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VORTICES IN THE CLASSICAL TWO-DIMENSIONAL ANISOTROPIC HEISENBERG MODEL

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ABSTRACT

The structure and dynamics of vortex spin configurations is considered for a two-dimensional classical Heisenberg model with easy-plane anisotropy. Using both approximate analytic methods based on a continuum description and direct numerical simulations on a discrete lattice, two types of static vortices (planar and out-of-plane) are identified. Planar (out-of-plane) vortices are stable below (above) a critical anisotropy. The structure of moving vortices is calculated approximately in a continuum limit. Vortex-vortex interactions are investigated numerically. A phenomenology for dynamic structure factors is developed based on a dilute gas of mobile vortices above the Kosterlitz-Thouless transition. This yields a central peak scattering whose form is compared with the results of a large-scale Monte Carlo-Molecular Dynamics simulation.

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INTRODUCTION

Two-dimensional magnetism has attracted heightened interest in the last few years because of: (i) the availability of much improved quasi-two-dimensional ferromagnetic and antiferromagnetic materials, including layered structures, magnetically-intercalated graphite and, most recently, Cu-based high-temperature superconductors ; (ii) rapidly increasing information on spin dynamics from inelastic neutron scattering, particularly at low frequencies and long wavelength ; and (iii) advances in numerical simulation capability on large lattices which can guide and test modeling of nonlinear structures and their dynamics.

Classical, anisotropic Heisenberg models are important for a large class of magnetic systems. Easy-plane (XY) symmetry is especially interesting because it admits vortex-like spin configurations and the possibility of a topological vortex-antivortex unbinding transition, as proposed by Kosterlitz and Thouless. The advances outlined above now allow us to seriously probe the dynamics associated with such a transition in real magnetic materials.

In this paper we consider the classical Heisenberg ferromagnet in two spatial dimensions and with easy-plane exchange anisotropy,

$$H = -J \sum_{(m,n)} (S_m^x S_n^x + S_m^y S_n^y + \lambda S_m^z S_n^z), \quad (I.1)$$

where J is a coupling constant and the summation is taken over the nearest neighbour square lattice sites. Our principal concern is to understand in detail the structure and dynamics of vortex spin configurations and their signatures in dynamic structure factors, $S(\vec{q}, \omega)$, as measured by inelastic neutron scattering.

In section (II) we review existing literature and show that continuum theory yields two types of static vortices: viz. "planar" (in which spin components are confined to

the XY plane) and "out-of-plane" (in which there is a pulse-shaped S_x distribution accompanying the vortex shape in S_x and S_y). In section III we study these vortices via a direct numerical simulation of the discrete system (I.1), using Landau dynamics and Landau-Gilbert damping. We find a critical λ (λ_c): for $\lambda > \lambda_c$ ($< \lambda_c$) the out-of-plane (planar) vortex is stable. By studying square, triangular and hexagonal lattices, we conjecture that λ_c increases with lattice coordination number. The exact numerical studies also support the qualitative vortex energy dependence on λ obtained in a perturbative continuum calculation.

Turning to vortex dynamics, an approximate analytic calculation in the continuum limit (section IV) suggests that asymmetric out-of-plane spin components develop for both vortex types, with the asymmetry occurring about the direction of vortex motion. This is confirmed by numerical studies on the lattice. Preliminary numerical studies of vortex-vortex interactions (Section V) reveal that the anisotropy parameter λ is also important for the competition between the attractive/repulsive force existing between a vortex-(anti)vortex pair and the pinning forces due to the discreteness of the lattice. For $\lambda > \lambda_c$, the forces between the pair easily dominate the pinning forces of the lattice but, for $\lambda < \lambda_c$, unless the pair separation is rather small, or λ is very near λ_c , the pinning forces of the lattice are predominant.

Finally, in section (VI) we consider a phenomenology based on a dilute gas of mobile vortices to calculate $S(\vec{q}, \omega)$ above the Kosterlitz-Thouless transition temperature. This suggests an intrinsic "central peak" component (i.e. spectral weight at $\omega \sim 0$). In particular we note that the correlation of S_x spin components ($S_{xx}(\vec{q}, \omega)$) is very sensitive to the vortex shape. Thus the velocity-dependence of the shape noted above has a direct influence. We compare our predictions with numerical simulations on a 100×100 square lattice using a combined Monte Carlo-molecular dynamics technique, and discuss the

relevance of dynamic vortices to the observed central peak structure.

Section VII contains a summary and concluding remarks.

II. Equations of motion and static solutions

The Hamiltonian given by (I.1) reduces to the well known isotropic Heisenberg and XY models for $\lambda = 1$ and 0, respectively. The classical spin vector, $S_n = \{S_n^x, S_n^y, S_n^z\}$, can be specified by two angles of rotation θ_n and Φ_n

$$S_n = S [\cos \theta_n \cos \Phi_n, \cos \theta_n \sin \Phi_n, \sin \theta_n]. \quad (II.1)$$

In a continuum approximation, Hamiltonian (I.1) can be written as

$$H = \frac{JS^2}{2} \int d^2r \left[[1 - \delta(1 - m^2)] \frac{(\nabla m)^2}{(1 - m^2)} + (1 - m^2)(\nabla \Phi)^2 + 4\delta m^2 \right] \quad (II.2)$$

where

$$\delta = 1 - \lambda \quad (II.3)$$

and $m = \sin \theta$. The variables m and Φ constitute a pair of canonically conjugate variables, which means that

$$\dot{\Phi} = \frac{\partial H}{\partial m}, \quad \dot{m} = -\frac{\partial H}{\partial \Phi}, \quad (II.4)$$

where H is the Hamiltonian density in (II.2).

The equations of motion obeyed by m and Φ can be obtained by using (II.4)

$$\frac{1}{JS} \frac{\partial m}{\partial t} = (1 - m^2) \Delta \Phi - 2m \nabla m \cdot \nabla \Phi \quad (II.5a)$$

$$\frac{1}{JS} \frac{\partial \Phi}{\partial t} = -\frac{\Delta m}{(1 - m^2)} + \delta \Delta m + m[4\delta - (\nabla \Phi)^2] - \frac{m}{(1 - m^2)^2} (\nabla m)^2. \quad (II.5b)$$

These equations agree with the ones obtained by Takeno and Homma¹ after an appropriate change of variables is performed. Those authors presented a general theory to

derive a classical spin system from the original quantum Hamiltonian for generalised Heisenberg models. However, only the one dimensional case was studied in detail.

We are mainly interested in studying nonlinear excitations in this two-dimensional system and we will start our discussion by considering static solutions to eqs.(II.5). Later in this paper, we will study the small distortions suffered by these objects due to their motion.

It can readily be seen that the set of expressions

$$m_p = 0 \quad (II.6a)$$

$$\Phi_p = q \tan^{-1} \left(\frac{y}{x} \right), q = \pm 1, \pm 2, \dots \quad (II.6b)$$

corresponds to a particular solution to eqs. (II.5). The condition expressed by (II.6a) requires $S_n^z = 0$, in which case Hamiltonian (I.1) reduces to the planar model and (II.6b) describes the usual vortex of the Kosterlitz-Thouless theory. Hereafter, we will refer to this solution as a planar vortex. The energy of a single planar vortex,

$$E_p = \pi J S^2 \ln(R_s/r_a), \quad (II.7)$$

has the well known logarithmic dependence on R_s , the size of the system. r_a is a constant of the order of a lattice spacing and corresponds to a cut-off for the radial integration.

Another particular static solution of eqs.(II.5) (for the two-dimensional case) has been obtained by other authors^{2,3} by noticing that taking (II.6b) for Φ one can obtain a static solution of (II.5a) by requiring m to be a function of the radial polar coordinate, i.e., $m = m(r)$. The explicit expression for $m(r)$ should be obtained from the remaining equation (II.5b). Analytical (instantons) solutions for the isotropic Heisenberg model

($\lambda = 1$) have been obtained by Belavin and Polyakov⁴ and also by Trimper⁵. Unfortunately, eq. (II.5b) cannot be solved analytically for general λ . However, for the conditions

$$m(r) = \begin{cases} \pm S, & \text{for } r = 0, \\ 0, & \text{for } r = \infty \end{cases} \quad (II.8)$$

asymptotic solutions can be given:

$$m_{out} = \begin{cases} pS \left(1 - \frac{a^2 r^2}{2r_v^2}\right), & \text{for } r \rightarrow 0 \\ cS \left(\frac{r_v}{r}\right)^{1/2} \exp(r/r_v), & \text{for } r \rightarrow \infty \end{cases} \quad (II.9a)$$

$$(II.9b)$$

where $p = \pm 1$ depending on the sign of m_{out} at the origin, and r_v is defined by

$$r_v = \frac{1}{2} \sqrt{\frac{\lambda}{1-\lambda}} \quad (II.10)$$

and is interpreted as being the "radius" of the vortex core. a and c are constants that can be fitted by matching the asymptotic solutions (II.9). [If we match at $r = r_v$ we obtain $a = \pi e/5$ and $c = 3\pi/10$]. Eqs.(II.9) were obtained for $q = \pm 1$ since this is the case of main interest. We will refer to this solution as the "out-of-plane" vortex.

The asymptotic solutions obtained by Takeno and Homma³ are of similar form although there are some differences between their expressions and ours, partially because they included an external field applied along the z -axis. Hikami and Tsuneto² arrived at slightly different vortex-like solutions because they neglected the contribution of a term $\delta \sin \theta \cos \theta \nabla \theta$ in their continuum Hamiltonian. Expressions identical to those in eqs.(II.9) were obtained by Nikiforov and Sonin⁶ for the Hamiltonian

$$H = -\tilde{J} \sum_{m,n} [S_m^x S_n^x + S_m^y S_n^y + S_m^z S_n^z] - \tilde{\delta} \tilde{J} \sum_m (S_m^z)^2, \quad (II.11)$$

i.e., with local instead of exchange anisotropy. For this model, the vortex radius is $\tilde{r}_v = 1/\sqrt{2\tilde{\delta}}$. Hamiltonians (I.1) and (II.11) become equivalent for $\lambda \rightarrow 1$, $\tilde{\delta} \rightarrow 0$ and, in

this limit, r_v and \bar{r}_v diverge. The difference between these two models becomes greater in the opposite limit, $\lambda \rightarrow 0$ and $\bar{\delta} \rightarrow 1$. In particular, we have $r_v = 0$ and $\bar{r}_v = 1/\sqrt{2}$ for $\lambda = 0$ and $\delta = 1$, respectively.

If we insert $\lambda = 0$ into (II.5), we do not obtain a decaying solution as in eq.(II.9b). Thus the only meaningful static vortex solution is the planar one — which is in agreement with our vortex radius definition [$r_v(\lambda = 0) = 0$]. It should be stressed that r_v is less than one lattice spacing for an appreciable range of λ ($r_v < 1$ for $\lambda \leq 0.8$). This leads us to consider whether the discrete nature of the lattice introduces effects that invalidate a continuum approach. Numerical simulation studies on a discrete lattice have been performed (section III) in order to obtain information about the behavior of vortex solutions as functions of λ . In particular, we have determined the ranges of λ for which the static planar and out-of-plane vortex solutions are stable.

The energy of a single out-of-plane vortex, E_{out} , is calculated in the Appendix. We find that, for $\lambda \ll 0.8$, E_{out} is higher than E_p and increases with λ . This λ dependence of E_{out} is in agreement with our simulation results, presented in section III.

III. Single-Vortex Simulations

In order to clarify the behavior of the two static vortex solutions identified in section II as functions of the anisotropy λ and the location of the vortex center on the lattice, simulation studies were performed on a 40×40 square lattice. The discrete equations of motion used in the numerical simulations are

$$\vec{S}_i = \vec{S}_i \times \vec{F}_i - \epsilon \vec{S}_i \times (\vec{S}_i \times \vec{F}_i), \quad (III.1)$$

$$\vec{F}_i = J \sum_{ij} (S_j^x \hat{x} + S_j^y \hat{y} + \lambda S_j^z \hat{z}). \quad (III.2)$$

The sum on j only runs over the nearest neighbors of i . The parameter ϵ is the strength of a Landau-Gilbert damping, which was included for testing vortex stability and for damping out spin waves generated from non-ideal initial conditions. Neumann or free boundary conditions were used for simulating single vortices. The equations for the xyz spin components were integrated using a fourth order Runge-Kutta scheme with a time step of 0.04 (in time unit \hbar/JS). Conservation of energy and spin length (to about 1 part in 10^5) served as checks of numerical accuracy.

The first set of simulations used a single planar vortex in a unit cell of the lattice as the initial condition. The equations of motion were integrated for several hundred time units, using a damping strength $\epsilon = 0.1$, for $0 \leq \lambda \leq 1$. We observe that for all $\lambda < (0.72 \pm 0.01)$ the planar vortex remains as the stable configuration; a bell-shaped out-of-plane spin component centered at the vortex center is seen to develop only for $\lambda > 0.72$. Figures [1(a,b)] show the stationary long-time configuration obtained for $\lambda = 0.80, 0.90$. They agree rather well with the asymptotic expressions given by (II.9). The radius of the area where m differs appreciably from zero — ~ 3 lattice sites for $\lambda = 0.80$ [$r_v(\lambda = 0.80) = 1$] and ~ 4.5 for 0.90 [$r_v(\lambda = 0.90) = 1.5$] — increases with λ in the same way that r_v does. Fitting eqs.(II.9) to the resulting out-of-plane structure we obtain $a = 0.39\pi$ and $c = 0.65\pi$ which are close to the values we find when matching the asymptotic solutions at $r = r_v$ (section II).

The stability of the planar vortex for small λ ($\lambda \ll 0.80$) can be established analytically by considering small perturbations, (Φ_i, m_i) , to the static vortex (Φ_p, m_p) . We use the ansatz

$$\Phi = \Phi_p + \Phi_i ; m = m_p + m_i \quad (III.3)$$

in the Hamiltonian (II.2) obtaining

$$\delta H = H(\Phi, m) - H(\Phi_p, m_p) = \pi JS^2 \int_{r_a}^{R_s} r dr \{ \lambda (\nabla m_1)^2 + m_1^2 \left(4\delta - \frac{1}{r^2} \right) + (\nabla \Phi_i)^2 \}. \quad (III.4)$$

The first and third terms in the integrand of (III.4) are always positive but the second term is positive only if $r > r_0$, where $r_0 = 1/\sqrt{2\delta}$. For $0 \leq \lambda \leq 3/4$, r_0 is inside the vortex core and integration from $r = r_a$ to R_s always yields $\delta H > 0$, i.e., the planar vortex is stable here.

Another set of single-vortex simulations was performed using a static *out-of-plane* vortex as initial condition. The initial configuration was specified by eq.(II.6b) for Φ and (A-3) for m (only the first two coefficients, α_1 and α_2 were taken). We find that the initial out-of-plane vortex relaxes to a planar one for $\lambda \leq 0.72$. Again, only for $\lambda > 0.72$, does the out-of-plane vortex stay as a stable configuration.

Complementary simulations were performed using triangular and hexagonal lattices. Similar behaviors were found: viz., there is a "critical" value λ_c above which the static out-of-plane vortex solution is the stable configuration; for $\lambda < \lambda_c$, the stable configuration is the planar vortex. The static limit of the equations of motion derived for these non-square lattices leads to asymptotic solutions identical to the ones given by eqs. (II.6) and (II.9) — this result could be expected since these equations are obtained in a continuum theory. Our numerical simulations give $\lambda_c \approx 0.62$ for the triangular lattice and $\lambda_c \approx 0.86$ for the hexagonal lattice. This suggests that the static planar vortex stability decreases with increasing coordination number.

A fourth set of single-vortex simulations using an out-of plane vortex as initial condition but considering different positions of the vortex-center was performed to give insight into how the energy of this vortex depends on the location of its center—relevant

for vortex dynamics. Three positions in a square lattice were considered: (a) at the center of a square formed by four neighbors; (b) at the center of a line joining two nearest neighbors; and (c) at one of the lattice sites. For small λ , the total energy is different for each of the cases, being lowest for case (a) and highest for (c). As λ increases the differences between these energies decrease, and for $\lambda \approx 0.7$ all these energies are close to each other. The λ -dependence of the energy can also be extracted from these simulations and agrees qualitatively with the behavior predicted by the calculations given in the Appendix.

IV. Single Moving Vortices

Above the Kosterlitz-Thouless transition temperature the system is in a disordered phase characterized by unbound vortices interacting with each other. Equations of motion for single moving vortices were derived by Huber⁷ and Nikiforov and Sonin⁶. In this section we will study the distortion suffered by the static vortex solutions given in Section III due to their motion. The procedure chosen is the one adopted in ref.[6] for Hamiltonian (II.11). We will also be interested in obtaining the energy of these moving vortices as a function of their velocity v .

We use an ansatz similar to the one given by eqs.(III.2) writing

$$\Phi = \Phi_0 + \Phi_1, \quad m = m_0 + m_1, \quad (IV.1)$$

where (Φ_0, m_0) denote the static solutions given by eqs.(II.6) and (II.9) and (Φ_1, m_1) are the distortions (assumed small) due to the vortex motion. Inserting (IV.1) into (II.5), we obtain

$$-\frac{\vec{v} \cdot \vec{\nabla} \Phi_0}{JS} = \frac{\Delta m_1}{(1 - m_0^2)} - \delta \Delta m_1 + \left[\frac{2m_0 \Delta m_0}{(1 - m_0^2)^2} - [4\delta - (\nabla \Phi_0)^2] + \frac{4m_0^2 (\nabla m_0)^2}{(1 - m_0^2)^3} \right]$$

$$+ \frac{(\nabla m_0)^2}{(1 - m_0^2)^2} \left] m_1 + 2m_0 \nabla \Phi_0 \cdot \nabla \Phi_1 + \frac{2m_0}{(1 - m_0^2)^2} \nabla m_0 \cdot \nabla m_1, \quad (IV.2a)$$

$$-\frac{\vec{v} \cdot \nabla m_0}{JS} = (1 - m_0^2) \Delta \Phi_1 - 2m_0 \nabla m_0 \cdot \nabla m_1 - 2m_0 \nabla m_1 \cdot \nabla \Phi_0 \quad (IV.2b)$$

after linearizing in m_1, Φ_1 and also in v . In eqs.(IV.2) we have used

$$\frac{\partial \Phi}{\partial t} = -\vec{v} \cdot \nabla \Phi, \quad \frac{\partial m}{\partial t} = -\vec{v} \cdot \nabla m \quad (IV.3)$$

for a steady state vortex motion with velocity \vec{v} .

It is clear from eqs.(II.5) that a moving vortex cannot be confined to the XY-plane. The moving structure must develop some out-of-plane spin component. Using eqs. (II.6) into (IV.2) we have

$$-\frac{\vec{v} \cdot \hat{e}_\Phi}{JSr} = -\lambda \Delta m_{1P} + m_{1P} \left[4\delta - \frac{1}{r^2} \right] \quad (IV.4a)$$

$$0 = \Delta \Phi_{1P}, \quad (IV.4b)$$

where \hat{e}_Φ is the unit vector for the Φ -coordinate. A particular solution of eq. (IV.4b) is given by $\Phi_{1P} = 0$ and the asymptotic behavior of m_{1P} can be obtained from eq. (IV.4a)

$$m_{1P} = \begin{cases} \frac{\vec{v} \cdot \hat{e}_\Phi}{JS} r = -\frac{v}{JS} r \sin(\phi - \alpha), & r \rightarrow 0 \\ -\frac{\vec{v} \cdot \hat{e}_\Phi}{4\delta JS} \frac{1}{r} = \frac{v}{4\delta JS} \frac{\sin(\phi - \alpha)}{r}, & r \rightarrow \infty \end{cases} \quad (IV.5a)$$

$$(IV.5b)$$

where α is the angle between the direction of the velocity \vec{v} and the x-axis. We notice that the moving vortex does not possess the circular symmetry exhibited by the static vortex since it depends on the polar coordinate Φ and is symmetric about the \vec{v} -direction. This symmetry could be expected if we want the profile to define a distinct direction for the velocity and is confirmed by our vortex-antivortex pair simulation (section V). We note that eq. (IV.4a) can be solved exactly in the $\lambda = 0$ limit leading to

$$m_{1P} = \frac{v}{JS} \frac{r \sin(\phi - \alpha)}{4\delta r^2 - 1}, \quad (IV.6)$$

which has the asymptotic behavior predicted by eqs. (IV.5). The above equation is an exact solution to (IV.4a) only for $\delta = 1$ but we can expect that it is a good approximation for $\delta \approx 1$. Eq. (IV.6) has a singularity (and changes sign) at $r^* = (1/4\delta)^{1/2}$ which for $\delta \approx 1$ is less than a lattice constant away from the vortex center. It is reasonable to assume that keeping the neglected nonlinear terms would suppress the divergence and force m_{1P} to cross zero near r^* to justify the assumption of small spatial derivatives. The reliability of our asymptotic $r \rightarrow 0$ solution is questionable but this will not affect our calculations because this solution will be used only in a negligible regime [$0 < r < r_v$, and $r_v < 1$ for $\lambda < 0.8$]. Also, we will be interested in correlation functions for small q only (section VI), where the asymptotic $r \rightarrow \infty$ solution is sufficient. Nevertheless, this question will be properly handled using a numerical simulation (section V).

Asymptotic expressions for the small corrections to the *out-of-plane* vortex due to its motion can be determined by substituting eqs. (II.6b) and (II.9) into eqs. (IV.2).

We obtain

$$m_{1OP} = -\frac{a^2 v}{3JS} r^3 \sin(\phi - \alpha) \quad (IV.7a)$$

$$\Phi_{1OP} = p \frac{v}{JS} r \cos(\phi - \alpha) \quad (VI.7b)$$

for $r \rightarrow 0$ and

$$m_{1OP} = \frac{v}{4\delta JS} \frac{\sin(\phi - \alpha)}{r}, \quad (IV.7c)$$

$$\Phi_{1OP} = \frac{cvr_v^{3/2}}{JS} \frac{e^{-r/r_v} \cos(\phi - \alpha)}{r^{1/2}} \quad (IV.7d)$$

for $r \rightarrow \infty$. As before, the out-of-plane component m is asymmetric about the direction of motion but now this asymmetry is a small correction to be added to the core shape given by eq. (II.9a), while in the previous case, eq. (IV.5) corresponds to the predicted shape for the out-of-plane component of a vortex moving with small velocities. The

