

KINK-ANTI-KINK SCATTERING FOR AN EASY-PLANE  
ONE-DIMENSIONAL ANTIFERROMAGNET

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A numerical investigation of collisions of kink-antikink ( $K\bar{K}$ ) pairs in an easy-plane classical antiferromagnetic chain is presented here, for the case of an applied field within the easy plane. An approximate kink profile as obtained from an earlier Ansatz was used as the initial condition for numerical integration on a discrete lattice. As a function of the applied magnetic field and kink Ansatz parameter  $\theta_A$ , which measures the tilt of the spins out of the easy plane, we have found distinct parameter regimes resulting in transmission, reflection, and annihilation of the  $K\bar{K}$  pair. Results for both the in-plane ( $XY$ ) and out-of-plane ( $YZ$ ) kinks are summarized, and comparison is made to  $K\bar{K}$  scattering in the easy-plane ferromagnet. Similarly to the case of the easy-plane ferromagnet  $\text{CsNiF}_3$ , it is found that these results imply difficulties in the interpretation of experiments on tetramethyl ammonium manganese trichloride (TMMC) in terms of classical soliton theory. For example, for fields from approximately 20 kG to 80 kG, the low velocity  $XY$  collisions generally result in pair annihilation to spin waves. For fields less than 20 kG, however, the low velocity  $K\bar{K}$   $XY$  pair transmits. Experimental results for TMMC are discussed in the light of these features.

## 1. Introduction: Solitons in One-Dimensional Magnets

There are a number of unresolved questions concerning the theoretical description of magnetic chain materials. In particular we consider those expected to support sine-Gordon soliton-like excitations (which we refer to here as kinks). Typical examples of these materials include easy-plane ferromagnets (EPF's)  $\text{CsNiF}_3$  (spin  $S=1$ ),  $(\text{C}_6\text{H}_{11}\text{NH}_3)\text{CuBr}_3$ , or "CHAB" ( $S=1/2$ ), and the easy-plane antiferromagnet (EPA)  $(\text{CD}_3)_4\text{NMnCl}_3$ , or TMMC ( $S=5/2$ ). In the presence of an applied magnetic field within the easy plane, a classical mechanics description using a nearest neighbour Hamiltonian with either exchange or single ion anisotropy leads approximately to a sine-Gordon (SG) equation of motion for the in-plane spin angle  $\phi$  (Mikeska 1978,1980). This approximate equation of motion requires the assumptions of slow spatial variations in the spin fields or sublattice spin fields for the antiferromagnet (continuum limit), small out-of-easy-plane spin motions, and of course supposes classical mechanics to be adequate. Generally, for small enough applied field and velocity, the predicted kink width will be small enough so that the continuum limit is a good approximation. While the out-of-plane angle  $\theta$  may be fairly small for some slowly moving kinks, it nevertheless introduces terms in the equations of motion ignored in the SG treatment (beyond terms linear in  $\theta$ ), which typically cannot be neglected for an accurate evaluation of the energy-velocity dispersion  $E(v)$ .

In fact, these terms can have a dramatic effect, changing the solutions qualitatively from the SG limit. For sufficiently large applied fields, greater than an anisotropy-dependent critical field  $B_c$  (Kumar 1982, see also Harada *et al* 1981), the easy-plane SG-like kinks acquire a negative effective mass, regardless of whether the

continuum limit was used (Wysin *et al* 1984,1986). For ferromagnetic (FM) coupling, these high field kinks have been shown numerically to *reflect* as a result of  $K\bar{K}$  collisions-- i.e., collisions of kink-antikink pairs of equal but opposite velocity (Wysin *et al* 1984). At fields below the critical field, the FM  $K\bar{K}$  pair can either transmit (at the smallest fields), annihilate (at intermediate fields), or reflect (at fields just below the critical field). This behaviour would not be expected in a pure SG system--only transmission of the pair could occur if the SG dynamics were a good approximation to the dynamics of the original complete Hamiltonian. These discrepancies can be traced to the terms in the magnetic Hamiltonian which are inherently nonlinear degrees of freedom (the out-of-plane angles), but which are approximated as linear degrees of freedom to obtain the SG Hamiltonian. The SG equation of motion includes the nonlinear dynamics of the in-plane angle  $\phi$ , while the out-of-plane angle  $\theta$  essentially becomes its conjugate momentum (i.e.  $\theta \approx \dot{\phi}$ ), an approximation which generally turns out to be inaccurate. These additional terms in the Hamiltonian also introduce non-zero frequency bound states in the kink spectrum which are responsible for the non-SG behaviour of the collisions.

A study of  $K\bar{K}$  collisions in the easy-plane *antiferromagnet* (AFM) is a natural extension of the above mentioned work. This study is similar to that for the ferromagnet, with the major difference being the need to include kinks from both the *XY* and *YZ* regimes of the dispersion curve (Flüggen and Mikeska 1983). We accomplished this in a natural way by employing a previously introduced Ansatz for the kink profile as the initial condition for the numerical integration (Wysin 1985, Wysin *et al* 1986). The kink changes smoothly from *XY* in character (small  $z$  spin components) to

$YZ$  (small  $x$  spin components) as a variational parameter  $\theta_A$  (which measures the out-of-plane tipping) is increased from zero towards  $\pi/2$ .

A priori it was not at all clear whether AFM  $K\bar{K}$  scattering should resemble  $K\bar{K}$  scattering in the FM. Here we have found some similarities between the two, especially if one considers the  $XY$  AFM kinks to be analogous to the FM kinks. The analogy can also be seen in the dispersion relationships for isolated kinks. Here we will review the single kink dispersions and present new  $K\bar{K}$  data to support this view.

We do not address the question of the adequacy of a classical mechanics vs. quantum mechanics description. Certainly if these spin systems are strongly quantum mechanical, then it is necessary to re-examine what is meant by "quantum soliton", especially since the SG soliton limit for these one-dimensional (1D) magnets is derived from a classical analysis. Quantum aspects of this problem have been partially studied in other articles. For example, Mikeska and Frahm (1986) and Fogedby *et al* (1986) have applied the semiclassical approximation for large spin to the quantum specific heat problem. The quantum corrections to the classical SG model have been reviewed by Johnson and Wright (1985); they point out that for the specific heat of CHAB and TMMC these corrections increase the disagreement of the theory with experiment, and cause only a slight improvement in the description of the specific heat of  $\text{CsNiF}_3$ . On the other hand, classical calculations using the full magnetic Hamiltonian for  $\text{CsNiF}_3$  (e.g. transfer matrix calculation of Pini and Rettori 1984) or for TMMC (e.g. Monte Carlo calculation of Jensen *et al* 1985) have demonstrated difficulties also in a classical description of these materials. Generally these classical calculations overestimate the magnitude of specific heat peaks when compared to experiment. It seems likely

that quantum effects restrict the spin motions more strongly than expected to the easy plane, thereby reducing the effective number of degrees of freedom, and making classical SG theory more appropriate than the full magnetic Hamiltonian theory. Emerging "numerically exact" quantum transfer matrix calculations for  $S=1/2$  (Wysin and Bishop 1986) also show this reduction in the effective number of degrees of freedom-- quantum transfer matrix specific heat peaks have close to the same magnitude as experiment and classical SG theory for CHAB. Since this question is not completely resolved even for static (thermodynamic) properties, especially for  $S=5/2$  TMMC, investigation of classical AFM  $K\bar{K}$  dynamics clearly is a useful tool.

The stability properties of the  $XY$  and  $YZ$  kinks are relevant for determining the allowed initial conditions. These stability regimes have already been established, partly numerically and partly by a linear stability analysis (Wysin *et al* 1986, see also Lemmens *et al* 1986 for an alternative view). These will be reviewed below in Section 2, along with the dispersion relations. In Section 3A we shall give a brief description of the numerical method and analysis, and a review of the FM  $K\bar{K}$  results. In Section 3B we present the new AFM  $K\bar{K}$  results, in terms of the three regimes labeled on dispersion curves and on a final state output "phase diagram". The similarities to FM  $K\bar{K}$  collisions will be noted, and the relevance of these results to TMMC experiments will be discussed in Section 4.

## 2. Review of Single Kink Dynamics

The nearest-neighbour Hamiltonian under consideration here includes an applied easy-plane field  $B=B_x$ , and single ion anisotropy  $A > 0$ ;

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

where  $J > 0$  is the nearest-neighbour exchange ( $J = 6.5$  K and  $A/J = 0.04$  for TMMC, Regnault *et al* 1982),  $n$  labels the lattice sites, and  $\mu_B$  is the Bohr magneton, and the  $xy$  plane is the easy plane. The continuum limit SG equations of motion derived from this Hamiltonian were given originally by Mikeska (1980), and Flüggen and Mikeska (1983). Later they were re-analyzed by Wysin *et al* (1986), who found that using a coordinate system with the  $x$  axis as the polar axis allows a more natural description of  $YZ$  kinks, while at the same time simplifying their stability analysis. Note that for the numerical integration presented here, it is most convenient to apply the discrete equations of motion in terms of  $xyz$  spin components rather than angles, *i.e.*,

$$\dot{\mathbf{S}}_n = \mathbf{S}_n \times [-J(\mathbf{S}_{n-1} + \mathbf{S}_{n+1}) + g \mu_B \mathbf{B} - 2AS_n^z \mathbf{2}], \quad (2)$$

since this allows for integration of the  $3N$  equations of motion without the evaluation of any trigonometric functions. In this way spin length and energy conservation both serve as checks of the numerical accuracy. (Note that there is no damping in this simulation.)

The energy-velocity dispersion relation for isolated kinks has been determined by three different methods:

- i) approximately from the SG limits, both  $XY$  and  $YZ$ ;
- ii) by numerical integration of the discrete equations of motion, using an appropriate

initial condition (either SG-like or from the Ansatz, below), combined with a time averaging procedure to remove spin waves;

iii) by applying a variational Ansatz, that assumes simple profiles for the spins on both the even and odd sub-lattices, as being SG profiles in tilted spin-space coordinates (Wysin *et al* 1986).

These all give similar qualitative results for the  $XY$  and  $YZ$  branches, however, the latter two show that the  $XY$  branch terminates where it meets the  $YZ$  branch, an important detail which is lost in the SG approach. Furthermore, the SG limit drastically overestimates the effective mass for  $XY$  kinks.

The numerical method directly gives stability information (Wysin *et al* 1986). Combined with a linear stability analysis for  $YZ$  kinks, it has been demonstrated that  $YZ$  kinks have a limited range of stability. At fields less than the critical field  $B_c$ , only  $YZ$  kinks with velocities greater than some minimum value  $v^*$  will be dynamically stable. If the field is equal to  $B_c$ , the minimum velocity  $v^*$  approaches zero. For fields greater than the critical field,  $v^*$  becomes negative. This is shown more clearly in Fig. 1; also see Wysin *et al* (1986) for a further explanation of  $YZ$  kink stability. At the same time, as the applied field is varied from below to above  $B_c$ , the  $XY$  branch continuously diminishes to a point (for  $B = B_c$ ), and re-emerges with downward curvature (implying negative effective mass) for fields greater than  $B_c$ . These negative effective mass  $XY$  kinks are also dynamically stable, as demonstrated in these numerical integrations.

The limited extent of the  $XY$  branch could be interpreted to mean that SG-like  $XY$  kinks with larger (absolute value) velocities are dynamically unstable. Note that it is possible to estimate the stability limit for the  $XY$  kinks from the linear stability analysis for  $YZ$  kinks, since the two dispersion curves end where they intersect. A linear stability analysis can be performed for moving as well as stationary SG-like  $YZ$  kinks: First order perturbation theory for the moving  $YZ$  kink linear stability problem estimates the velocity  $v^*$  at which the  $XY$  branch meets the  $YZ$  branch, as (Wysin *et al* 1986)

$$v^*/c_0 = \frac{2}{\pi} \frac{B_c}{B} \left[ 1 - \left( \frac{B}{B_c} \right)^2 \right], \quad (3a)$$

where

$$c_0 = 2JS/\hbar, \quad (3b)$$

and the critical field is

$$B_c = [8AJS^2]^{1/2}/(g\mu_B). \quad (4)$$

The lattice spacing is used as the unit of length here. Note that for  $B < B_c$ , when  $v^* > 0$ , the  $XY$  effective mass is positive, while for  $B > B_c$ , when  $v^* < 0$ , the  $XY$  effective mass is negative. Equation (3a) is an approximate expression which is most accurate for  $B$  near  $B_c$ . Also note that one cannot determine  $v^*$  by equating the predicted SG  $XY$  and  $YZ$  energies for a given field; the SG theory predicts that the branches do not cross except for  $B$  very near  $B_c$ . The non sine-Gordon behaviour manifests itself by strongly changing the effective masses of the  $XY$  kinks.

The  $XY$  kinks are in many ways analogous to the kinks of the easy-plane ferromagnet. The EPF kink's effective mass changes sign at a corresponding critical



field, the absolute values of the effective masses are much smaller than predicted by SG theory, and they are also *dynamically* stable even for fields greater than the critical field. And while the  $XY$  kinks obey dynamics very different from SG-like, the  $YZ$  kinks, on the other hand, can be described quite accurately using SG dynamics outside of the unstable regimes mentioned. The EPA  $YZ$  kinks have no natural analogue in the ferromagnet.

With the above points in mind, we can hope that these EPA  $K\bar{K}$  numerical collision experiments will answer the following questions:

- i) Generally, what outcomes are possible for EPA  $K\bar{K}$  collisions, of either  $XY$  or  $YZ$  type?
- ii) Is the behaviour of  $XY$   $K\bar{K}$  collisions similar to that of the  $K\bar{K}$  collisions of the EPF?
- iii) How do we characterize the behaviour of  $YZ$   $K\bar{K}$  collisions?

To prepare for the presentation of our results, we first review the EPF  $K\bar{K}$  scenario.

### 3. *Kink-Antikink Collisions*

#### 3A. *Ferromagnetic $K\bar{K}$ Method and Results*

The main features of EPF  $K\bar{K}$  collisions have been given earlier (Wysin *et al* 1984). The numerical method used for either ferro- or antiferro-magnetic coupling is essentially the same. The method used for the ferromagnet will be reviewed next, and modifications necessary to study the antiferromagnet will be described later.

The discrete equations of motion for the EPF were integrated numerically on a lattice of 80 to 180 spins, a larger number being necessary for kinks of greater width

(where the kink width  $w \approx \sqrt{JS/g\mu_B B}$ ). The initial condition was taken to be a single SG kink profile, corresponding to an SG velocity  $v_{SG}$ . By using Neumann boundary conditions for the  $xyz$  components, the kink interacts with its mirror image opposite velocity antikink at the boundary. In this way we need only half as many lattice points as compared to using a SG  $K\bar{K}$  profile on a lattice with periodic boundary conditions, in addition to saving a factor of two in CPU time. The Numerical method was a standard fourth order Adams-Bashforth-Moulton predictor-corrector scheme with mop-up. (For example, see Ceschino and Kuntzmann 1966.) The profile was allowed to evolve until approximately twice the time for the kink to reach the boundary. By viewing the time evolution of the profile and spatial averages (denoted with  $\langle \rangle$ ) of the in-plane and out-of-plane angles, it was possible to classify the final state according to whether the  $K\bar{K}$  pair underwent

- i) SG-like transmission, with monotonically increasing or monotonically decreasing  $\langle \phi \rangle(t)$ ; or
- ii) reflection, with a reversal of the slope of  $\langle \phi \rangle(t)$ ; or
- iii) breather formation or annihilation, with oscillatory  $\langle \phi \rangle(t)$ .

The final state was found to be dependent on both the initial SG velocity  $v_{SG}$  and the applied field (for a fixed value of anisotropy ratio  $A/J$ ). Results are summarized in Figure 4 of Wysin *et al* (1984), in terms of an output state phase diagram with four different regimes. The SG-like transmission regime covers only a small portion of the diagram--generally the collision behaviour is unlike sine-Gordon dynamics. Regimes III and IV in the figure both involve  $K\bar{K}$  reflection. However, in regime IV negative effective mass kinks reflect with no change in velocity, while in regime III positive

effective mass kinks reflect, *with a velocity change* (but no change in energy; there are two types of regime III kinks with equal energy but different velocity). Also, a detail not illustrated in the breather formation regime of Figure 4 (Wysin *et al* 1984) is the existence of at least one SG-like transmission window. With such a rich variety of non-SG behaviour for these equal but opposite velocity collisions, we also expect a similar variety for unequal velocity  $K\bar{K}$  pairs.

### 3B. EPA $K\bar{K}$ Collisions

For this case we used 101 to 501 lattice sites, with the kink width varying as  $w \approx 2JS/(g\mu_B B)$  for  $XY$  kinks and as  $w \approx \sqrt{J/(2A)}$  for  $YZ$  kinks. Using a fixed ratio  $2A/J=0.04$ , the field ranged from  $B/B_c=0.10$  to  $B/B_c=1.50$ . For TMMC, this corresponds to  $9.0 \text{ kG} \leq B \leq 140 \text{ kG}$ , with  $B_c \approx 90 \text{ kG}$ . The initial condition was an Ansatz profile for some specified value of a parameter  $\theta_A$ , where  $\theta_A$  determines the tilt of the spins out of the easy plane on the A-sublattice (Wysin *et al* 1986). The resulting profile could correspond to either an  $XY$  or  $YZ$  kink, depending on whether  $\theta_A$  was near zero or  $\pi/2$ . At some intermediate value of  $\theta_A$ , the Ansatz kink switched from the  $XY$  branch to the  $YZ$  branch. A given combination of  $\theta_A$  and  $B/B_c$  then determined the initial velocity, energy, and width of the kink.

Neumann boundary conditions were applied to the  $xyz$  spin components, but now the spatial derivatives on each sublattice were separately set to zero at the boundaries. Integration proceeded until about twice the time necessary for the kink to interact with its mirror image antikink at the boundary. Classification of the type of collision was based on viewing the time evolution of the spin profile and the spatial averages of in-plane and out-of-plane angles. The tilt of the two spins at the center of one kink, one

on each sublattice, measured from the easy plane, provided another diagnostic.

Possible outcomes of collisions include SG-like transmission, annihilation, and reflection. Typical cases of each of these are shown in Figures 2-6. The profiles are viewed in either  $z$ -polar or  $x$ -polar spherical coordinates, depending on which was visually more convenient. These results are summarized in Figures 7,8 and 9, as indicated on the single kink dispersion curves. An alternative representation of the summarized data is the final state phase diagram of Figure 10.

The results for low velocity  $XY$  kinks are similar to those for ferromagnetic kinks. Generally, for low fields  $B < 0.2B_c$  there is SG-like transmission. At higher fields but still with  $B < B_c$  the low velocity pairs annihilate, or possibly form breathers, and the higher velocity  $XY$  kinks undergo SG-like transmission. For  $B > B_c$ , the negative effective mass  $XY$  kinks reflect, as in the ferromagnet. Most of the cases tested for  $YZ$   $K\bar{K}$  pairs resulted in transmission, consistent with their nearer to SG behaviour. The exceptions included some cases at small velocity for  $B > B_c$ , where annihilation occurs. Other annihilation cases, at the  $XY$  to  $YZ$  boundaries for  $B > B_c$  may be artifacts of the Ansatz initial condition.

#### 4. Discussion

Typically the dynamic behaviour of isolated kinks in easy-plane magnets has been seen to be only poorly described by a sine-Gordon equation. Generally the effective kink mass is modified by additional terms in the equations of motion not included in the simplified SG picture. These additional terms also are responsible for introducing internal bound states in the kink spectrum which are very important for collisions. In

