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## ASPECTS OF CLASSICAL EXCITATIONS IN TWO-DIMENSIONAL MAGNETIC SYSTEMS

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### ABSTRACT

Dynamic properties of classical spin excitations in models for quasi-two-dimensional materials are described. Included are spin configurations for vortex and vortex-like excitations from continuum limit equations of motion, together with comments about their stability. Models studied are the anisotropic ferro- and antiferromagnets, and an easy-plane ferromagnet with 4-fold in-plane symmetry breaking. Results from numerical simulations of the dynamic structure function  $S^{\alpha\alpha}(\vec{k}, \omega)$  are shown and compared with phenomenological theories.

### 1. INTRODUCTION

#### 1.1 Low-Dimensional Models

Understanding the dynamic properties of excitations in magnetic models is a challenging and exciting enterprise, and from the theoretical viewpoint, analysis for systems in one or two dimensions can in many cases be carried out with more details than would be possible in three dimensions. From the experimentalists' perspective, there exist a wide variety of real materials which can be quite accurately described in terms of strong spin-spin interactions acting only along one or two of the crystal axes, thereby imposing a lower effective dimensionality.<sup>1-4</sup> For these materials, at temperatures above a transition temperature where the full three-dimensional interactions become relevant, the spin degrees of freedom can be described by a Hamiltonian with a lower effective dimensionality  $d < 3$ . Then the material is called "quasi-d-dimensional."

#### 1.2 Quasi-One-Dimensional Magnets and Solitons

Historically, the most well known quasi-one-dimensional magnetic materials<sup>1</sup> are the spin-1 easy-plane ferromagnet  $\text{CsNiF}_3$ , and the spin-5/2 easy-plane antiferromagnet  $(\text{CH}_3)_4\text{NMnCl}_3$ , known as TMMC. These and

other materials have been thoroughly studied experimentally and analyzed in terms of nearest neighbor classical spin chain Hamiltonians possessing soliton modes.<sup>5-7</sup> The analysis of equilibrium and dynamic properties for such models is a mature and still active field (for example, see the article by D.P. Landau herein). Usually the interactions are anisotropic, perhaps with an Ising (easy-axis) or planar (easy-plane) symmetry. Presence of Ising anisotropy will lead to the possibility of static soliton-like excitations, involving rotations of the spin field through  $\pi$ , connecting regions having the two energetically equivalent alignments along the Ising axis. With planar anisotropy, there is the possibility of static soliton-like excitations involving in-plane rotations through  $2\pi$  for ferromagnets or  $\pi$  for antiferromagnets. These typically will be better defined if there is a small applied magnetic field within the easy plane, breaking the symmetry in that plane.

Quite generally, with reasonable continuum limit assumptions, magnetic Hamiltonians in one dimension map approximately onto the one-dimensional sine-Gordon (sG) equation.<sup>5-7</sup> Therefore, phenomenological descriptions involve an "ideal gas" of sG solitons moving within (and perturbing) a background field of small amplitude spin waves.<sup>8</sup> Within this sG description, contributions to the dynamic structure function,  $S^{\alpha\alpha}(\vec{k}, \omega)$ , as measured in inelastic neutron scattering, are expected due to solitons (peaks at  $\omega = 0$ ), spin waves (peaks at finite  $\omega$ ) and multi-spinwave processes (which can also contribute to  $\omega = 0$  intensity). In terms of gross features this description is probably valid for many materials. However, there are known difficulties. Corrections are expected due to deviations from sG dynamics.<sup>9,10</sup> The mapping onto the sG equation is approximate---spins tilt out of the easy plane for "planar" systems, an effect not fully accounted for in the sG equation. Also there could be quantum effects, and higher order soliton-spinwave interaction effects. However, if we consider quantum effects to be small (expected for  $S \geq 1$ ), then numerical spin dynamics integrations are a productive way to avoid the sine-Gordon mappings and at the same time obtain accurate results for  $S^{\alpha\alpha}(\vec{k}, \omega)$ . Conveniently, at this time available computing power is appropriate for performing these spin dynamics calculations for

reasonably large systems in two dimensions (100 x 100) as well as for one-dimension.

### 1.3 Quasi-Two-Dimensional Magnets and Vortices

Understanding of the statics and dynamics of quasi-two-dimensional magnets is not so thoroughly developed. However, the variety of challenging models and materials and possibilities for topological excitations is much greater than for one dimension. Some typical examples of quasi-two-dimensional magnets include<sup>2</sup>  $\text{BaCo}_2(\text{AsO}_4)_2$ , an XY ferromagnet,  $\text{BaNi}(\text{PO}_4)_2$ , an XY antiferromagnet, and  $\text{Rb}_2\text{CrCl}_4$ , an XY ferromagnet with in-plane symmetry-breaking.<sup>3</sup> Also, there is the nearly isotropic Heisenberg ferromagnet  $\text{K}_2\text{CuF}_4$ , and the XY ferromagnet  $\text{CoCl}_2$  intercalated in graphite.<sup>4</sup> Among the available materials spin-S values range from 1/2 to 2, with interesting exchange and crystal field anisotropies on triangular, honeycomb and square lattices.

For two-dimensional models, in addition to spin waves and solitons (or now, "domain walls"), there can also be "vortex" excitations involving a singular point in the spin field, which has a nonzero curl. All of these can be expected to make contributions to  $S^{\alpha\alpha}(\vec{k}, \omega)$ . The gross features should be well described by a phenomenological model, in terms of an ideal gas of walls, vortices, and spinwaves weakly interacting. For a simple model such as one with planar anisotropy but no applied fields (e.g., XY model), only vortices and spinwaves are present, and an ideal gas phenomenology has been developed by Mertens et al.<sup>11</sup> to describe the dynamics above the vortex unbinding<sup>12</sup> transition temperature (Kosterlitz-Thouless transition temperature  $T_{KT}$ ). Static vortices are responsible for zero frequency intensity in  $S^{\alpha\alpha}(\vec{k}, \omega)$ , that is, a central peak. The phenomenology can be compared with numerical simulations of  $S^{\alpha\alpha}(\vec{k}, \omega)$ , however, an exact separation of central peak intensity into vortex and multi spinwave components is difficult. The numerical simulations suggest that corrections to the ideal gas phenomenology are needed, especially for the out-of-plane spin component correlations. However, for  $T > T_{KT}$ , the phenomenology assumes unperturbed vortices moving with a Boltzmann distribution of velocities, but at present it is not completely understood how strongly the vortex-spinwave or vortex-vortex interactions modify the

correlations, nor are the dispersion relation and velocity distribution of moving vortices actually known.

Ideally, one should consider the linearized perturbation about a vortex solution to obtain the vortex-spinwave scattering properties and vortex stability with respect to perturbations. In practice, this leads to a 4th order eigenvalue problem for which the bound states are not known. Instead, numerical integrations can be used, starting from a vortex initial condition, to indicate the dynamic stability. Similarly, numerical simulations have been used to indicate properties for traveling vortices. Any information about dynamic properties of isolated vortices obtained in this way will be helpful in improving phenomenological models, and offer guidance for other models involving more complex anisotropic interactions.

There are three primary goals for this paper: i) to review the classical mechanics description of spin waves, domain walls, and especially, vortices in several magnetic models; ii) to present some results relating to stability of vortices (as derived from continuum theory) when placed on a lattice; iii) to present results for  $S^{\alpha\alpha}(\vec{k},\omega)$  for these models, in the light of available phenomenology theories. The models considered are the anisotropic Heisenberg model (ferro and antiferromagnetic exchange), and a model for  $\text{Rb}_2\text{CrCl}_4$ , which is an easy-plane ferromagnet with 4-fold in-plane symmetry breaking anisotropy. The intention is to give an idea of the remarkable assortment of excitations in the various models, concentrating on their spin configurations, stability and dispersion properties, and the implications of these for their contributions to dynamic space-time correlation functions.

## 2. ANISOTROPIC HEISENBERG MODELS: XY TO ISOTROPIC FERROMAGNETS

For spin variables  $\vec{S}_i$ , where  $i$  labels a lattice site in two dimensions, a simple Hamiltonian is

$$H = - J \sum_{(i,j)} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z) , \quad (1)$$

where the sum is over nearest neighbor pairs  $(i,j)$  and the parameter  $\lambda$  measures the degree of exchange anisotropy. Here we consider only planar

anisotropy, with  $0 \leq \lambda \leq 1$ . As  $\lambda$  ranges from 0 to 1 the model changes smoothly from the XY model to the isotropic Heisenberg model.

The discrete equations of motion resulting from (1), obtained most easily through classical Poisson brackets, are

$$\frac{d\vec{S}_i}{dt} = \vec{S}_i \times \vec{F}_i \quad (2)$$

$$\vec{F}_i = J \sum_{(i,j)} (S_j^x \hat{x} + S_j^y \hat{y} + \lambda S_j^z \hat{z}). \quad (3)$$

The sum in (3) involves only the nearest neighbors of site  $i$ . This form of the differential equations is used for numerical integrations due to its simplicity and lack of trigonometric function evaluations. Using these equations, and assuming small dynamic fluctuations from a state with  $\vec{S} = S(1,0,0)$  leads to the spinwave dispersion relation for an excitation with wavevector  $(k_x, k_y)$ ,

$$(\omega/2JS)^2 = (2-c)(2-\lambda c); \quad c = \cos k_x a + \cos k_y a \quad (4)$$

where  $a$  is the lattice spacing. This dispersion has an interesting feature. For small wavevectors, we have

$$\omega \approx JS(ka)^2 \quad \text{for} \quad \lambda = 1 \text{ (Heisenberg)} \quad (5)$$

$$\omega \approx 2JS(ka) \quad \text{for} \quad \lambda = 0 \text{ (XY)}. \quad (6)$$

This point is that for intermediate values of  $\lambda$ , there is a mixture of linear and quadratic wavevector dependencies, with a crossover from linear to quadratic  $k$ -dependence at adequately large  $k$ .

### 2.1 A Continuum Limit

A crossover effect for the continuum solutions as  $\lambda$  ranges from 0 to 1 might also be expected, especially since a planar vortex is not expected for the isotropic model. The continuum limit<sup>13</sup> can be studied by using spin variables in terms of the spherical coordinates:

$$\vec{S}(\vec{r}) = S(\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta). \quad (7)$$

In a lowest order continuum limit derived from a square lattice, the coupled equations of motion for the  $\theta(\vec{r})$  and  $\phi(\vec{r})$  fields are

$$\dot{\theta} = JS (\cos\theta \nabla^2\phi - 2\sin\theta \vec{\nabla}\phi \cdot \vec{\nabla}\theta) \quad (8)$$

$$\begin{aligned} \dot{\phi}\cos\theta = & -JS \{ [|\nabla\theta|^2 + |\nabla\phi|^2 - 4 + \lambda (4 - |\nabla\theta|^2)] \sin\theta \cos\theta \\ & + (\sin^2\theta + \lambda \cos^2\theta) \nabla^2\theta \} \end{aligned} \quad (9)$$

These equations have two types of soliton-like vortex solutions<sup>14</sup> (or, an "instanton" when  $\lambda = 1$ ).

## 2.2 Planar Vortices

Angle  $\phi$  measures the spin angle projected on the easy xy plane, while angle  $\theta$  measures the tilting of the spins up out of the xy plane. In the XY limit one expects a static planar solution, with  $\theta = 0$  and  $\dot{\theta} = \dot{\phi} = 0$ . This exactly satisfies (9) and then (8) simplifies to the Laplace equation, for any value of  $\lambda$ :

$$\nabla^2\phi = 0 \quad (10)$$

This has a simple "planar vortex" (or antivortex) solution

$$\begin{aligned} \phi &= \pm \tan^{-1}(y/x) + \phi_0 \\ \theta &= 0 \end{aligned} \quad (11)$$

where  $\phi_0$  is an arbitrary constant. The energy depends logarithmically on the system size  $R$  and a short distance cut-off  $r_a$ ,

$$E_{pl} = \pi JS^2 \ln(R/r_a). \quad (12)$$

This is the well known vortex (antivortex) of the XY model, but it also exists for nonzero  $\lambda$ . The vortex is singular at its center; the spin direction is undefined there. The antivortex differs from the vortex only in the sense of the circulation in the spin field.

In a system in thermodynamic equilibrium, it is expected that these are created as vortex-antivortex pairs, where the cost in energy depends logarithmically on the separation of their centers. In the Kosterlitz-Thouless transition for the XY model, it becomes possible to lower the free energy by creating pairs when the creation energy  $\Delta U_{\text{pair}}$  can be counterbalanced by the entropy term  $T\Delta S_{\text{pair}}$ . This occurs at a transition temperature<sup>15</sup>  $T_{KT} \approx 0.8 JS^2$  for  $\lambda=0$ . It is useful to see whether

