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AUTHOR(S): G. M. Wysin
A. R. Bishop
J. Oitmaa

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Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Easy-Plane Antiferromagnetic Kinks

G. M. Wysin^{*}, A. R. Bishop and J. Oitmaa[†]

Center for Nonlinear Studies and Theoretical Division
Los Alamos National Laboratory
Los Alamos, NM 87545, USA

Abstract

We present an Ansatz for kink excitations in an easy-plane classical antiferromagnetic chain with a magnetic field in the easy plane. The Ansatz includes the in-plane (XY) and out-of-plane (YZ) kinks as belonging to one continuously connected energy dispersion curve. Results of the Ansatz calculation are compared with a numerical simulation and with a linear stability analysis for YZ kinks.

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I. Introduction

Recently there has been considerable experimental and theoretical interest in the low temperature properties of 1-D easy-plane antiferromagnets, such as spin-5/2 TMMC [1-5]. In particular, in the presence of an applied field in the easy plane, the spin Hamiltonian is taken to be [2]:

$$H = \sum_n [J\vec{S}_n \cdot \vec{S}_{n+1} + A(S_n^z)^2 - g\mu_B B_x S_n^x] \quad , \quad (1)$$

where J and A are positive, g and μ_B are the Lande g factor and the Bohr magneton respectively. Neutron scattering experiments [3] on TMMC have shown an interesting crossover behavior of the in-plane and out-of-plane spin wave dispersion as the field is increased. At a "crossover" or "critical" field B_c , there is a switching of the hard axis from the dipole anisotropy axis to the applied field axis [4].

This switching is also expected to affect the relative energies of the nonlinear soliton, or "kink" excitations. These kink excitations have been described in a continuum limit by an approximate mapping to the sine-Gordon (sG) equation, and are rotations of the spins through π around either the z -axis (XY kinks) or the field axis (YZ kinks) [5]. At the critical field the stationary XY and YZ kinks have equal energies, as do the in-plane and out-of-plane spin waves at the zone boundaries.

Previously XY and YZ kinks have been considered to be distinct solutions of the equations of motion, belonging to separate energy dispersion branches. Alternatively, here we review an Ansatz which includes the two as distinct limits of a single continuously connected dispersion curve [6,7]. Also we compare with results of a numerical integration of the discrete equations of motion, as well as presenting a linear stability analysis for YZ kinks.

II. Continuum sG Limit

Properties of continuum limit XY and YZ kinks have been given elsewhere [2,5]. Here we present a slightly different analysis for the YZ kinks.

In order to look for the YZ kink solution, it is best to use spherical polar coordinates where the field direction is the polar axis, in order to take the symmetry of the desired solution properly into account. So if the spins are parameterized in terms of x-polar spherical coordinates, then the equation of motion governing the YZ kinks has been shown to be [6,7]:

$$2(\phi_{zz} - \frac{1}{4}\phi_{tt}) = \alpha \sin 2\phi \quad ; \quad \alpha \equiv 2A/J \quad . \quad (2)$$

This is a sG equation with $c = 2$, with the small angles θ, ϕ given in terms of Θ and Φ . The YZ kink solution is

$$\theta = \frac{1}{2}\pi \quad ; \quad \phi = \pm 2 \tan \exp \zeta \quad ; \quad (3a)$$

$$\zeta \equiv \gamma\sqrt{\alpha}(z - vt) \quad ; \quad \gamma \equiv (1 - \frac{1}{4}v^2)^{-1/2} \quad . \quad (3b)$$

The YZ kink energy is approximately $E_{YZ} = 2\gamma\sqrt{\alpha} JS^2$. Note that the field determines the width and energy of XY kinks, whereas the anisotropy does so for YZ kinks. Both XY and YZ sG kink energies increase monotonically with velocity.

A linear stability analysis [6,7] of YZ sG kinks leads to the following decoupled eigenvalue equation for $\tilde{\theta}$ (where one has assumed small perturbations $\tilde{\theta}$, $\tilde{\phi}$, $\tilde{\theta}$ and $\tilde{\phi}$ from the sG profile, and $\beta \equiv g\mu_B B_x / JS$):

$$-\gamma^2 \tilde{\theta}_{\zeta\zeta} + (1 - 2 \operatorname{sech}^2 \zeta - \frac{\beta\gamma v}{2\sqrt{\alpha}} \operatorname{sech} \zeta) \tilde{\theta} = \lambda \tilde{\theta} \quad (4)$$

An instability is indicated by a bound state solution to this Schrodinger problem with an imaginary eigenfrequency, where the eigenfrequency ω is related to the eigenvalue by $\omega^2 = 4\alpha(\lambda - 1) + \beta^2$. For $v = 0$, there is a $\operatorname{sech} \zeta$ bound state, with zero eigenvalue. This corresponds to $\omega^2 = \beta^2 - 4\alpha$, however, and can have $\omega^2 < 0$ if $\beta < \beta_c \equiv 2\sqrt{\alpha}$, indicating a structural instability for fields less than the critical field.

For nonzero v , the potential for $\tilde{\theta}$ is modified. The effect of nonzero v can be taken into account through first order perturbation theory. A short

calculation shows that the stability criterion becomes $v/c > (4\alpha - \beta^2)/(\pi\beta\sqrt{\alpha})$.

III. The Variational Ansatz

The XY and YZ kinks can be connected through a variational Ansatz, made in terms of the xyz spin components in a manner similar to that done for the easy-plane ferromagnetic kinks [8]. Further motivation and details of this Ansatz calculation are given elsewhere [6,7]. Essentially, a kink profile can be represented by a trajectory of the spin vectors on the unit sphere, plus information about the distribution of the spin vectors along the trajectory. Specifically, there will be one trajectory for each sublattice, and we assume that the A sublattice spin trajectory lies in a plane at an angle θ_A to the easy plane, while the β sublattice spin trajectory lies in a plane at angle θ_B . The distribution of the spins along these trajectories is taken to be sG-like; the angular position within these tilted planes being $\phi = 4 \tan^{-1} \exp[(z - vt)/w]$, where w is a width variational parameter. Thus the Ansatz involves three parameters: θ_A , θ_B and w , and for given α and β , these are determined by locating the extrema of the Lagrangian.

IV. Results and Discussion

In Figure 1 we show $E(v)$ as obtained from this Ansatz using $\alpha = 0.04$ as appropriate for TMMC and for fields $\beta = 0.3, 0.4$ and 0.5 ($\beta_c = 0.4$), and for $0 < \theta_A < \pi$. We also show results from numerical integration of the equations of motion on a discrete lattice, using Ansatz profiles as initial conditions, and time averaging the kinks in their own reference frame to remove spin wave contributions to the energy (a result of having only an approximate traveling wave initial condition).

It is found from these numerical studies that the stable kink profile given by the Ansatz can correspond to either an XY or YZ kink, depending on θ_A ; the XY and YZ branches are continuously connected. Also, for $\beta < \beta_c$, where static YZ kinks are unstable, there can be stable moving YZ kinks, consistent with the linear stability analysis results.

From the numerical integrations, XY kinks are stable above and below the critical field, for $\alpha = 0.04$, $0.08 \leq \beta \leq 0.6$ and $|v/c| < 1$. Even for $\beta > \beta_c$, they show no tendency to decay to lower energy YZ kinks. Whether they can be viewed as slightly perturbed sG kinks is doubtful, especially for $\beta > \beta_c$. The situation is the same as in the ferromagnet above the critical field, where the

kinks are dynamically stable but move in a direction opposite to that predicted by sG theory [9]. We conclude the XY kinks are not adequately described by sG theory, and that there is no structural instability at the critical field.

For small velocities $v \ll c$, a two parameter Ansatz for YZ kinks (putting $\theta_A + \theta_B = \pi$) reproduces the velocity dependence of the energy given by sG theory. sG theory adequately describes the YZ branch. Static YZ kinks are stable only if $\beta > \beta_c$. Dynamic YZ kinks require a minimum applied field to be stable, where this minimum field decreases with increasing velocity.

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- * Permanent address: LASSP, Cornell University, Ithaca, NY
14853
- † Permanent address: The University of New South Wales,
P.O. Box 1, Kensington, NSW 2033, Australia.
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Figure Caption

Figure 1 Kink energy vs. velocity as obtained from the Ansatz calculation (drawn curves) and the numerical integration (data points) with $\alpha = 0.04$ and $\beta = 0.3$ (dashed, \square), $\beta = \beta_c = 0.4$ (solid, Δ) and $\beta = 0.5$ (dotted, \times). There are distinguishable XY and YZ segments of each dispersion curve, although at $\beta = \beta_c$ the XY segment is degenerate (a point at $v = 0$).

