Solitons in planar ferromagnets with biquadratic exchange

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We study the influence of biquadratic exchange on the soliton excitations of the one-dimensional easy-plane Heisenberg ferromagnet using a classical approximation in the continuum limit. Their energy is found to be significantly affected particularly for the more localized configurations, where a fourth-order expansion is necessary for accurate results.

The influence of solitonlike excitations in the properties of magnetic chains has been the subject of continued interest in recent years, particularly in view of the role played by recent developments in the theory of nonlinear systems[1] and the fact that some model substances have been investigated in detail via neutron scattering experiments[2] as well as bulk specific-heat measurements.[3] Much attention has been focused upon the magnetic salt $CsNiF_3$, which is considered the best example of a planar one-dimensional ferromagnetic system.[4] The usual Hamiltonian used to describe this system is the one-dimensional easy-plane Heisenberg ferromagnet

$$\mathscr{H}_0 = -J\sum_n \mathbf{S}_n\cdot\mathbf{S}_{n+1} + A\sum_n (S_n^z)^2 - g\mu_B H\sum_n S_n^x \quad (1)$$

for an infinite chain directed along the z axis with sites labeled by n. $J>0$ is the exchange integral; the second term has $A>0$ and corresponds to the single ion uniaxial anisotropy due to the crystalline field, and it constrains the spins to lie in a plane perpendicular to the chain axis. The last term is the usual Zeeman energy for an in-plane magnetic field.

The Hamiltonian (1) has been extensively studied,[5] particularly at low temperature with spins considered as classical variables and the chain approximated by a continuum. Corrections, both quantum and due to the discreteness of the chain, have been considered as well as the instabilities that appear at high T and strong magnetic fields.[6] In this work we report results of studying the effect on the behavior of solitons of adding a biquadratic exchange term $(\mathbf{S}_n\cdot\mathbf{S}_{n+1})^2$ to the Hamiltonian (1). The necessity of including such a term for spins higher than $\frac{1}{2}$ goes back to Schrödinger,[7] who showed that for spin 1 (which is the case of $CsNiF_3$) the permutation operator was

$$(\mathbf{S}_i\cdot\mathbf{S}_j)^2 + \mathbf{S}_i\cdot\mathbf{S}_i - 1 ,$$

and an interpretation in terms of a superexchange mechanism was given by Anderson.[8] The influence of this additional term on the thermodynamic properties has been studied by a number of authors,[9] and the existence of soliton excitation in uniaxial anisotropic ferromagnets was established by Ferrer[10] using the coherent state formalism.

We take then the Hamiltonian

$$\mathscr{H} = -J\sum_n (\mathbf{S}_n\cdot\mathbf{S}_{n+1}) + A\sum_n (S_n^z)^2 - g\mu_B H\sum_n S_n^x - \alpha J\sum_n (\mathbf{S}_n\cdot\mathbf{S}_{n+1})^2 \quad (2)$$

with $J>0$, $A>0$, and α a parameter that measures the strength of the biquadratic exchange, in the classical approximation. The evolution governed by the Hamiltonian (2) is given by Hamilton's equations which become partial differential equations in the long-wavelength limit. For weak magnetic fields and small out-of-plane motions the sine-Gordon equation obtains[11] when $\alpha=0$. In our case, $\alpha\neq0$, writing

$$\mathbf{S}(z,t) = S(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) , \quad (3)$$

with $\theta=\theta(z,t)$, $\phi=\phi(z,t)$, and keeping terms up to second order in lattice spacing over wavelength we obtain

$$\dot\theta = -J(1+2\alpha S^2)Sa^2(\phi''\sin\theta + 2\theta'\phi'\cos\theta) + g\mu_B H\sin\phi ,$$
$$\dot\phi\sin\theta = J(1+2\alpha S^2)Sa^2[\theta'' - (\phi')^2\sin\theta\cos\theta] + 2AS\sin\theta\cos\theta + g\mu_B H\cos\theta\cos\phi . \quad (4)$$

Here, an overdot denotes time differentiation, a prime denotes space differentiation and a is the lattice spacing. These equations are the same as the ones obtained by Wysin *et al.*[6] when $\alpha=0$. Thus, to this order, the effect of the biquadratic exchange is to renormalize the exchange energy J to $\tilde J = J(1+2\alpha S^2)$. In the sine-Gordon limit ($g\mu_B H \ll 2AS$, $\theta\sim\pi/2$), Eq. (3) simplifies to

$$\phi'' - \frac{1}{c^2}\ddot\phi = m^2\sin\phi ,$$

$$\cos\theta = \frac{1}{2AS}\dot\phi ,$$

with

$$c^2 = 2Aa^2S^2\tilde J ,$$

and

$$m^2=g\mu_B H/\tilde{J}Sa^2 \ .$$

The energy of the soliton is

$$E=8JS^2\gamma\frac{g\mu_B H(1+2\alpha S^2)^{1/2}}{(JS)^{1/2}}$$

[where $\gamma=(1-u^2/c^2)^{-1/2}$ and u is the speed of the soliton] which shows that biquadratic exchange raises the soliton energy for $\alpha>0$ and lowers it for $\alpha<0$, say by 10% for $\alpha=-0.1$. Thus, even a small amount of superexchange energy considerably alters the energy of soliton excitations in a linear magnetic chain, its influence easily being of the same order of magnitude as quantum corrections.[11] This also suggests that the biquadratic term may affect crucially the stability analysis concerning out-of-plane excursions.[6,12,13] In this report, however, we confine ourselves to magnetic fields sufficiently low so that the sine-Gordon soliton is stable.

To second order then, biquadratic exchange, although it significantly changes the energy, does not qualitatively change the nature of soliton. In order to have a more detailed understanding of the influence of this term, we have carried out the continuum approximation to fourth order in lattice spacing over wavelength. We do this because for higher magnetic fields solitons become more localized (Fig. 1) and the biquadratic term weights more heavily those configurations, suggesting that higher derivative contributions may become important.

The Hamiltonian (2) becomes, to fourth order,

$$\mathcal{H}=\int_{-\infty}^{\infty}\frac{dz}{a}\left[-J(1+2\alpha S^2)\frac{a^4}{4!}\mathbf{S}\cdot\mathbf{S}''''-\alpha\frac{Ja^4}{4}(\mathbf{S}\cdot\mathbf{S}'')^2 -J(1+2\alpha S^2)\frac{a^2}{2}\mathbf{S}\cdot\mathbf{S}''+A(S^z)^2 -g\mu_B H(S^x-S)\right] . \quad (5)$$

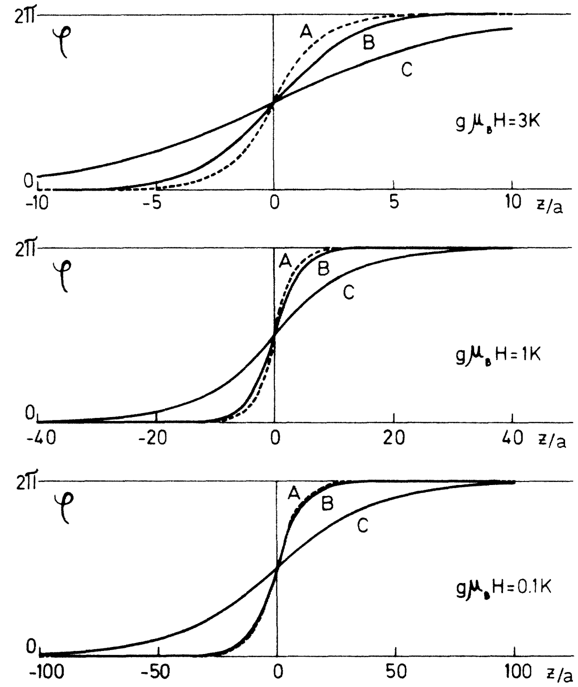

FIG. 1. Soliton profiles as function of z/a for three values of magnetic field. A: (dashed lines) second-order approximation, $\alpha=-0.4$; B: fourth-order approximation, $\alpha=-0.4$; C: $\alpha=1.0$, second and fourth order essentially coincide. Note the change of horizontal scale for the different magnetic fields: as the latter go up, localization sharply increases.

In this approximation the effect of biquadratic exchange is more than a mere renormalization of the exchange energy appearing in the usual bilinear expression. Using (3) the evolution equations are

$$\dot\theta=-J(1+2\alpha S^2)\frac{a^4S}{12}[\phi''''\sin\theta-4(\theta')^3\phi'\cos\theta-4\theta'\phi'''\cos\theta+6\theta''\phi''\cos\theta +8\theta'\phi'''\cos\theta-6(\theta')^2\phi''\sin\theta+4\theta'''\phi'\cos\theta -12\theta'\theta''\phi'\sin\theta-6(\phi')^2\phi''\sin\theta-4(\phi')^3\theta'\cos\theta] +\alpha Ja^4S^3[3(\phi')^2\phi''\sin^3\theta+4\theta'(\phi')^3\sin^2\theta\cos\theta+2\theta'\theta''\phi'\sin\theta+(\theta')^2\phi''\sin\theta+2(\theta')^3\phi'\cos\theta] -J(1+2\alpha S^2)a^2S(\phi''\sin\theta+2\theta'\phi'\cos\theta)+g\mu_B H\sin\phi \ , \quad (6)$$

$$\dot\phi=-J(1+2\alpha S^2)\frac{a^4S}{12}[6(\theta')^2\theta''\cos\theta-\theta''''\cos\theta+6\theta''(\phi')^2\cot\theta\cos\theta +12\theta'\phi'\phi''\cot\theta\cos\theta-6(\theta')^2(\phi')^2\cos\theta +3\phi'\phi'''\cos\theta+3(\phi'')^2\cos\theta-(\phi')^4\cos\theta] +\alpha Ja^4S^3[(\phi')^4\sin^2\theta\cos\theta-\theta''(\phi')^2\sin\theta-2\theta'\phi'\phi''\sin\theta-(\theta')^2(\phi')^2\cos\theta-3(\theta')^2\theta''\operatorname{cosec}\theta] -J(1+2\alpha S^2)a^2S[(\phi')^2\cos\theta-\theta''\operatorname{cosec}\theta]+2AS\cos\theta+g\mu_B H\cos\phi\cot\theta \ . \quad (7)$$

As a first step towards the full understanding of these formidable equations we have looked at static, in-plane ($\theta=\pi/2$) configurations. In this case the equation to be solved for ϕ is

$$2F\phi'''' - 12B(\phi')^2\phi'' + 2C\phi'' - D\sin\phi = 0 , \qquad (8)$$

with Hamiltonian

$$\mathscr{H} = \int_{-\infty}^{\infty} \frac{dz}{a}[-F(\phi'')^2 - B(\phi')^4 + C(\phi')^2 + D(1-\cos\phi)] , \qquad (9)$$

where

$$F = \frac{a^2}{12}C = J(1+2\alpha S^2)\frac{a^4S^2}{24} ,$$

$$B = J(1+8\alpha S^2)\frac{\alpha^4 S^2}{24} ,$$

$$D = g\mu_B HS .$$

We have solved (8) numerically with boundary conditions

$$\phi \underset{z\to+\infty}{\longrightarrow} \pi , \quad \phi \underset{z\to-\infty}{\longrightarrow} 0 ,$$

corresponding to a soliton (kink), and found the energy of those solutions with (9), using parameters adequate for $CsNiF_3$: $J=23.6$ K, $A=5$ K, $S=1$.

Results are given in Figs. 1 and 2. We have considered magnetic fields $g\mu_B H=0.1$, 1.0, and 3.0 K, to stay below the critical field $B=\frac{3}{2}A$ where sine-Gordon solitons become unstable. As was expected, the fourth-order contributions of the biquadratic term change the energy of the static solitons by as much as a factor of 2 with respect to $\alpha=0$ for $g\mu_B H=3$.

To sum up, we have found that biquadratic exchange affects the solitons energy in one-dimensional magnetic chains such as $CsNiF_3$ significantly, and that corrections found in a fourth-order approximation in lattice spacing over wavelength can also be noticeable. The agreement of sine-Gordon results with experiment is greatly improved with a small, negative, biquadratic term.

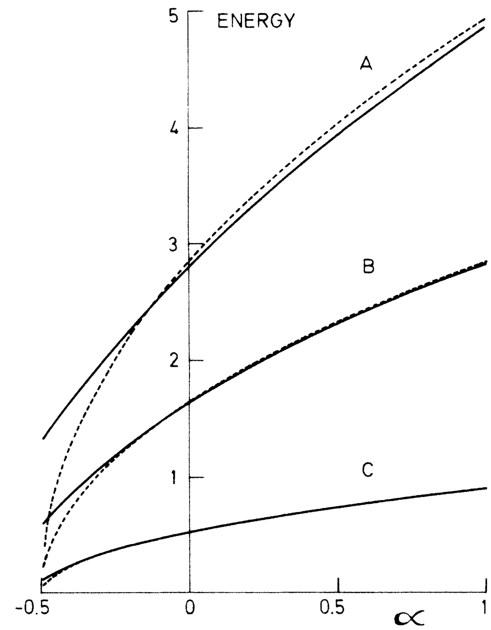

FIG. 2. Energy (in units of JS^2) of static solitons in the second-order (dashed line) and fourth-order (solid line) approximation in lattice spacing over wavelength as a function of α, the parameter measuring the strength of biquadratic superexchange, for three different magnetic fields; A: $g\mu_B H=3$ K; B: $g\mu_B H=1$ K; C: $g\mu_B H=0.1$ K.

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[1] See for instance, *Solitons and Condensed Matter Physics,* edited by A. R. Bishop and T. Schneider (Springer, New York, 1978); *Physics in One Dimension,* edited by J. Bernasconi and T. Schneider (Springer, New York, 1981).

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