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LETTER TO THE EDITOR

Interaction induced deformation of two coupled XY spin chains

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Abstract. We study two coupled XY spin chains in the continuum limit with ferromagnetic interaction both along and between the chains. We find 2π twist soliton solutions for the difference in orientation angle of the spins along the chains. If we allow the chains to be elastic, they will deform (move apart) in the region of the soliton in order to reduce magnetic energy. The extent of deformation is a result of a balance between the gain in magnetic energy and elastic energy cost. We also generalize these results to the case of a soliton lattice.

The interaction between two neighbouring spin chains is important in determining the physical properties of a material, e.g. CuO chains in high temperature superconductors or quasi-one-dimensional magnetic materials under pressure. Here we consider two coupled XY spin chains [1] at a distance d from each other. The XY plane is perpendicular to the chain direction, z. The interaction between the spins along, as well as between, the chains, is ferromagnetic. The Hamiltonian is given by the following expression:

$$H = -J_0 \sum_i S_i^{(1)}.S_{i+1}^{(1)} - J_0 \sum_i S_i^{(2)} S_{i+1}^{(2)} - J(d) \sum_i S_i^{(1)} S_i^{(2)} \tag{1}$$

where $S_i^{(1)}$ and $S_i^{(2)}$ denote spin in chains 1 and 2, respectively. J_0 and $J(d)$ are the interaction constants along and between the chains, respectively. We will assume that $J_d = C/d^2$, where C is a constant. The actual form of J_d as a function of d is not relevant to the magnetoelastic effect discussed in this article.

Because $S^2 = 1$, we will use the angle representation for each spin which takes into account the normalization condition $S_i = (\cos\theta_i, \sin\theta_i)$. Now we can take the continuum limit in equation (1) which leads to the following expression:

$$H = \int \left\{ \frac{1}{2} J_0 \left[(\nabla_z \theta_1)^2 + (\nabla_z \theta_2)^2 \right] + 2J(d) \sin^2 \frac{\theta_2 - \theta_1}{2} \right\} \mathrm{d}z. \tag{2}$$

Here $\theta_1 = \theta_1(z)$, $\theta_2 = \theta_2(z)$ and in the process of taking the continuum limit we have omitted constant terms that merely renormalize the energy: $S_{1,i}^2$, $S_{1,i+1}^2$, $S_{2,i}^2$, $S_{2,i+1}^2$ and $-J(d)$.

The Euler–Lagrange equations for θ_1 and θ_2 are as follows:

$$\frac{J_0}{2} \frac{\mathrm{d}^2\theta_1}{\mathrm{d}z^2} = -J(d) \sin(\theta_2 - \theta_1) \tag{3a}$$

$$\frac{J_0}{2} \frac{\mathrm{d}^2\theta_2}{\mathrm{d}z^2} = J(d) \sin(\theta_2 - \theta_1). \tag{3b}$$

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Now we substract equation (3a) from (3b) and introduce the new variable $\Delta\theta = \theta_2 - \theta_1$. We obtain the following sine–Gordon equation

$$\frac{\mathrm{d}^2\Delta\theta}{\mathrm{d}z^2} = 4\frac{J(d)}{J_0}\sin\Delta\theta \tag{4}$$

which has a nontrivial 2π soliton solution

$$\Delta\theta(z) = 4\arctan\left[\exp(-\frac{z}{\xi})\right] \qquad \xi = \frac{1}{2}\sqrt{\frac{J_0}{J(d)}} = \frac{d}{2}\sqrt{\frac{J_0}{C}} \tag{5}$$

with $\Delta\theta(-\infty) = 0$ and $\Delta\theta(+\infty) = 2\pi$. If we now add equations ($3a$) and ($3b$) we get the following equation for the sum of the angles $\theta_1 + \theta_2$:

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}(\theta_1 + \theta_2) = 0 \tag{6}$$

with the solution $\theta_1 + \theta_2 = C_0 z + D$, where D is a constant, and the boundary conditions $\theta_1(\pm\infty) = \theta_2(\pm\infty) =$constant, which assure the convergence of the energy in (2) is satisfied by $C_0 = 0$.

Using equations (2) and (5), the total magnetic energy of the soliton is given by $E = 3J_0/\xi$. Each chain contributes J_0/ξ, as does the coupling between the chains.

At the centre of the soliton (i.e. $\Delta\theta = \pi$), the contribution to the energy from the interaction term is at a maximum and the total energy will be most sensitive to the interaction constant $J(d)$ in this region. If we now allow the distance between the chains to vary, i.e. $d = d(z)$ and keep at the same time the boundary conditions fixed, $d(-\infty) = d(+\infty) = d_0$, the system will try to reduce its energy by moving the two chains further apart in the region around the centre of the soliton (figure 1). This is rather natural because, as one might predict, near the centre of the soliton, $\theta_2 - \theta_1 \simeq \pi$ and the system tries to reduce energy by increasing d. This will cost elastic energy and the exact shape of the two spin chains will depend on the balance between the magnetic and elastic energy. The full Hamiltonian of the system has the form:

$$H = H_{magn} + H_{elast}$$

where H_{elast} has the form

$$H_{elast} = 2\kappa \int \left(\frac{\mathrm{d}y}{\mathrm{d}z}\right)^2 \mathrm{d}z \tag{7}$$

and $y(z)$ is the distance of the distorted spin chain at a point z from the original straight line.

If we take as an ansatz $y(z) = \alpha\,\mathrm{sech}\,(z/\xi)$ for the distortion of each chain we get $H_{elast} = 4\kappa\alpha^2/3\xi$. Now we proceed to show that for distorted chains the gain in magnetic energy more than compensates the cost of elastic energy. The magnetic energy of distorted chains is given by

$$H_{magn} = \frac{3J_0}{\xi} - \pi\frac{\alpha}{d}\frac{J_0}{\xi}. \tag{8}$$

In the above expression we have assumed that $\alpha/d \ll 1$. It suffices that $\pi(\alpha/\mathrm{d})(J_0/\xi) > (4\kappa\alpha^2/3\xi)$ and deforming the chains will become energetically favourable. This can be reached easily for soft elastic chains.

Next, we write down the periodic (soliton lattice) solution of equation (4) for appropriate boundary conditions

$$\Delta\theta_L(z) = 2\arccos\left[\mathrm{sn}\left(\frac{z}{k\xi}, k\right)\right] \tag{9}$$

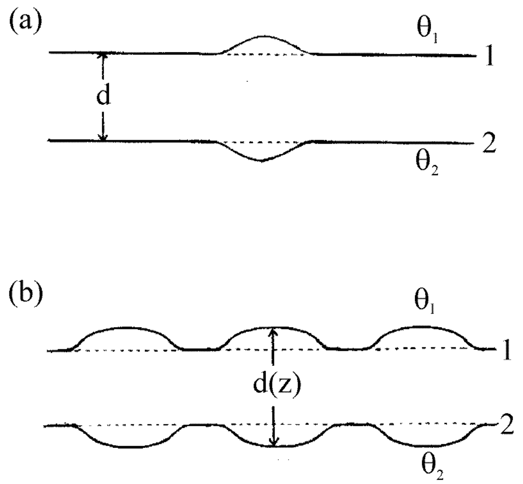

Figure 1. (a) Two coupled XY spin chains with deformation in the region of a 2π twist soliton in the difference angle $(\theta_1 - \theta_2)$. (b) Two coupled XY spin chains with deformation for a soliton lattice in the difference angle $(\theta_1 - \theta_2)$.

with the periodicity $4l = 4\xi k K(k)$, where k is the modulus of the Jacobian elliptic function sn (sine amplitude), and $K(k)$ is the complete elliptic integral of the first kind. In the limit $k \to 1$, as $\lim_{k\to1} K(k) \to \infty$, the half period $2l$ tends to infinity and we recover the single soliton solution of equation (5).

The total magnetic energy per soliton of the soliton lattice is given by

$$H_{magn} = \frac{3J_0}{k\xi}\left(E - \frac{1}{3}k'^2 K\right) \tag{10a}$$

where $E(k)$ is the complete elliptic integral of the second kind. Each chain contributes $J_0 E/k\xi$ to the magnetic energy whereas the coupling between the chains contributes $J_0/k\xi(E - k'^2 K)$. In the single soliton limit ($k \to 1$), lattice solution (equation (9)) and the lattice energy (equation (10a)) reduce to the results obtained above (equation (5) and $3J_0/\xi$). Unlike the single soliton case, the contribution to the total energy from each chain is greater than the coupling term because of soliton interaction. Asymptotically, when the solitons are very far apart ($l \gg \xi$, $k' \to 0$), the interaction energy (in addition to the single soliton energy) is

$$H_{magn} = \frac{3J_0}{\xi}\left[1 + \frac{4}{3}\left(\frac{l}{2\xi}\right)\exp\left(\frac{-l}{2\xi}\right)\right] \tag{10b}$$

with $E = 3J_0/\xi$ being the magnetic energy of a single soliton. The form of the repulsive interaction indicates that the soliton lattice is stable only for $l > 2\xi$.

If we take as an ansatz $y(z) = \beta cn(z/k\xi, k)$ for the periodic distortion of each chain we get

$$H_{elast} = \frac{4\kappa\beta^2}{3k^3\xi}[k'^2 K + (2k^2 - 1)E]. \tag{11}$$

In the limit $k \to 1$ equation (11) reduces to the elastic energy of the single soliton (with $\beta \to \alpha$). Again, we show that for periodically distorted chains, the gain in magnetic energy is more than the cost of elastic energy. The magnetic energy of periodically distorted chains is

$$H_{magn} = \frac{3J_0}{k\xi}\left(E - \frac{1}{3}k'^2 K\right) - \frac{2\beta J_0}{d\xi k^2}[kk' + (2k^2 - 1)\arcsin k]. \tag{12}$$

Here we have assumed that $\beta/d \ll 1$. Note that equation (12) reduces to equation (8) in the limit $k \to 1$ (and $\beta \to \alpha$). It suffices that

$$3kJ_0[kk' + (2k^2 - 1)\arcsin k] > 2\kappa\beta d[k'^2 K + (2k^2 - 1)E]$$

and periodically deforming the chains will become energetically favourable. Again, this can be reached easily for soft elastic chains.

Similar magnetoelastic effects have been predicted [2] in the context of Heisenberg spins on the surface of a cylinder. However, in that study the cylinder shrinks in the region of the soliton whereas in the present case the two chains move away in the region of the soliton. Examples of one-dimensional magnets with XY spin chains include ferromagnetic material $CsNiF_3$ [3], antiferromagnetic materials $CsCoCl_3$ [4] and TMMC [5]. A particular example of coupled XY chains is the quasi-one-dimensional magnet $Pr(C_2H_5SO_4)_3.9H_2O$ (or $PrEtSO_4$) [6]. Neutron scattering, NMR, electron-spin-echo and optical absorption experiments indeed provide evidence for magnetic solitons in these materials.

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