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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,

$$H = -J \sum_{(m,n)} (S^x_m S^x_n + S^y_m S^y_n + \lambda S^z_m S^z_n), \qquad (I.1)$$

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_z 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 occuring 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_z spin components ($S_{zz}(\vec{q},\omega)$) 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

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

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

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

where

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

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

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

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)

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

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

These equations agree with the ones obtained by Takeno and Homma[1] 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

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

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

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,

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

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