## Soliton instability in a one-dimensional magnet

Pradeep Kumar Physics Department, University of Florida, Gainesville, Florida 32611 (Received 27 April 1981)

Neutron scattering experiments on planar one-dimensional magnets have been analyzed in terms of sine-Gordon solitons. We show here that at high magnetic fields the sine-Gordon soliton becomes unstable. This results in the spins becoming nonplanar at the center of the soliton. The change is discontinuous and contains hysteretic effects.

The neutron scattering experiments show solitonlike excitations<sup>1,2</sup> in a planar ferromagnet, e.g., CsNiF<sub>3</sub>. The purpose of this Brief Report is to show that these solitons have a unique instability. The instability can be caused by increasing the magnetic field. The resulting effects are discontinuous and resemble a first-order phase transition. As the magnetic field increases, the instability appears at a critical field which is higher than the corresponding critical field at which the original soliton is restored. It should be possible to see this instability in neutron scattering experiments.

A one-dimensional, planar ferromagnet is described by the Hamiltonian<sup>2</sup>

$$H = -J \sum_{i < j} \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_j + A \sum_i (S_i^z)^2 - \vec{\mathbf{S}} \cdot \vec{\mathbf{H}} \quad , \tag{1}$$

where the spins are measured in units of the Bohr magneton  $\mu_B$ . The sum over *j* is restricted to the nearest neighbors only. The external magnetic field *H* is taken to be in the *x* direction while the chain direction is along the *z* axis. The exchange constant *J* and the anisotropy energy *A* are known and for CsNiF<sub>3</sub> take the values 23.6 and 4.5 K, respectively.<sup>3</sup> The spin dynamics is described by the usual Bloch's equations. The character of nonlinear excitations is best seen if we treat the spins classically and write the Hamiltonian in terms of the polar angles  $\theta$  and  $\phi$ :

 $\vec{S} = s(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ ,

$$H = \int_{-\infty}^{\infty} \frac{dz}{a} \left\{ \frac{Ja^2s^2}{2} (\theta_z^2 + \sin^2\theta \phi_z^2) + As^2\cos^2\theta - sH\sin\theta\cos\phi \right\} ,$$
(2)

where a gradient expansion has been done. *a* denotes the nearest-neighbor distance and the subscripts imply differentiation. If now the anisotropy field is minimized by putting  $\theta = \pi/2$  everywhere, the resulting energy for  $\phi$  has degenerate minima at  $\phi = 2n\pi$ , *n* is an integer. It then gives rise to a sine-Gordon (SG) soliton.<sup>2,4</sup> It is a screw-type soliton in which the spins rotate in the *xy* plane as one

progresses along the chain direction. The neutron scattering experiments<sup>1</sup> have been analyzed in terms of this SG soliton and the results are satisfactory.

The point here is that as the magnetic field is increased, the SG soliton becomes unstable. The new structure consists of a  $[0, 2\pi]$  structure for  $\phi$  and in the center  $\theta$  swings out to  $\theta \le \pi$  (Fig. 1). The origin of this effect can be seen from Eq. (2). The anisotropy energy indeed prefers  $\theta = \pi/2$ . Yet the magnetic field term is such that at the center of the soliton  $(\phi = \pi)$  the preferred values for  $\theta$  are  $n\pi$ . Furth-



FIG. 1. Soliton profile is shown as a function of  $z/\xi$ . A SG soliton shown in the upper part consists of  $\phi$  going from 0 to  $2\pi$  over a length scale of order 1 and  $\theta$  remains  $\pi/2$  everywhere. The distorted soliton shown in the lower part consists of a narrow transition region and  $\theta$  is inhomogeneous.

25

483

©1982 The American Physical Society

(4c)

more the gradient energy term for  $\phi$  is decreased if  $\theta$  departs from  $\pi/2$ . Since the gradient energy for SG soliton is also proportional to magnetic field, the magnetic field prefers  $\theta \neq \pi/2$  at the center of the soliton and above a critical value of the field, the distorted soliton becomes the ground state. This new

structure is lower in energy by as much as 30% and is only half as wide as an SG soliton.

Let us first do a linear stability analysis of the SG soliton. If  $\phi(z) = \phi_0(z) + \phi_1$  and  $\theta(z) = \pi/2 + \psi(z)$  where  $\phi_0(z) = 2 \sin^{-1} \operatorname{sech}(z/\xi_0)$  and  $\xi_0^2 = Ja^2s^2/SH$ , Eq. (2) becomes

$$H = E_0 + \int_{-\infty}^{\infty} \frac{dz}{a} \left( \frac{Ja^2 s^2}{2} (\phi_{1z})^2 + sH[1 - 2\operatorname{sech}^2(z/\xi_0)] \phi_1^2/2 \right) + \int_{-\infty}^{\infty} \frac{dz}{a} \left[ \frac{Ja^2 s^2}{2} (\psi_z)^2 + \left[ As^2 + \frac{sH}{2} - 3sH\operatorname{sech}^2 z/\xi_0 \right] \psi_1^2 \right] \right]$$
(3)

where  $E_0 = -NsH + 8(JHs^3)^{1/2}$  is the energy of a single soliton. The second term describes the usual fluctuations of a SG soliton and can be written as  $\sum_n \lambda_n \phi_n^2$ . The  $\lambda_n$  include a bound state  $\lambda_0 = 0$ ; the so called translational mode and the continuum of scattering states. For our purposes all  $\lambda_n > 0$  and the SG soliton is stable against  $\phi$  fluctuations. Interestingly enough,  $\psi$  fluctuation energy, if written as  $\sum_n \mu_n \psi_n^2$  consists of fluctuation eigenvalues and eigenvectors of the famous " $\phi^{4}$ " field theory. The lowest eigenvalue  $\mu_0$  is given by  $2As^2 - 3SH$  and becomes negative for  $H > H_c^1 = \frac{2}{3}AS = 18$  kG (for CsNiF<sub>3</sub>). This field is not inordinately high. However to my knowledge no experiments have been performed in this field region.

In other words, the  $\psi$  fluctuations consist of a bound state that condenses for  $H > H_c^1$ . The amplitude of this condensed state can be determined only by going to higher-order nonlinear terms. It turns out that the terms quartic in  $\psi_n$  are no help at all. Indeed they go negative at a much lower field. Two conclusions can be drawn from the result: (a) an expansion in powers of  $\psi_n$  is insufficient and one must do a full nonlinear analysis and (b) there exists another critical field  $H_c^{II} < H_c^{I}$  such that for  $H_c^{II} < H < H_c^{I}$ ; the distorted ground state is lower in energy than the SG soliton. Since the latter is stable against small  $\psi$  fluctuations, the two states must be separated by an energy barrier.

I do a variational calculation for the full nonlinear analysis. The bound-state wave function is given by  $\psi = \operatorname{sech}^2 z/\xi_0$ . An obvious nonlinear extension is to assume  $\sin \phi/2 = \operatorname{sech} z/\xi$  and  $\sin \psi/2 = \alpha \operatorname{sech}^2 z/\xi$  and then treat  $\alpha$  and  $\xi$  as variational parameters. It is relatively easy to minimize H with respect to  $\xi$ ; the resulting  $\alpha$  dependent energy E and the width  $\xi$  are given in terms of  $E_{SG} = 8(JS^3H)^{1/2}$  and  $\xi_0$ ; the corresponding quantities for a sine-Gordon soliton

$$E/E_{\rm SG} = (F_1F_2)^{1/2}, \quad \xi/\xi_0 = (F_1/F_2)^{1/2}, \quad (4a)$$

where

$$F_{1} = 1 + 2\left[2 - \left(\frac{1-\alpha}{\alpha}\right)^{1/2} \tan^{-1}\left(\frac{\alpha}{1-\alpha}\right)^{1/2} - \left(\frac{1+\alpha}{\alpha}\right)^{1/2} \tanh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{1/2}\right] - 2\alpha^{2}\left(\frac{16}{15} - \frac{256}{315}\alpha^{2}\right) , \qquad (4b)$$

$$F_2 = 1 - (\frac{2}{5} - \frac{4}{3}\beta)\alpha^2 - \frac{32}{35}\beta\alpha^4 , \quad \beta = As/g\mu_B H ,$$

where for CsNiF<sub>3</sub>, g = 2.4 so that  $\beta = 28$  kG/H. The energy ratio  $E/E_{SG}(\alpha)$  is plotted in Fig. 2 for  $\beta = 1.0$ and 1.7. For  $\beta > 1.8$ ,  $\alpha = 0$  is the global energy minimum of the system, subject to the boundary conditions that  $\phi \rightarrow [0, 2\pi]$  for  $z \rightarrow [-\infty, +\infty]$ . For  $\beta < 1.8$ , the minimum at  $\alpha \neq 0$  becomes lower in energy.<sup>5</sup> Notice however that the energy scale near  $\alpha = 0$  is tenfold larger for  $\beta = 1.7$ . The energy barrier is indeed very small and is never higher than 0.3%. For  $\beta < 1.5$ , and  $\alpha \neq 0$  state is the only energy minimum. The angle  $\psi_0 = 2 \sin^{-1} \alpha$  measures the maximum excursion of  $\theta$  near the center of the dis-

torted soliton. For  $\beta = 1.7$ ,  $\psi_0 = 66^\circ$  and increases as  $\beta$  decreases.

There remains the question however whether the class of functions chosen for  $\phi$  and  $\psi$  describe the lowest minimum of the free energy. Undoubtedly, it must do so for small  $\alpha$ . For large  $\alpha$ , the sech<sup>2</sup>z/ $\xi$  function is such that the length scale for  $\psi(z)$  is half of that for  $\phi(z)$ . This must cost in gradient energy. We therefore try another class of solutions where  $\sin\psi/2 = \alpha \operatorname{sech} z/\xi$  and  $\phi$  is unchanged. Again the energy is minimzed with respect to  $\xi$  first; the resulting  $\alpha$  dependent quantities are identical to Eq. (4a).



FIG. 2. Energy of a distorted soliton in terms of the pure SG energy as a function of  $\alpha$ . For  $\beta = 1.0$ , there is only one minimum at  $\alpha = 0.63$ . For  $\beta = 1.7$ , it has two minima, at  $\alpha = 0$  corresponding to an SG soliton and  $\alpha = 0.55$ . The energy scale near  $\alpha = 0$  has been expanded tenfold to show the small energy barrier. The value of  $\theta$  at the soliton center is given by  $\pi/2 + 2\sin^{-1}\alpha$ . The  $\theta$  profile here is  $\sin(\theta/2 - \pi/4) = \alpha \operatorname{sech}^2 z/\xi$ .

Equations (4b) and (4c) are replaced by

$$F_1 = 2 - \left(\frac{1 - \alpha^2}{\alpha^2}\right)^{1/2} \tan^{-1} \left(\frac{\alpha^2}{1 - \alpha^2}\right)^{1/2} - \frac{8}{3} \alpha^2 (1 - \frac{4}{5} \alpha^2) ,$$
(5a)

$$F_2 = 1 - (\frac{1}{3} - 2\beta)\alpha^2 - \frac{4}{3}\beta\alpha^4 \quad . \tag{5b}$$

While the qualitative features are similar to Fig. 2 the energy minima are indeed lower. The critical  $\beta$ are different now. The  $\alpha = 0$  energy minimum becomes lower than the  $\alpha = 0$  min for  $\beta < 2.44$ . The  $\alpha = 0$  minimum becomes unstable for  $\beta < \frac{4}{3}$ . Clearly these functions are not a good description near  $\alpha = 0$ . A reasonable description of the system can be obtained if we use Eqs. (5) for the large  $\alpha$  branch of the solutions and Eqs. (4) for the small  $\alpha$  case. Since the changes are discontinuous we expect this description to be accurate. Finally, we show in Fig. 3 the energy, the maximum excursion angle  $\alpha = \sin\psi_0/2$ and the width of the distorted texture as a function of  $\beta$ . They are only weakly affected by magnetic field.



FIG. 3. Energy ratio, the width ratio, and  $\alpha$  are shown here as a function of  $\beta$ (= 28 kG/H for CsNiF<sub>3</sub>) for the distorted soliton. The  $\theta$  profile here is sin( $\theta/2 - \pi/4$ ) =  $\alpha$  sechz/ $\xi$ .

To summarize then, in a planar ferromagnet, the SG solitons are unstable at large magnetic fields and form a texture where the spins rise out of the plane. As H increases, for  $H > H_c^{II}$ , the nonplanar texture has lower energy. However it is separted by a low-energy barrier from the planar spin soliton. Hence on the increasing field path, the instability sets in at  $H_c^{I}$ . As the field is decreased, the SG soliton (planar spins) is restored for  $H < H_c^{II}$ . Temperature effects however probably round off this hysteresis to a large extent.

The observation of this instability could be limited by the magnetization saturation at large fields. They scale with H/T. Our estimates indicate they are small. The experiment most sensitive to this instability is perhaps magnetic resonance. It measures the frequency for a uniform spin fluctuations. For a SG soliton, the frequence is are  $\omega = 0$  or  $\omega = \gamma H$ ; the Larmor frequency,  $\gamma$  is the gyromagnetic ratio. And therefore magnetic resonance is not too effective in determining the presence of solitons. On the other hand, the distorted texture has characteristic frequency shifts which can be used as a label to study the instability. Magnetic resonance should also describe the interaction of the distorted texture with spin waves, etc. In neutron scattering, the elastic scattering measures the energy and width of the soliton.<sup>6</sup> The change in energy at the transition is only 10%. However the width reduces by a factor of  $\frac{1}{2}$  and should be observable. Needless to say that the measurement of the dynamic structure factor (in inelastic scattering) would provide all the information.

There is an interesting relationship between this problem and the polyacetylene problem.<sup>7</sup> The latter is a nonlinear coupled fermion-boson problem equivalent to the Gross-Neveu model in particle physics. This problem is a nonlinear coupled boson field problem, albeit a classical version. The experiment corresponding to doping in polyacetylene<sup>8</sup> here is spin tipping. For  $H < H_c^{II}$  at 90° spin tip would go back to the SG soliton and unshifted resonance fre-

- <sup>1</sup>J. K. Kjems and M. Steiner, Phys. Rev. Lett. <u>41</u>, 1137 (1978). For a review see M. Steiner, J. Appl. Phys. <u>50</u>, 7395 (1979).
- <sup>2</sup>H. J. Mikeska, J. Phys. C <u>11</u>, L29 (1978).
- <sup>3</sup>M. Steiner, J. Villain, and C. G. Windsor, Adv. Phys. <u>25</u>, 87 (1976).
- <sup>4</sup>For an extensive review of solitons in one-dimensional condensed matter physics see K. Maki, Prog. Low Temp.

quencies. For  $H > H_c^{II}$ , the spin tip would create distorted solitons and shifted resonance frequencies.

I am thankful to Alan Bishop for educating me in the ways of one-dimensional magnets and J. Krumhansl for encouraging and stimulating discussions. This work was supported by National Science Foundation under Grant No. DMR-8006311 and by the Research Corporation.

Phys. (in press).

- <sup>5</sup>For decreasing magnetic field, the SG soliton appears at  $\beta \leq 2.4$ . Since the energy barrier near  $\alpha = 0$  is very small, the difference must be quite small.
- <sup>6</sup>A. R. Bishop, J. Phys. A (in press).
- <sup>7</sup>R. Jackiw and J. R. Schrieffer (unpublished); H. Takayama, Y. R. LinLiu, and K. Maki, Phys. Rev. B <u>21</u>, 2388 (1980).
- <sup>8</sup>W. P. Su and J. R. Schrieffer (unpublished).