lattice constant. The temperature-normalized anisotropy is

\[
y_4 = \frac{h_4}{2k_B T}.
\]

Due to approximations made in the Villain model, the maximum value of \( y_4 = 1 \) corresponds to a clock model with effectively infinite anisotropy.\textsuperscript{22}

The fugacity of a vortex, or the density of vortices, is dependent upon the vortex core energy \( E_c \):

\[
Y = y_0 e^{-\frac{\pi^2 K}{2}} \approx y_0 e^{-\frac{E_c}{\pi k_B T}}.
\]

\( y_0 \) is a small parameter that is renormalized by the flow described by the RG equations. It has been introduced into the Villain model (where \( y_0 = 1 \)), to create the generalized Villain model. In the regions \( K > 2/\pi \), \( y_0 \) is renormalized to zero and is an irrelevant parameter. In the region \( K < 2/\pi \), \( y_0 \) is renormalized to unity and is a relevant parameter. In this way, it can be shown\textsuperscript{22} that the generalized Villain model formally reproduces the results for isotropic 2DXY system as described by the Villain model. By introducing \( y_0 \), it was possible to display a dual symmetry between \( y_0 \) and \( y_4 \) in the
anisotropic 2DXY model. This was instrumental in the original derivation of the RG equations.

While introducing $y_0$ was necessary, it is problematic when relating the system of equations to a physical system. This is because $y_0$ is a phenomenological, and not a physical, parameter. For this reason, it is useful to recast the equations in terms of the fugacity $Y$, and a modified physical, parameter $Y_4$ that maintains the dual relation with $Y$:

$$Y_4 = y_4e^{-2K^{-1}}. \quad (7)$$

A line of fixed points of the RG equations occurs when $y_0 = y_4 = 0$, regardless of the value of $K$. A second line occurs when $y_0 = \pm y_4$; $K = 2/\pi$. Jose et al.\(^{(22)}\) have shown that, in an infinite system, this second line of fixed points mark second-order phase transitions for systems of different microscopic fourfold anisotropy. These transitions have non-universal exponents that depend upon the anisotropy, and, in the limit of strong anisotropy, cross over to 2D Ising transitions.

The RG equations\(^{(2)}\) to\(^{(4)}\) that include fourfold anisotropy will be solved for a finite system in two steps. In Section III, the equations are solved by expansion about the critical coupling $K = 2/\pi$. This is referred to as the “critical approximation” and is routinely used to study critical properties. This step is necessary because the fixed point is the only place where boundary conditions are known precisely. RG equations valid at the fixed points can be used to determine the values of constants of integration, and to tune parameters in the equations to values appropriate for ultrathin films. The solutions confirm that a finite-size KT transition can be preserved in the presence of fourfold anisotropy, and that, because the fixed point is approached only logarithmically in the system size $L$, the renormalization flow does not approach the critical point closely. In Section IV, a second approximation is used. This is referred to as the “perturbative approximation”. It is not as good close to the fixed point (where the flow does not proceed in a finite system), but is valid across the broad temperature range of the finite-size transition where the flow does proceed. This provides a more accurate calculation of the effective coupling, vortex density, anisotropy, and ultimately, the magnetic susceptibility.

III. RENORMALIZED COUPLING NEAR THE CRITICAL COUPLING, IN THE PRESENCE OF FOURFOLD ANISOTROPY

A. Flow equations

This section extends previous work\(^{(13,30)}\) by including the effects of fourfold anisotropy. The coupling in the RG equations is expanded about its value at the fixed point, to lowest order in the parameter $x$:

$$x = \pi K - 2, \quad (8)$$

$$Y = y_0e^{-\frac{\pi + 2}{\sqrt{3}x}}, \quad Y_4 = y_4e^{-\frac{\pi + 2}{\sqrt{3}}} \quad (9)$$

This yields the equations to lowest order in $x$ for small $x$:

$$\frac{dx}{d\ell} = \gamma^2 \left[ -\left( x + \frac{2}{\sqrt{3}} \right)^2 Y^2 + Y_4^2 \right] \rightarrow \gamma^2 \left( -Y^2 + Y_4^2 \right), \quad (10)$$

with $\gamma = 4\pi$,

$$\frac{dY}{d\ell} = -xY \quad (11)$$

$$\frac{dY_4}{d\ell} = \frac{2}{2 + x} xY_4 \rightarrow xY_4 \quad (12)$$

Using eqs.\(^{(11)}\) and \(^{(12)}\) to substitute for one power of $Y$ and $Y_4$, respectively, eq.\(^{(10)}\) can be written as a perfect differential that can be integrated to give

$$x^2(\ell) = \gamma^2 \left[ Y^2(\ell) + Y_4^2(\ell) \right] + C, \quad (13)$$

where $C$ is a constant of integration. Taking the ratio of eqs.\(^{(11)}\) and \(^{(12)}\) gives an expression independent of $x$ that can be integrated to yield

$$Y(\ell)Y_4(\ell) = D \quad (14)$$

where $D$ is a second constant of integration. The known parameter values at the fixed point $x = 0, Y = \pm Y_4$ require that

$$Y|_{x=0} = Y_4|_{x=0} = \sqrt{D}, \quad (15)$$

and indicate that an infinite system with bare anisotropy $\eta_4$ flows to a fixed point where $Y_4 = \sqrt{D}$.

The constant $C$ is determined by substituting eq.\(^{(14)}\) into eq.\(^{(13)}\) and using the known values at the fixed point, to give $C = -2\gamma^2 D$. This value describes a flow line leading to the fixed point. This value of $C$ therefore defines the separatrix between different types of flow leading away from this fixed point (for a system with this anisotropy). The flow for systems near the separatrix is investigated\(^{(13,31)}\) by allowing the integration constant $C$ to deviate from the separatrix by a small amount proportional to the reduced temperature, $t = (T - T_S)/T_S$, where $T_S$ gives flow on the separatrix to the phase transition represented by the fixed point. Then

$$C = -2\gamma^2 D - \alpha t, \quad (16)$$

where\(^{(15,16)}\) $\alpha = (\pi/b)^2$ and $b = 1.846...$. It can be shown\(^{(17)}\) that negative values of $t$ correspond to flow away from the fixed point to a low temperature phase with high anisotropy and vanishing vortex density (fugacity). Positive values of $t$ give flow to a high temperature phase with vanishing anisotropy and high vortex density. This type of behaviour led to the original identification of a topological transition at $t = 0$ in the isotropic system\(^{(18)}\).

Finally, the value of $C$ is used to complete the square in eq.\(^{(13)}\) to yield an equation that describes the flow near the critical coupling.

$$\pm \sqrt{x(\ell)^2 + \alpha t} = \gamma[Y(\ell) - Y_4(\ell)]$$

$$= \gamma[Y(\ell) - \frac{D}{Y(\ell)}] = \gamma[\frac{D}{Y_4(\ell)} - Y_4(\ell)]. \quad (17)$$
B. Tuning to physical parameters of ultrathin films

To follow the renormalization of a specific system with a specific value of fourfold anisotropy it is necessary to follow the flow line with the specific value of \( D \) for this system. This value of \( D \) is determined by the initial conditions \( x(0) \), \( Y(0) \), and \( Y_d(0) \) for the system, where \( \gamma(0) \) indicates that renormalization begins at the microscopic level where \( L = 1 \) and \( L = \ln L = 0 \). To accomplish this, all variables are expressed in terms of the initial value \( x(0) \). In the case of \( Y(0) \) and \( Y_d(0) \), this requires using the definition of \( x \) to substitute for the temperature:

\[
k_B T = \frac{\pi J}{x(0) + 2}.
\]

In addition, the number of free parameters is reduced by introducing the ratio of the microscopic fourfold anisotropy to the bare exchange, \( \lambda = h_4/J \), so that

\[Y_d(0) = \lambda \left( \frac{x(0) + 2}{2\pi} \right) e^{-\frac{x^2}{2\pi^2}}.\]

An approximate expression for the energy of a vortex core is given by

\[Y(0) = e^{-\frac{2\lambda}{\pi}(x(0) + 2)}.\]

When the initial conditions fall on the separatrix \( t = 0 \) for a system with a particular value of the microscopic anisotropy, the flow proceeds to the fixed point and the corresponding value of \( D \) can be identified. According to eq. (17), this occurs when

\[x(0) = \pm \gamma[Y(0) - Y_d(0)].\]

After substituting from eq. (20) and (19), this equation can be solved for \( x_\lambda(0) \) for the value of \( \lambda \) that characterizes the bare system, and the corresponding value of \( D_\lambda \) can be found using eq. (14):

\[D_\lambda = Y_\lambda(0) Y_{d\lambda}(0).\]

The upper and lower roots in eq. (21) correspond to whether or not \( Y_d(0) > Y_{d\lambda}(0) \). The condition \( Y_\lambda(0) = Y_{d\lambda}(0) \) divides these cases, and represents a system with initial conditions at the fixed point at \( x = 0 \). It presumably stays at the fixed point under geometric scaling.

Initial conditions for systems with a wide range of \( \lambda \) are collected in Table I. It turns out that only the positive root of eq. (21) is relevant, as this root produces \( x_\lambda(0) \) up to \( \lambda = 7.3 \). Under the assumptions of the generalized Villain model, the maximum value of \( y_d \) is unity. According to eq. (9), this implies a maximum value of \( \sqrt{D_\lambda} = \exp(-\pi) \), \( D \approx 1.9 \times 10^{-3} \). Therefore, table entries for \( \lambda > 1 \) are certainly not well-founded. This is consistent with the Monte Carlo simulations of Taroni et al. who showed a gradual cross over from finite-size KT behaviour to Ising-like behaviour begins in the range \( 0.1 < \lambda < 0.5 \). Ultrathin metallic films on single-crystal substrates have anisotropies with the order of magnitude \( 10^{-2} > \lambda > 10^{-3} \), giving \( 2 \times 10^{-8} < D < 2 \times 10^{-5} \). This is consistent with KT behaviour.

### Table I

| \( \lambda = h_4/J \) | \( x_\lambda(0) \) | \( Y_\lambda(0) \) | \( Y_{d\lambda}(0) \) | \( D_\lambda \) |
|-----------------|----------------|----------------|----------------|----------------|
| 7.3             | 0              | 0.101          | 0.101          | 1.02 \times 10^{-2} |
| 3.0             | 0.215          | 0.0790         | 0.0620         | 4.90 \times 10^{-4} |
| 1.0             | 0.421          | 0.0625         | 0.0287         | 1.79 \times 10^{-4} |
| 0.1             | 0.595          | 0.0512         | 0.00366        | 1.87 \times 10^{-5} |
| 0.01            | 0.620          | 0.0497         | 3.81 \times 10^{-4} | 1.89 \times 10^{-5} |
| 0.001           | 0.623          | 0.0495         | 3.81 \times 10^{-5} | 1.89 \times 10^{-5} |
| 0               | 0.623          | 0.0495         | 0              | 0              |
Following Bramwell and Holdsworth to this occurs when the anisotropy is screened away. According to fig. (1), due to the unbinding of the vortex-antivortex pairs, and to an endpoint where the vortex density gets very large. The finite-size transition ends when the system moves to an endpoint where the formation of vortex-antivortex pairs starts to be significant. According to eq. (25), occurs at

\[ x \rightarrow 0 \]

when

\[ \omega_{c,0} = \alpha t_0 + 2\gamma^2 D = \left[ \frac{\pi}{2 \ln L} \right]^2 \]  

(27)

Substituting the expression for \( x(\ln L) \) from eq. (25) into eq. (17) leads to quadratic equations for \( Y(\ln L) \) and \( Y_4(\ln L) \). The solutions are most usefully expressed in terms of the scaled variable \( \omega/\omega_{c,0} \):

\[ x = \frac{1}{\ln L} \frac{\pi}{2} \sqrt{\frac{\omega}{\omega_{c,0}}} \tan \left( \frac{\pi}{2} \sqrt{\frac{\omega}{\omega_{c,0}}} \right). \]

(28)

\[ F(\omega/\omega_{c,0}) = \frac{1}{(\gamma \ln L)^2} \frac{(\pi/2)^2 \omega/\omega_{c,0}}{\sin^2 \left[ \frac{\pi}{2} \sqrt{\omega/\omega_{c,0}} \right]} \]

(29)

Then

\[ Y^2 = \frac{1}{2} F(\omega/\omega_{c,0}) + \frac{1}{2} \sqrt{F^2(\omega/\omega_{c,0}) - 4D^2} \]

(30)

\[ Y_4^2 = \frac{1}{2} F(\omega/\omega_{c,0}) - \frac{1}{2} \sqrt{F^2(\omega/\omega_{c,0}) - 4D^2}. \]

(31)

These expressions for \( x, Y \) and \( Y_4 \) are plotted in fig. (1), using scaled variables that exhibit (near) universal curves. Each of the plots has a curve for \( \ln L = 4 \) and for \( \ln L = 9 \). Only in part (c) for \( Y_4 \) is there an indication that the curves do not overlap precisely. For \( D \leq 1.9 \times 10^{-5} \), curves generated using the exact solutions in Appendix A are indistinguishable within the linewidth from the approximate solution shown in fig. (1).

The finite-size transition ends when the system moves to an endpoint where the vortex density gets very large due to the unbinding of the vortex-antivortex pairs, and the anisotropy is screened away. According to fig. (1), this occurs when \( \omega/\omega_{c,0} \rightarrow 4 \), independent of system size. Following Bramwell and Holdsworth, this corresponds to \( x \rightarrow -\infty \), and according to eq. (25), occurs at

\[ \omega_{c,L} = \alpha t_L + 2\gamma^2 D = \left[ \frac{\pi}{\ln L} \right]^2. \]

(32)

In a finite system, the correlation length \( \xi \) is limited by the system size. This implies that the correlation length is maximum near \( \omega_{c,L} \), where the paramagnetic vortex gas forms. In the presence of fourfold anisotropy, eq. (32) can be used to show that it scales as

\[ \xi \sim L \exp \left( \frac{\pi}{\sqrt{\omega}} \right) \]  

for \( \omega > \omega_{c,L} \).

(33)

Since \( D \) is small for thin ferromagnetic films, the difference between this relation and the form found for the isotropic system, will be very difficult to observe.

These results confirm that the finite-size KT transition in ultrathin ferromagnetic films survives the inclusion of fourfold anisotropy, and that a second order transition is
not expected. The effective coupling, correlation length, and transition points are those found previously for the isotropic system, if \( \omega \to \omega + 2 \gamma^2 D \equiv \omega \). The principle new finding is the expression in eq. (31) for \( Y_4 \). These qualitative conclusions are not surprising, given the previous simulations by Taroni et al.\(^{27}\).

However, it is also clear from fig.(1) that there are important quantitative problems with the calculated system properties. The effective exchange coupling goes to zero \( (x = -2) \) before the vortex gas forms at \( \omega_{c,L} (x \to -\infty) \). The condition \( K = 0 \) is marked in fig.(1b) by the circular dots for systems with sizes increasing by integer values of \( \ln L \) from 4 to 9. At larger values of \( \omega < \omega_{c,L} \) the coupling becomes large and antiferromagnetic, a situation that is unphysical. Thus the calculation is certainly not reliable near \( \omega_{c,L} \), and is unlikely to be reliable outside the region near \( \omega = 0 \) where \( x \) is indeed a small expansion parameter. Another example can be seen in part (c) of the figure, where the anisotropy goes to zero with a discontinuity in slope and becomes complex above \( \omega_{c,L} \), rather than approaching zero as a smooth and continuous real function. These are indications that the critical approximation will not be sufficient for a quantitative description of the system across the full width of the peak created by the finite-size transition, including for the calculation of the magnetic susceptibility.

**IV. RENORMALIZED COUPLING ACROSS THE FINITE-SIZE TRANSITION IN THE PRESENCE OF FOURFOLD ANISOTROPY**

**A. Flow equations**

In order to explore the entire range of the finite-size transition, it is better to retain the original RG equations and work directly with a normalized, effective coupling \( \pi K/2 \equiv \delta = 1 + x/2 \) within the range \( \delta > 0 \). Then the RG equations are:

\[
Y = y_0 e^{-\pi \delta}, Y_4 = y_4 e^{-\frac{\pi}{2}}(34)
\]

\[
\frac{d\delta}{d\ell} = \frac{1}{2} \gamma^2 (Y^2 - Y_4^2), \quad (35)
\]

\[
\frac{dY}{d\ell} = -2(\delta - 1)Y, \quad (36)
\]

\[
\frac{dY_4}{d\ell} = \frac{2(\delta - 1)}{\delta} Y_4. \quad (37)
\]

Expressed in these variables, the flow equations have a fixed point at \( \delta = 1 \), \( Y = \pm Y_4 \).

These equations are not amenable to a closed solution. However, an approximation is suggested by the solution in the critical approximation in Section III. Because the renormalization flow approaches the fixed point logarithmically in \( L \) (see eq. (25)), finite systems do not get very close to the fixed point. Rather, they follow a path where \( (Y/Y_4)^2 \gg 1 \) in the pertinent range of reduced temperature. According to eq. (30) and (31), this ratio is smallest in the limit of \( \omega \to 0 \), where it ranges from 430 for \( \ln L = 4 \) to 17 for \( \ln L = 9 \). This suggests neglecting the term in \( Y_4^2 \) in eq. (35) to find a solution for \( \delta(\ell) \) and \( Y(\ell) \), and using these to find \( Y_4(\ell) \) as a perturbation through the ratio of eq. (36) and (37). The relevant equations in this approximation are

\[
\frac{d\delta}{d\ell} = -\frac{1}{2} \gamma^2 \delta^2 Y^2, \quad (38)
\]

\[
\frac{dY}{d\ell} = -2(\delta - 1)Y, \quad (39)
\]

\[
\frac{dY_4}{Y_4} = -\frac{dY}{\delta Y}. \quad (40)
\]

This approach will be termed the “perturbative approximation”. It is important to reiterate that although eq. (38) to (40) do not display the fixed point of the original RG equations, they are a very good approximation in the region some distance from the fixed point where the renomalization flow carries a finite system.

Rearranging eq. (39) as an expression for \( Y \), and substituting for one power of \( \ln \delta \) in eq. (38) in the region where they are both valid. This gives

\[
C = 2\gamma^2 D + \omega - 8 = \omega - 8. \quad (42)
\]

Incorporating this in eq. (41), provides a final expression for the fugacity in the perturbative approximation:

\[
\gamma^2 Y^2 = 8(\ln \delta + \frac{1}{\delta} - 1) + \omega. \quad (43)
\]

**B. Finite-size transition**

Substituting the expression for \( Y^2 \) from eq. (43) into eq. (38), and separating variables gives

\[
-d\ell = \frac{d\delta}{4[\delta^2 \ln \delta + \delta(1 - \delta)] + \frac{1}{2} \omega \delta^2} \quad (44)
\]

Because of the presence of \( \ln \delta \), this integral cannot be performed analytically. However, the denominator is
FIG. 2. The function $f(\delta)$ in the square brackets of eq. (44) is illustrated, along with various approximations to it. The solid line indicates the exact function. The dashed line $1/2(\delta-1)^2$ is the quadratic function used in the critical approximation in Section III. The remaining two lines are piecewise approximating polynomials for the regions $\delta > 3/4$ and $0 < \delta < 3/4$.

well-behaved so long as $\delta > 0$, and various approximations are instructive. These approximations are illustrated in fig. (2), where the term $f(\delta)$ in square brackets in eq. (14) is plotted. The solid line is the exact function, and the purely quadratic function $1/2(\delta-1)^2$ is the critical approximation for small $x$ ($\delta \approx 1$) used in the previous section. The figure makes it clear why this approximation is unreliable near $\delta \approx 0$, where the free vortex gas forms.

A simple and effective representation of $f(\delta)$ is achieved by piecewise polynomials. In the range $\delta \geq 3/4$, the polynomial $1/2(\delta-1)^2$ is used. Then eq. (44) has the form

$$\int_{\delta_i}^{\delta_f} \frac{d\delta}{\delta X(\delta)} = -\ln L,$$

(45)

where $X(\delta) = a + b\delta + c\delta^2$ with $a = 2$, $b = -4 + \omega/2$ and $c = 2$. This integral is given in Appendix B in eq. (B.9). Its qualitative form is more easily seen in the limit $\omega \ll 4$, where the expression simplifies to

$$\delta = 1 + \frac{\sqrt{\omega}}{2\tan[\sqrt{\omega}\ln \left[L \frac{\delta^2}{(1-\delta)^2 + \omega^2}\right]]}. \quad (46)$$

This coupling is closely related to eq. (25) in the same limit, but represents an important qualitative change. While there is only a modest difference near $\delta \approx 1$, the behaviour at $\delta \approx 0$ is very different. The implicit equation for $\delta$ includes a term in $\ln \delta$ that rules out solutions for $\delta \leq 0$. Thus the system approaches the limit of vanishing exchange coupling ($\delta = 0$) asymptotically in $\omega$.

FIG. 3. a) The normalized effective coupling $\delta(\omega)$ is plotted for both the critical and perturbative approximations to the RG equations, for the case $\ln L = 7$ and $D = 1.9 \times 10^{-5}$. For the latter, the solid line is a numerical integration of eq. (44) and the long dash line that almost overlaps with the solid line is the polynomial approximation that gives eq. (B.9) and (B.12). The result in the critical approximation is given by eq. (25). b) The polynomial approximation is used to plot $\delta(\omega)$ for the same value of $D$ and a range of system sizes $L$.

In the range $3/4 \geq \delta > 0$ in fig. (2), $f(\delta)$ is reasonably approximated by the polynomial $3\delta^2 - 1.73\delta + 0.77$. This is again of the form in eq. (44), but the algebra is more complicated. The result is given in Appendix B in eq. (B.13), and is qualitatively similar to eq. (46) with the substitution of a generalized expression for

$$\ln L \to \ln L(\omega) = \ln L + g(\omega), \quad (47)$$

where $g(\omega)$ is a function that arises from matching the two polynomial approximations at $\delta = 3/4$, and is given in eq. (B.13).

These various expressions for $\delta(\ln L)$ are compared in fig. (3a) as a function of $\omega$ for parameters appropriate for ultrathin Fe/W(001) films $^{29,31}$, $D = 1.9 \times 10^{-5}$ and $\ln L = 7$. The solid curve is a numerical integration of the relation in eq. (44). The polynomial approximation to it is given by the long dash line. As can be seen, the
closed expressions in eq. (B.9) and (B.12) reproduce the exact result very well. The two curves nearly overlap; the deviation is greatest at the matching point $\delta = 3/4$ and for large $\omega$ as $\delta \to 0$. The effective exchange coupling approaches $\delta = 0$ asymptotically, as is appropriate for a finite system, and there is no region where the coupling becomes antiferromagnetic.

The result in the critical approximation, given by eq. (25), is also shown as a short dash line in fig. (3a). Bramwell et al.\(^{18}\) have shown, using the critical approximation, that the effective critical exponent of the magnetization, given by

$$\frac{\partial \ln M}{\partial \ln t} \bigg|_{\delta=1} = \frac{\partial \delta (t)}{\partial \ln t} \bigg|_{\delta=1},$$

has a universal value 0.231..., and that this prediction is well supported by experiment.\(^{27}\) Comparing the two approximations, there is a small shift in the region near $\delta = 1$, but the slopes of the curves are very nearly the same.\(^{19}\) For this reason, the value of the effective critical exponent will not be affected. Fig. (3b) shows $\delta (\omega)$ for a range of system sizes.

### C. Width of the finite-size transition

The onset of the formation of vortex-antivortex pairs continues to occur when the value of the coupling is equal to the value at the fixed point ($\delta = 1, x = 0$). In the perturbative approximation, an expression for $\omega_0$ can be found from eq. (B.9), as it applies for $\delta > 3/4$. As $\delta \to 1$, a small angle approximation for the tangent at an angle slightly less than $\pi/2$ gives

$$\frac{\pi}{2\sqrt{\omega_0}} - \frac{1}{4} = \ln[L \left(\frac{4}{\omega_0}\right)^{1/4}].$$

The values of $\omega_0$ are plotted against the system size in fig. (4a), using a solid line. The dashed lines are the results of the critical approximation in eq. (27) and (32). The scaling properties of $\delta$ in the perturbative approximation are revealed by reploting fig. (3b) as a function of the scaled parameter $\omega/\omega_0$ in fig. (4b). A second scaling point occurs at the point of inflection of all of the curves, $\omega/\omega_0 = 4.61... \equiv \beta$, at which point $\delta = 0.395...$ independent of the system size. For the finite system, this point of steepest descent is all that remains of the instantaneous jump in the coupling observed at $T_{KT}$ in the isotropic, infinite system. It is identified as $\omega_L$ and the values are plotted in fig. (4b) using a solid line.

The scaling $\omega_L = \beta \omega_0$ can be used with eq. (49) to determine the scaling of the correlation length

$$\xi \sim L = \left(\frac{\omega}{4\beta e}\right)^{1/3} \exp\left[\frac{\pi \sqrt{7}}{2\sqrt{\omega_0}}\right], \omega \geq \omega_L.$$  

This displays the exponential singularity associated with a KT transition. The constant in the exponential factor has been altered by a factor of $\sqrt{7}/2 = 1.07$ from that found in the critical approximation. The prefactor to the exponential has no singularity and does not affect the scaling behaviour substantially within the range $\omega \geq \omega_L$ where the estimate applies.
D. Screening of the anisotropy

With solutions for $\delta(\omega)$ and $Y(\omega)$ derived under the condition that $Y^2 \gg Y_4^2$, it is now possible to solve for $Y_4(\omega)$ as a perturbation using eq.(40). First, note from eq.(45) that $\gamma Y$ is the square root of the function $h(\delta)$, where

$$h(\delta) = 8(\ln \delta + \frac{1}{\delta} - 1) + \omega. \quad (51)$$

Using this relation, eq.(40) can be written as

$$\frac{dY_4}{Y_4} = -\frac{1}{4}\delta(\ell) \frac{dh[\delta(\ell)]}{d\delta} d\ell. \quad (52)$$

As the variables $Y_4$ and $\ell$ are separated, integration leads to

$$Y_4(ln\, L, \omega) = A \exp \left[ -2 \int_0^{\ln L} \frac{1}{\delta(\ell, \omega)} - 1 \, d\ell \right]. \quad (53)$$

The integration constant $A$ can be determined in the limit $\delta \to 1$, where the critical and perturbative approximations are both valid. Then, from eq.(14),

$$Y_4(ln\, L, \omega_0) = \frac{D}{Y(ln\, L, \omega_0)} = A \exp \left[ -2 \int_0^{\ln L} \frac{1}{\delta(\ell, \omega_0)} - 1 \, d\ell \right], \quad (54)$$

since $\delta = 1$ at $\omega_0$. This notation is understood to mean that $\omega_0$ is a constant in the integral and takes the value appropriate for the system size of the endpoint $L$. According to eq.(43),

$$Y(ln\, L, \omega_0) = \frac{\sqrt{\omega_0}}{\gamma}. \quad (55)$$

Using these results, eq.(53) can be written as

$$Y_4(ln\, L, \omega) = Y_4^0 \exp \left[ -2 \int_0^{\ln L} \frac{d\ell}{\delta(\ell, \omega)} \right], \quad (56)$$

with $Y_4^0 = \frac{\gamma D}{\sqrt{\omega_0}} \exp \left[ 2 \int_0^{\ln L} \frac{d\ell}{\delta(\ell, \omega_0)} \right]. \quad (57)$

The fugacity $Y(\omega)$ from eq.(43) and the anisotropy $Y_4(\omega)$ from eq.(56) are plotted against $\omega/\omega_0$ in fig.(5a) and (5b), respectively. Each fugacity curve shows no clear marker of the finite-size transition, but $\omega_L$ is indicated by the scaling point and the dashed line. The inset shows the same curves with $Y$ for different system sizes normalized by $\gamma/\sqrt{\omega_0}$, still plotted against $\omega/\omega_0$. b) The anisotropy $Y_4$ from eq.(56) for different system sizes is plotted against the scaled parameter $\omega/\omega_0$. The anisotropy goes to zero smoothly and continuously just beyond $\omega_L$. In the insert, $Y_4$ is scaled by $\sqrt{\omega_0}/\gamma D$. $\omega/\omega_0 < \sim 2$, in good agreement with the critical approximation in fig.(1b) in this range.

The anisotropy $Y_4(\omega)$ plotted in fig.(5b) approaches zero smoothly and continuously, where it has the functional form of an exponential of the exponential function. In the inset, the anisotropy is scaled by $\sqrt{\omega_0}/\gamma D$ to allow direct comparison with fig.(1c). The near universal curve for $\omega < \sim 2$ observed in the critical approximation is seen here as well. The anisotropy extends well beyond $\omega_L$, especially for smaller system sizes. This again reflects the fact that smaller systems contain a more truncated distribution of vortex sizes.
V. THE MAGNETIC SUSCEPTIBILITY

A. Contribution due to fluctuations in the scalar magnetization

Archambault et al. have studied the magnetic susceptibility in a finite-size, isotropic 2DXY system, and demonstrated that a broad peak occurs as the spatial range over which the effective coupling varies diverges until it is limited by the system size. Their analysis uses the harmonic 2DXY model (which is almost equivalent to the Villain model) on a \( L \times L \) square lattice of \( N \) spins with no explicit fourfold anisotropy term. The lattice spacing is unity. They find that the vector magnetization has a well-defined scalar magnitude \( M \) in the spin wave region at low temperature. The magnetization rotates “slowly” in the isotropic XY plane, so that in finite spin systems the scalar magnetization is a well-defined quantity on experimental time scales despite the lack of anisotropy. They suggest that when magnetic properties such as the magnetic susceptibility or critical behaviour are measured in an applied field, the field pins the direction of the magnetization so that the relevant fluctuations are in the magnitude of the magnetization.

Defining the scalar magnetization in terms of the in-plane unit spins \( S_i \) at site \( i \),

\[
M = \frac{1}{N} \sum_i \vec{S}_i \cdot \sum_i \vec{S}_i, \tag{58}
\]

they calculate the susceptibility per spin, \( \chi/N \), as the fluctuations in the scalar magnetization:

\[
\frac{\chi T}{N} = \langle M^2 \rangle - \langle M \rangle^2. \tag{59}
\]

They work in units where the Boltzmann constant is unity. In the low temperature spin wave region, the magnetization has the form

\[
\langle M \rangle = \exp \left( -\frac{G(0)}{2K} \right), \tag{60}
\]

where \( G(0) \) is the 2D Green’s function for the square lattice, evaluated at the origin (see Appendix C). The second moment of the scalar magnetization is

\[
\langle M^2 \rangle = \frac{1}{N} \sum_r M^2 \exp \left( \frac{G(r)}{K} \right), \tag{61}
\]

so that

\[
\frac{\chi T}{N} = \frac{1}{N} \sum_r \left[ \exp \left( -\frac{G(0)}{K} \right) \exp \left( \frac{G(r)}{K} \right) \right] - \exp \left( -\frac{G(0)}{K} \right). \tag{62}
\]

This expression is generalized to higher temperature in the range of the finite-size Kosterlitz-Thouless transition by replacing the bare coupling \( K \) by the effective coupling \( K_{ef}(r, \omega) \equiv 2\delta(r, \omega) / \pi \) as determined by the renormalization group equations. A choice must be made for the value \( K_{ef}(r) \) to be used in the final term in eq. (62), as it is outside the sum over \( r \). Because \( G(0) \) is dominated by fluctuations at small wavevector, the choice \( K_{ef}(L) \) is made.

Archambault et al. show that a series expansion of the exponential in \( G(r) \) converges very quickly. When only the first term beyond unity is kept, then the susceptibility can be divided into a part \( \chi_S \) due to spin waves,

\[
\frac{\chi_S T}{N} = \frac{1}{N} \sum_r \frac{\pi^2 G^2(r)}{8 \delta^2(r)} \exp \left( -\frac{\pi G(0)}{2\delta(r)} \right), \tag{63}
\]

and a part \( \chi_V \) due to vortices,

\[
\frac{\chi_V T}{N} = \frac{1}{N} \sum_r \left[ \exp \left( -\frac{\pi G(0)}{2\delta(r)} \right) \right] - \exp \left( -\frac{\pi G(0)}{2\delta(L)} \right). \tag{64}
\]

Because a characteristic experimental thin film system size \( L \) is \( L \approx c^2 \), eqs. (63) and (64) for the susceptibility can be evaluated in the continuum limit. This is outlined in Appendix C.

A comparison of the magnetic susceptibility calculated using \( \delta \) for a system with fourfold anisotropy, determined in both the critical and perturbative approximations in

FIG. 6. The calculated magnetic susceptibility is plotted against \( \omega \) using values of the effective exchange coupling \( \delta(\omega) \) determined in the critical approximation (dashed line) and perturbative approximation (solid line) to the RG equations. The curves are for a system size \( \ln(L) = 7 \) and \( D = 1.9 \times 10^{-3} \). The solid dot indicates the point beyond which the exchange coupling is no longer ferromagnetic in the critical approximation, and the susceptibility calculation diverges.
the previous sections, is shown in fig.(6). The system parameters are \( \ln(L) = 7 \) and \( D = 1.9 \times 10^{-5} \). (A small jump in the solid curve near \( \omega = 0.11 \) occurs at the point where the perturbative approximation for \( \delta \) moves from one piecewise polynomial to another.) Both curves are in qualitative agreement, in that the susceptibility is small in the spin wave region, begins to increase near \( \omega_0 \approx 0.40 \), where vortex pairs begin to form, and has a broad peak over the entire range of the finite-size transition.

There are, however, important quantitative differences. In the critical approximation, the susceptibility has a larger amplitude and reduced full-width at half maximum, and the position of the peak is significantly below \( \omega_{cL} \approx 0.18 \). The curve terminates just past its peak, at the point where \( \delta = 0 \) and eq.(63) and (64) diverge. Although the high temperature tail of the curve is predicted to have an exponential dependence on \( \omega^{-1/2} \) from general arguments leading to eq.(63), it is not possible to demonstrate this characteristic functional dependence of the vortex gas. In contrast, in the perturbative approximation \( \delta \to 0 \) asymptotically so that the system remains ferromagnetic, and the expressions for the susceptibility remain well defined. The position of the curve maximum is very nearly at \( \omega_L \approx 0.16 \) and the form of the high temperature tail can be determined in detail. These differences, and the changes in the values of \( \omega_0 \) and \( \omega_L \), are important for quantitative fitting of experimental data to extract magnetic properties and properties of the vortex distribution.

For these reasons, further analysis of the magnetic susceptibility is restricted to that calculated using the perturbative approximation. The sum of the spin and vortex contributions are shown in fig.(7a) for a range of system sizes. It can be seen that the susceptibility per spin gets narrower and smaller as the system size increases. In part (b) of the figure, the susceptibilities are plotted against \( \omega/\omega_0 \), and scaled by a factor of \( L^{5/16} \). While scaling by \( L^{5/16} \) is not an exact property of the curves, it does allow a convenient comparison of the shape of the susceptibility curve with system size. It is clear that the susceptibility peak becomes narrower in larger system sizes because the high temperature side is cut off more sharply. This is due to the inclusion of larger vortices that more completely destroy the magnetization stabilized by finite-size effects.

It can also be seen that while the peak maximum occurs near \( \omega_L \), where \( \delta(\omega) \) has a point of inflection, the peak position disperses somewhat with size.

The high temperature tail of the susceptibility is expected to scale as \( \chi \sim \xi^{2-\eta} \). According to eq.(50), it will therefore depend on reduced temperature as \( \exp[(2-\eta)/(1.07\pi \omega^{-1/2})] \), independent of system size. This behaviour is illustrated in fig.(7a). The slope of the curves ranges from 6.17 to 6.24 for system sizes of \( \ln(L) = 5 \) to 9, respectively. If the predicted value of \( \eta = 1/4 \) at \( T_{KT} \) is used, then the slope is expected to be 5.88. Because the slopes in fig.(7a) are determined significantly above \( T_{KT} \), the value of \( \eta \) is likely to be less than 1/4 and dependent on the temperature range. If this is indeed the case, then a value of \( \eta = 0.16 \pm 0.01 \) is derived from the slopes.

**B. Contribution due fluctuations in the magnetization direction**

With the inclusion of explicit fourfold anisotropy, the direction of the magnetization may no longer be determined by the applied field, but rather by the magnetic easy axes. It is then important to distinguish between the susceptibility with a small field applied along the magnetization (as in the previous section), and with a field
applied perpendicular to the magnetization. Experimental measurements are expected to include both.

The anisotropy can be represented by an anisotropy field $H_{an}$, and a small oscillating field $H_{opp}$ can be simultaneously parallel and perpendicular to an easy axis. The effective field $H^{eff}$ along which the scalar magnetization is aligned in equilibrium is

$$H^{eff} = H_{opp} + H_{an}. \tag{65}$$

For definiteness, the x-axis is chosen along an easy axis, and the angle $\phi$ of the magnetization is measured from this axis. Applying a field along the y-axis and measuring the magnetic response along the y-axis gives the measured susceptibility tensor component $\chi_{yy}^{app}$.

$$\frac{1}{\chi_{yy}^{app}} = \frac{\partial H_{opp}^{app}}{\partial M_y} = \frac{\partial H^{eff}}{\partial M_y} - \frac{\partial H_{an}^{en}}{\partial M_y}, \tag{66}$$

where the anisotropy field is derived from the anisotropy energy density $E_{an}$.

$$H_{an}^{en} = -\frac{\partial E_{an}(M,\phi)}{\partial M_y}. \tag{67}$$

Recalling that the effective field is by definition parallel to the magnetization in equilibrium, the reciprocal of the effective susceptibility component can be expressed in planar circular components as

$$\frac{\partial H^{eff}}{\partial M_y} = \frac{\partial M}{\partial M_y} \cdot \frac{\partial}{\partial M} H^{eff} \sin \phi = \sin^2 \phi \cdot \frac{\partial H^{eff}}{\partial M}. \tag{68}$$

$\partial H^{eff}/\partial M$ is just the (reciprocal of the) susceptibility due to fluctuations of the scalar magnetization calculated in the previous section for the finite-size KT transition. For consistency of notation with previous sections, this susceptibility will be referred to simply as $\chi$. Combining the results of eqs. (66) to (68), the experimentally measured susceptibility per spin is

$$\frac{\chi_{yy}^{app}}{N} = \frac{\chi/N}{\sin^2 \phi + \frac{\partial E_{an}(M,\phi)}{\partial M^2} \chi/N}. \tag{69}$$

From eq. (1) and (34), the anisotropy energy density calculated for a single spin can be written as

$$E_{an} = 2TY_4[1 - \cos 4\phi]. \tag{70}$$

Using planar circular co-ordinates once again to perform the partial derivatives in eqs. (67) and (66) yields

$$\frac{\chi_{yy}^{app}T}{N} = \frac{\chi T/N}{\sin^2 \phi + \frac{32Y_4}{N^2} \chi^2 T/N \cos^2 \phi \cos 4\phi}. \tag{71}$$

With the oscillating field applied along the y-axis, the low temperature domains with magnetization aligned along the easy axis parallel to the y-axis have $\phi = \pi/2$, and

$$\frac{\chi_{yy}^{app}T}{N} \rightarrow \frac{\chi T}{N} = \frac{\chi || T}{N}. \tag{72}$$

This is the result from the previous section.

For domains aligned along the easy axis parallel to the x-axis, $\phi = 0$ at low temperatures where the anisotropy persists, and the susceptibility is given by

$$\frac{\chi_{yy}^{app}T}{N} < M >^2 \equiv \frac{\chi_L T}{N}. \tag{73}$$

As the temperature increases, $Y_4$ decreases and goes to zero near $\omega_L$. In the absence of anisotropy in eq. (71), the scalar magnetization aligns with the applied field, giving $\phi = \pi/2$. Then the susceptibility is once again given by eq. (72). For a sample with a distribution of both domain types, the susceptibility will be given by a linear combination of the limiting forms $\chi ||$ and $\chi_\perp$.

The transverse susceptibility $\chi_\perp T/N$ is plotted in fig. (5b) for a range of system sizes. The susceptibility is scaled in the same way as the plot of $\chi || T/N$ in fig. (7) to allow comparison. It can be seen that the transverse susceptibility due to angular fluctuations about the easy axis is much larger than the longitudinal susceptibility due to fluctuations of the magnitude of the magnetization. In addition, the low temperature limit (near $\omega = 0$) of $\chi_\perp$ increases much more quickly as the system size is decreased, than does $\chi ||$. However, as the anisotropy is screened near and above $\omega_L$, $\chi_\perp T/N$ goes quickly to zero and the longitudinal susceptibility is dominant. As a result, the high temperature tail of the susceptibility displays the characteristic functional form of a KT transition regardless of the domain orientations at low temperature. This is consistent with an isotropic paramagnetic vortex gas.

This behaviour can be seen in part (b) of the figure. The curve labeled $\chi || T/N$ represents a low temperature domain with the magnetization aligned with the applied field, whereas that with a small admixture of $\chi_\perp$ represents a situation where the field direction is slightly misaligned with the magnetization. These two curves are shown more clearly in the insert to the figure, using a magnified scale. These curves look very much like the experimental curves categorized as Type I in the experimental investigations of Fe/W(001) films by Atchison et al. The third curve, with a large admixture of $\chi_\perp$, represents a situation where there are equal portions of low temperature domains aligned along each of the two easy axes. This curve is similar to those categorized as Type II in the experimental study, including the observed factor of roughly ten in amplitude compared to Type 1 measurements. Although the precise numerical factors for the admixtures in fig. (5b) are not fitted, but rather chosen for illustrative purposes, the similarity between these first-principles calculations and the experimental measurements is very encouraging. These results suggest the possibility that the difference between Type I and Type II measurements in the finite-size KT transition to have do with the low temperature domain distribution in the film and the distinction between $\chi ||$ and $\chi_\perp$ introduced by the fourfold anisotropy.
VI. CONCLUSIONS

The magnetic response of the finite, anisotropic 2DXY model has been investigated using the renormalization group equations, by extending previous work on the infinite, anisotropic model and the finite, isotropic model. This has permitted an improved calculation of the effective exchange coupling, vortex density and anisotropy throughout the $\sim 10K$ range of the finite-size KT transition in a ferromagnetic film with fourfold anisotropy. These results permit in turn a quantitative calculation of the longitudinal susceptibility due to fluctuations in the magnitude of the magnetization, and in addition a first calculation of the transverse susceptibility due to driven oscillations of the magnetization direction about a fourfold easy axis in a 2DXY ferromagnetic film. Combining these responses shows great promise for the quantitative analysis of recent measurements of the susceptibility of Fe/W(001) ultrathin films with fourfold anisotropy, and opens opportunities for a more detailed experimental study of spin wave and vortex excitations in these films.

Solving the RG equations in the critical approximation confirms previous numerical simulations that showed that a finite-size KT transition is preserved so long as the ratio of the microscopic fourfold anisotropy to the bare exchange does not exceed $\lambda \approx 0.5$. They also confirm that the temperature range within which the critical approximation is valid is considerably narrower than the finite-size KT transition itself, so that the coupling, fourfold anisotropy and magnetic susceptibility found in this way provide qualitative insight, but are not quantitatively reliable.

The results of the critical approximation validate solving the RG equations by treating the fourfold anisotropy as a perturbation. This approximation proves to be quantitatively reliable across the full temperature width of the finite-size KT transition. A principle finding is that the coupling no longer exhibits physically unreasonable behaviour (moving from ferromagnetic to antiferromagnetic, and then diverging), but rather approaches zero asymptotically. The universal jump of the coupling seen in an infinite system becomes instead an inflection point of steepest descent where the coupling strength is independent of system size. This point is identified as $\omega_L$, where the unbinding of vortex-antivortex pairs becomes significant. The dependence of $\omega_L$ on system size implies that the correlation length and magnetic susceptibility retain the exponential temperature dependence characteristic of the KT transition.

The new findings for the coupling permit an improved calculation of the magnetic susceptibility, $\chi_{||}$, of the fluctuations in the magnitude of the magnetization. Furthermore, the fourfold anisotropy $Y_4(\ell, \omega)$ calculated in the perturbative approximation no longer exhibits an unphysical cusp, or becomes complex, near $\omega_L$. The improved results for the anisotropy and scalar magnetization are used to find the transverse susceptibility, $\chi_\perp$, for angular fluctuations of the magnetization about an easy axis. Together, these susceptibility components give a more complete account of the magnetic response of the 2DXY model with fourfold anisotropy.

An initial comparison to the measurements of the magnetic susceptibility of Fe/W(001) ultrathin films is very encouraging. Suitable combinations of $\chi_{||}$ and $\chi_\perp$ are in good qualitative agreement with, for instance, fig. (1a) and (4a) in Atchison et al. They confirm previous numerical simulations. In particular, the two distinct shapes of the measured susceptibility termed Type
I and Type II by those authors agree well with the combinations of $\chi_1$ and $\chi_2$ expected for situations where low temperature magnetic domains are aligned along single or multiple fourfold easy axes. Because $\chi_2 \to 0$ near $\omega_1$, both types of measurements exhibit the exponential dependence on temperature characteristic of a finite-size KT transition, indicating an isotropic high temperature phase. The experimental value of $\eta = 0.12 \pm 0.09$ in the temperature range where the exponential dependence is observed is consistent with the present calculations, where $\eta = 0.16 \pm 0.01$. The implication is that careful fitting of Type I measurements can be used to understand details of vortex pair formation, and fitting of Type II measurements can be used to study the evolution of the anisotropy in the finite-size KT transition. This process is underway.

These results open numerous opportunities to study spin wave and vortex properties in an ultrathin ferromagnetic film. The RG treatment of the 2DXY model uses an effective medium approach, where the presence of vortices and bound vortex pairs alters the medium in which spin waves propagate. Therefore, these calculations can be a basis for interpreting the imaginary, dissipative components of the measured susceptibility. For example, $Y_2(\xi, \omega)$ can be used to determine the energy barrier to dissipative domain switching due to an applied field. Also, the variation of the domain wall energy and activation energy for domain wall pinning in the effective medium are determined by a combination of $Y_2(\xi, \omega)$ and $\delta(\xi, \omega)$. These dissipative process can be studied as the system moves from a low temperature system dominated by spin wave excitations to one dominated by vortices. The imaginary component of the susceptibility above the transition may provide information on the dynamics of the vortex gas itself. These investigations are underway.

**APPENDIX A. EXACT SOLUTION IN THE CRITICAL APPROXIMATION**

This appendix gives the exact solution of eq. (23) in terms of the Jacobi elliptic functions. Beginning with

$$-\int d\ell = \int_{x_i}^{x_f} \frac{dx}{\sqrt{x^2 + \alpha t + \alpha t + 4\gamma^2 D}},$$  \hspace{1cm} (A.1)

a standard transformation will show that this is an elliptic integral of the first kind. Since the flow is from a larger positive initial value of $x_i$ to a final value near $x_f = 0$, it is advantageous to write the integral in a form where it is dominated by the endpoint near $x_f = 0$. Then it is insensitive to the initial value and the scaling properties will not depend it, as is expected. This can be accomplished through the co-ordinate transformation $z = 1/x$.

Then

$$-\int d\ell = \int_{1/x_i}^{1/x_f} \frac{-dz}{\sqrt{1 + \alpha tz^2} \sqrt{1 + (\alpha t + 4\gamma^2 D)z^2}}.$$  \hspace{1cm} (A.2)

Letting $\nu = \sqrt{\alpha t + 4\gamma^2 D} z$,

$$\sqrt{\alpha t + 4\gamma^2 D} \int d\ell = \int_{\sqrt{\alpha t + 4\gamma^2 D} \nu}^{\sqrt{\alpha t + 4\gamma^2 D} \nu} \frac{d\nu}{\sqrt{(1 + \nu^2)(1 + (k')^2 \nu^2)}},$$  \hspace{1cm} (A.3)

where $(k')^2 = (\alpha t)(\alpha t + 4\gamma^2 D)$. This is a well-known transformation of the standard form of elliptic integrals of the first kind, obtained by letting $\nu = \tan \phi$. Then

$$\sqrt{\alpha t + 4\gamma^2 D} \int d\ell = \int_{\arctan(\sqrt{\alpha t + 4\gamma^2 D} / x_f)}^{\arctan(\sqrt{\alpha t + 4\gamma^2 D} / x_f)} \frac{d\phi}{\sqrt{1 - k^2 \sin^2 \phi}},$$  \hspace{1cm} (A.4)

where $k^2 = 1 - (k')^2 = (4\gamma^2 D) / (\alpha t + 4\gamma^2 D)$. At this point, as the value of $x_i$ is not important, let $x_i \to \infty$. Recalling that the upper limit of $\ell$ is in units of the lattice constant, the integral becomes

$$\sqrt{\alpha t + 4\gamma^2 D} \ln L = F(\phi_f, k),$$  \hspace{1cm} (A.5)

with $F(\phi_f, k)$ the elliptic integral of the first kind, $\phi_f = \arctan(\sqrt{\alpha t + 4\gamma^2 D} / x_f)$, and $x_f = x(\ln L)$.

The expression in eq. (A.5) can be formally written in a way that isolates $x(\ln L)$ by using the inverse elliptic function $\text{am}(u, k)$. If

$$u = F(\phi_f, k),$$  \hspace{1cm} (A.6)

then the inverse function is defined as

$$\phi_f = \text{am}(u, k).$$  \hspace{1cm} (A.7)

In the present case,

$$x(\ln L) = \frac{\sqrt{\alpha t + 4\gamma^2 D}}{\tan[\text{am}(\sqrt{\alpha t + 4\gamma^2 D} \ln L, k)]}.$$ \hspace{1cm} (A.8)

Although the inverse elliptic integral cannot be solved analytically, some general results can be extracted by employing the Jacobi elliptic functions $\text{sn}(u, k)$, and $\text{cn}(u, k)$, defined as

$$\text{sn}(u, k) = \sin[\text{am}(u, k)] = \sin \phi_f,$$ \hspace{1cm} (A.10)

$$\text{cn}(u, k) = \cos[\text{am}(u, k)] = \cos \phi_f.$$ \hspace{1cm} (A.11)

First note that, for the present problem,

$$uk = (\sqrt{\alpha t + 4\gamma^2 D} \ln L) \sqrt{\frac{4\gamma^2 D}{\alpha t + 4\gamma^2 D}} = \sqrt{4\gamma^2 D} \ln L \equiv B,$$

where $B$ is a constant for a given system of size $L$ and anisotropy $h_4 \to \sqrt{D}$. Then the expression for $x(\ln L)$ can be written as

$$x(\ln L) = \sqrt{\frac{4\gamma^2 D}{k}} \frac{\text{cn}(B/k, k)}{\text{sn}(B/k, k)}.$$ \hspace{1cm} (A.13)
The condition for the beginning of the finite-size transition when \( k = k_0 \), is that \( K = 2/\pi \), or \( x = 0 \). This corresponds to the transcendental equation when \( k = k_0 \),

\[
\text{cn}(B/k_0, k_0) = 0, \text{ or } B/k_0 = \kappa(k_0),
\]  

(A.14)

where \( \kappa(k_0) \) is the complete elliptic integral of the first kind. Similarly, the end of the finite-size transition occurs when \( x \to -\infty \) at \( k = k_L \).

\[
\text{sn}(B/k_L, k_L) = 0, \text{ or } B/k_L = 2\kappa(k_L).
\]  

(A.15)

From this latter result, the form of the correlation length at and above \( t_L \) is

\[
\xi \sim L = \exp \left[ \frac{2\kappa(k_L)}{\sqrt{\alpha t + 4\gamma^2 D}} \right]; \quad t > t_L
\]  

(A.16)

To determine the functional form of \( Y_4(\ln L) \) and \( Y(\ln L) \) in this temperature range, eq. (4.17) can be combined with eq. (A.13) to give

\[
x^2 = \frac{4\gamma^2 D \text{cn}^2(B/k, k)}{k^2 - \text{sn}^2(B/k, k)} = \gamma^2 (\frac{D}{Y_4} - Y_4)^2 - \alpha t.
\]  

(A.17)

Using the property \( \text{cn}^2(u, k) = 1 - \text{sn}^2(u, k) \), and reversing the sign of the square in \( Y_4(\ln L) \),

\[
\frac{4\gamma^2 D}{k^2 \text{sn}^2(B/k, k)} - \frac{4\gamma^2 D}{k^2} = \gamma^2 (\frac{D}{Y_4} + Y_4)^2 - 4\gamma^2 D - \alpha t.
\]  

(A.18)

Recalling the definition of \( k^2 \), the second term on the left side cancels with the last two terms on the right. The third Jacobi elliptic function \( \text{dn}(u, k) = \sqrt{1 - k^2 \text{sn}^2(u, k)} \),

(A.19)

is used to substitute for \( \text{sn}^2(B/k, k) \). Then the square root of both sides can be taken to give

\[
\frac{2\sqrt{D}}{\sqrt{1 - \text{dn}^2(B/k, k)}} = \frac{D}{Y_4} + Y_4.
\]  

(A.20)

This quadratic equation, and the corresponding quadratic equation for \( Y_4 \), can be solved for two physical roots:

\[
\frac{Y_4}{\sqrt{D}} = \sqrt{\frac{1 - \text{dn}(B/k, k)}{1 + \text{dn}(B/k, k)}},
\]  

(A.21)

\[
\frac{Y}{\sqrt{D}} = \sqrt{\frac{1 + \text{dn}(B/k, k)}{1 - \text{dn}(B/k, k)}}.
\]  

(A.22)

### APPENDIX B. POLYNOMIAL APPROXIMATION OF THE INTEGRAL EXPRESSION FOR \( \delta(\ell) \)

The critical approximation uses the quadratic approximation \( f(\delta) = 1/2(\delta - 1)^2 \). When this expression is used in eq. (4.14) of the perturbative approximation, the integral for \( \delta(\ell) \) become

\[
\frac{d\delta}{4[\frac{1}{2}(1 - \delta)^2] + \frac{1}{2}\omega \delta^2} = \frac{d\delta}{X(\delta)} = -d\ell,
\]  

(B.1)

where

\[
X(\delta) = a + b\delta + c\delta^2.
\]  

(B.2)

with \( a = 2, b = -4 \) and \( c = 2 + \frac{\omega}{2} \). This standard integral yields the expression

\[
\delta = 1 + \frac{\sqrt{\omega}}{2\tan[\sqrt{\omega(\ln L)}]},
\]  

(B.3)

For comparison, the solution for the critical approximation, given by eq. (4.25), is

\[
\delta = 1 + \frac{\sqrt{\omega}}{2\tan[\sqrt{\omega(\ln L)}]}.
\]  

(B.4)

A better representation of \( f(\delta) \) is given by two-piecewise polynomials. For \( \delta \geq 3/4 \), the integral expression for \( \delta(\ell) \) in eq. (4.14) is well-approximated by

\[
\frac{d\delta}{4[\frac{1}{2}(1 - \delta)^2] + \frac{1}{2}\omega \delta^2} = -d\ell.
\]  

(B.5)

The integral in \( \delta \) is now of the form

\[
\int_{\delta_i}^{\delta_f} \frac{d\delta}{X(\delta)}
\]  

(B.6)

with \( a = c = 2, \) and \( b = -4 + \omega/2, \) and the discriminant \( q = 4ac - b^2 = \frac{1}{2}\omega(8 - \frac{1}{2}\omega) \). The solution is

\[
\frac{1}{2a} \ln \frac{\delta^2}{\delta_i^2} |_{\delta_i}^{\delta_f} - \frac{b}{a\sqrt{q}} \arctan \left[ \frac{2c\delta + b}{\sqrt{q}} \right] |_{\delta_i}^{\delta_f},
\]  

(B.7)

Evaluating this expression in the limit \( \delta_i \to \infty \) is well-behaved, and gives

\[
\frac{1}{2a} \ln c + \frac{b}{a\sqrt{q}} \frac{\pi}{2}.
\]  

(B.8)

After considerable algebra, the following closed expression for \( \delta_f = \delta(\ell) \) is obtained:

\[
\delta = 1 - \frac{\omega}{8} + \frac{\sqrt{\frac{\omega}{4}(8 - \frac{\omega}{2})}}{4\tan[\frac{\sqrt{\frac{\omega}{4}(8 - \frac{\omega}{2})}}{2 - \frac{\omega}{4}} \ln[L(\frac{\delta^2}{(1 - \delta)^2} + \frac{\omega}{4})]}}.
\]  

(B.9)

In the limit that \( 8\omega \ll 1 \), this reduces to eq. (4.19).
For $\delta \leq 3/4$, the polynomial approximation to $f(\delta)$ in fig. (2) is given by

$$\delta[\delta^2 - 1.73\delta + 0.77] = \delta[(\frac{7}{8} - \delta)^2 + \frac{1}{40}\delta^2]. \quad (B.10)$$

This leads to an integral for $\delta(\ell)$ of the same form as eq. (B.6), but with $a = (7/4)^2, b = -7 + (1/10 + \omega/2), c = 4$ and

$$q = (\frac{1}{10} + \frac{\omega}{2})(14 - (\frac{1}{10} + \frac{\omega}{2})). \quad (B.11)$$

After considerably more algebra, the result is

$$\delta = \frac{6.9 - \frac{\omega}{2}}{8} + \sqrt{\left(\frac{1}{10} + \frac{\omega}{2}\right)(13.9 - \frac{\omega}{2})}$$

$$8\tan\left[\frac{49}{10}\sqrt{\left(\frac{1}{10} + \frac{\omega}{2}\right)(13.9 - \frac{\omega}{2})}\right] \ln L(\omega) + \frac{8}{49} \ln\left(\frac{2}{(1 - \omega^2 + \omega^2)}\right) \quad (B.12)$$

In this expression,

$$\ln L(\omega) = \ln(L) + \frac{1}{4} \ln\left[\frac{9}{1 + 3\omega}\right] - \frac{8}{49} \ln\left[\frac{9}{2(1 + 3\omega) + \frac{1}{2}}\right]$$

$$- \frac{(2 - \frac{\omega}{2})}{\sqrt{\left(\frac{1}{10} + \frac{\omega}{2}\right)(13.9 - \frac{\omega}{2})}} \arctan\left[-\frac{\sqrt{\left(1 + \frac{\omega}{2}\right)(13.9 - \frac{\omega}{2})}}{0.9 - \frac{\omega}{2}}\right]$$

$$+ \frac{16}{49} \frac{(6.9 - \frac{\omega}{2})}{\sqrt{\left(\frac{1}{10} + \frac{\omega}{2}\right)(13.9 - \frac{\omega}{2})}} \arctan\left[-\frac{\sqrt{\left(1 + \frac{\omega}{2}\right)(13.9 - \frac{\omega}{2})}}{0.9 - \frac{\omega}{2}}\right]. \quad (B.13)$$

The complicated expression for $\ln L(\omega)$ arises due to matching the two quadratic approximations at $\delta = 3/4$. Note that both of the arctangent functions return angles in the 2nd quadrant.

**APPENDIX C. EVALUATION OF THE SUSCEPTIBILITY**

In the low temperature, spin wave limit of the harmonic model, Archambault et al.\cite{32} show that the magnetization is of the form

$$\langle M \rangle = \exp\left(-\frac{G(0)}{2K}\right), \quad (C.1)$$

where $G(0)$ is the Green’s function propagator for the square lattice, evaluated at the origin. That is,

$$G(r) = \frac{1}{N} \sum_{q \neq 0} e^{-iq \cdot r}/\epsilon_q, \quad (C.2)$$

evaluated at $r = 0$. In this Fourier sum over wavevectors $q$ in 2D,

$$\epsilon_q = 4 - 2\cos q_x - 2\cos q_y. \quad (C.3)$$

A discrete evaluation gives

$$G(0) = \frac{\ln(bN)}{4\pi}, \quad (C.4)$$

where\cite{32} $b = 1.845...$, as before. Because of this logarithmic dependence on system size, the 2DXY model has intrinsic finite-size effects, with

$$\langle M \rangle = \left(\frac{1}{6N}\right)^{\frac{1}{\nu_r}} \quad (C.5)$$

converging very slowly even for macroscopic $N$.

**A. The vortex susceptibility**

Since the experimental system\cite{32} has $L \approx 7$, the continuum limit of the sum should be a very good approximation. Because $\delta$ is a function of the scalar $\ln L$ in the perturbative approximation, there is no differentiation between the in-plane $x$ and $y$ axes, and the integral can be most easily performed in circular, planar co-ordinates $(\rho, \theta)$. In moving from a square to a circular system while maintaining the number of spins,

$$N = L^2 = \frac{\pi}{4} D^2, \quad (C.6)$$

where $D/2 = L/\sqrt{\pi}$ is the maximum value of $\rho$. The minimum value of $\rho$, corresponding to the bare lattice spacing before geometric scaling, is $1/\sqrt{\pi}$. In the continuum limit, the vortex susceptibility in eq. (64) is

$$\chi_v T \langle N \rangle = \frac{1}{N} \int_0^{2\pi} d\theta \int_{\frac{\rho}{\sqrt{\pi}}}^{\infty} \rho d\rho \exp\left(-\frac{\pi G(0)}{2\delta(\ln 2\rho)}\right)$$

$$- \exp\left(-\frac{\pi G(0)}{2\delta(\ln D)}\right). \quad (C.7)$$

Using the change of variables $\ell = \ln 2\rho$,

$$\chi_v T \langle N \rangle = \frac{\pi}{2N} \int_{\frac{ln D}{\sqrt{\pi}}}^{ln D} d\ell \exp(2\ell) \exp\left(-\frac{\pi G(0)}{2\delta(\ell)}\right)$$

$$- \exp\left(-\frac{\pi G(0)}{2\delta(\ln D)}\right). \quad (C.8)$$

Finally, substituting for $G(0)$ and $N$,

$$\chi_v T \langle N \rangle = \frac{2}{D^2} \int_{\frac{ln D}{\sqrt{\pi}}}^{ln D} d\ell \exp(2\ell) \exp\left(-\frac{\ln(\sqrt{b\pi D}/2)}{4\delta(\ell)}\right)$$

$$- \exp\left(-\frac{\ln(\sqrt{b\pi D}/2)}{4\delta(\ln D)}\right). \quad (C.9)$$

Recall that this is an equation for $\chi_v(\omega)$ because of the implicit temperature dependence of $\delta(\ell, \omega)$. In the low temperature limit, the coupling $\delta$ renormalizes very slowly with size, so that it is essentially constant. Then the vortex susceptibility is identically zero.
B. The spin wave susceptibility

In the continuum limit, the expression for the spin wave susceptibility in eq. (63) can be written as

\[
\chi_s T \frac{\pi^2}{N} = \frac{\pi^2}{8N} \int_{\pi}^{\pi} \frac{d\rho}{\delta^2(\ln 2\rho)} \exp \left( -\frac{\pi G(0)}{2\delta(\ln 2\rho)} \right)
\]

This can be integrated by parts by identifying

\[
dv = \int_{0}^{2\pi} d\theta d\rho G^2(\rho, \theta),
\]

so that

\[
v = \int d\rho \int_{0}^{2\pi} d\theta d\rho G^2(\rho, \theta) \equiv \sum_{r=1}^{N} G^2(r).
\]

In this expression, \(N(\rho) = \pi \rho^2\) limits the sum to the spins within a disc of radius \(\rho\). A numerical summation shows that

\[
\sum_{r=1}^{N} G^2(r) = \frac{1}{N} \sum_{q \neq 0} \left( \frac{1}{eq} \right)^2 = \frac{N}{c},
\]

with \(c = 258.59\). Letting

\[
u = \frac{\pi^2}{8N} \frac{1}{\delta^2(\ln 2\rho)} \exp \left( -\frac{\pi G(0)}{2\delta(\ln 2\rho)} \right),
\]

\[
d\nu = \frac{\pi^2}{8N} \left( \frac{\pi G(0)}{2\delta^3} - 2 \right) \frac{1}{\delta^3} \exp \left( -\frac{\pi G(0)}{2\delta} \right)d\delta.
\]

Collecting these together,

\[
\frac{\chi_s T}{N} = \frac{\pi^2 N(\rho)}{8cN} \frac{1}{\delta^2(\ln 2\rho)} \exp \left( -\frac{\pi G(0)}{2\delta(\ln 2\rho)} \right)
\]

According to Archambault et al.,

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39 The validity of this approximation is clear a posteriori from the fact that in a finite-size transition both $x$ and $\alpha t$ are not simultaneously small in comparison to $D$; that is, the system does not get close to the critical point.
40 The notation $t_L$ is used here, rather than $t_C$ as used in ref. 18, to reinforce that the separation of $t_0$ and $t_L$ is a finite-size effect.
41 The value of $D$ is relevant only in that it is small enough for the approximation in eq. (38) to (40) to hold, since $D$ and $\alpha t$ occur only in the combination $\omega$.
42 Compare eq. (46) and (25).
43 Here, the symbol $\beta$ does not represent a critical exponent.
44 This section continues to use the same units as ref. 32. For SI units factors of the saturation magnetization $M_S$ and magnetic permeability $\mu_0$ must be included.
45 Again, in this section units with $k_B = 1$ and lattice constants of unit length are used.