

Solitons in a generalized classical antiferromagnetic chain

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Abstract We study non linear excitations in the one-dimensional classical anisotropic antiferromagnetic Heisenberg model including fourth-order anisotropic terms, interchain interaction and a Moriya-Dzyaloshinskii term.

1. Introduction

Non-linear modes in one-dimensional ferromagnets have been extensively studied in recent years, there being an enormous literature concerning this subject¹. It is known, however, that in antiferromagnets, where we have two equivalent sublattices, the dynamics of nonlinear excitations is different in several aspects². The most interesting model to study theoretically is the one-dimensional classical anisotropic Heisenberg antiferromagnet. Mikeska² has considered various combinations of external magnetic fields and single-ion anisotropies. Kimura and de Jonge³ considered the case of positive and negative axial anisotropy. Costa and Pires⁴ have studied the model with the magnetic field in an arbitrary direction, and the case of two anisotropies has been investigated extensively by Pires and coworkers⁵. Pandit et al.⁶ have considered the antiferromagnet with a single-ion anisotropy and a Dzyaloshinskii-Moriya term.

In the present paper we carry out a detailed study of some aspects, not considered before in the literature, of the dynamics of non-linear excitations (soliton modes) in a one-dimensional classical anisotropic antiferromagnetic Heisenberg model. At this point it is important to mention that there are some equivalences between the theories for solitons in one-dimensional magnets and domain walls in the ordered phase of three-dimensional magnets⁷. In section 2 we will consider

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the inclusion of fourth-order anisotropy constants and interchain interactions. In section 3 we will study the interesting case when we have a Moriya-Dzyaloshinskii term leading to a weak ferromagnetic moment. The presence of such a moment makes it possible to control the motion of the soliton by means of an external magnetic field.

2. Equations of motion

We start with the Hamiltonian of an array of weakly coupled spin chains

$$H = 2J \sum_{n,i} \left[\vec{S}_{n,i} \cdot \vec{S}_{n+1,i} + d(S_{n,i}^z)^2 + b(S_{n,i}^y)^2 + B_1(S_{n,i}^z)^4 + B_2(S_{n,i}^y)^4 + B_3(S_{n,i}^z S_{n,i}^y)^2 \right] + 4J' \sum_{\substack{n \\ i \neq i'}} \vec{S}_{n,i} \cdot \vec{S}_{n,i'} \quad (1)$$

where i labels the chain and n a site along the chain, d and b are the second order and B_1, B_2, B_3 the fourth-order anisotropy constants. The intrachain exchange constant J is much larger than J' , the interchain exchange. We will consider only the situation where the temperature is higher than the Néel temperature, and assume $J, d, b > 0$ and all the anisotropy parameters small compared to unity. The classical ground state configuration of eq. (1) is Ising-like, $\vec{S} = (\pm S, 0, 0)$.

Following Mikeska⁷ we write \vec{S} as

$$\vec{S}_m = (-1)^m S \{ \sin(\theta_m + (-1)^m v_m) \cos(\phi_m + (-1)^m \alpha_m), \sin(\theta_m + (-1)^m v_m) \sin(\phi_m + (-1)^m \alpha_m), \cos(\theta_m + (-1)^m v_m) \} \quad (2)$$

where m is any site in the crystal, θ and ϕ are the angles giving the sublattice magnetization, and v and α describe the deviations from perfect anti-alignment, and can therefore be assumed to be small at low temperatures. Substituting eqs. (2) into (1) we can keep only terms up to second order in the small quantities v, α and the spatial variation of θ and ϕ . The variables v and α are then eliminated with $\partial\theta/\partial t$ and $\partial\phi/\partial t$, which can be derived from the equation of motion of the spins. Using the continuum approximation we obtain

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$$\begin{aligned}
\chi = JS^2 \int dV \left\{ \frac{1}{a} \left[\left(\frac{\partial \theta}{\partial z} \right)^2 + \sin^2 \theta \left(\frac{\partial \phi}{\partial z} \right)^2 \right] + \frac{J'}{Ja'} \left[\left(\frac{\partial \theta}{\partial x} \right)^2 + \left(\frac{\partial \theta}{\partial y} \right)^2 \right. \right. \\
+ \left. \left. \sin^2 \theta \left(\frac{\partial \phi}{\partial x} \right)^2 + \sin^2 \theta \left(\frac{\partial \phi}{\partial y} \right)^2 \right] + \frac{4}{S^2} P_0^2 + \frac{4}{S^2} \frac{P_\phi^2}{\sin^2 \theta} + 2d \cos^2 \theta \right. \\
+ 2b \sin^2 \theta \sin^2 \phi + 2\beta_1 \cos^4 \theta + 2\beta_2 \sin^4 \theta \sin^4 \phi + \\
\left. + 2\beta_3 \cos^2 \theta \sin^2 \theta \sin^2 \phi \right\}, \quad (3)
\end{aligned}$$

where the canonical momenta P_θ and P_ϕ are given by

$$P_\theta = \frac{1}{8J} \frac{\partial \theta}{\partial t}, \quad P_\phi = \frac{1}{8J} \sin^2 \theta \frac{\partial \phi}{\partial t},$$

and $\beta_i = S^2 B_i$ ($i = 1, 2, 3$), a is the intrachain lattice constant, a' the interchain distance and z is the coordinate along the chain.

The equations of motion can be obtained directly from the Hamiltonian eq.

(3). We obtain

$$\begin{aligned}
\tilde{\nabla}^2 \theta - \frac{1}{c^2} \frac{\partial^2 \theta}{\partial t^2} = \sin \theta \cos \theta (\tilde{\nabla} \phi)^2 - \frac{1}{c^2} \sin \theta \cos \theta \left(\frac{\partial \phi}{\partial t} \right)^2 \\
- 2d \cos \theta \sin \theta + 2b \sin \theta \cos \theta \sin^2 \phi - 4\beta_1 \cos^3 \theta \sin \theta \\
+ 4\beta_2 \sin^3 \theta \cos \theta \sin^4 \phi - 2\beta_3 \sin^2 \phi \cos \theta \sin \theta (\sin^2 8 - \cos^2 0), \quad (4)
\end{aligned}$$

$$\begin{aligned}
\tilde{\nabla}^2 \phi - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = -2 \cot \theta \left[(\tilde{\nabla} \theta) \cdot (\tilde{\nabla} \phi) - \frac{1}{c^2} \left(\frac{\partial \theta}{\partial t} \right) \left(\frac{\partial \phi}{\partial t} \right) \right] \\
+ 2b \sin \phi \cos \phi + 4\beta_2 \sin^2 \theta \sin^3 \phi \cos \phi + 2\beta_3 \cos^2 \theta \sin \phi \cos \phi, \quad (5)
\end{aligned}$$

where

$$c = 4JS \quad \text{and} \quad \tilde{\nabla} = \vec{i} \frac{\partial}{\partial z} + \alpha \left(\vec{j} \frac{\partial}{\partial x} + \vec{k} \frac{\partial}{\partial y} \right)$$

with

$$\alpha = J'a/Ja'.$$

Under the prescribed boundary conditions (i.e. the spins are aligned along the x axis for $z \rightarrow \pm\infty$) there can exist two types of moving solitons. Type I

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corresponds to $\phi = \pi/2$, that is the soliton is in the XY plane. Type II corresponds to $\phi = 0$ and the soliton is in the XZ plane. Since the solutions are similar, let us consider just type I solitons. Restricting ourselves to solitons propagating along the chain, i.e. taking $\phi = \phi(z, t)$ eq. (5) becomes

$$\frac{\partial^2 \phi}{\partial z^2} - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = 2b(1 + 2p \sin^2 \phi) \sin \phi \cos \phi, \quad (7)$$

where $p = \beta_2/b$. If we restrict ourselves to the study of stationary-profile solutions, writing $\xi = z - ut$, we can write eq. (7) as

$$\frac{d^2 \phi}{d\xi^2} = m^2 (1 + 2p \sin^2 \phi) \sin \phi \cos \phi, \quad (8)$$

with

$$m^2 = 2b(1 - u^2/c^2)^{-1} \quad (9)$$

For $b > 0$, $\beta_2 > 0$, $p < 1$, we find on integrating eq.(8)

$$\tan \phi = (1 + p)^{-1/2} \operatorname{cosech}(m\xi). \quad (10)$$

Taking eq.(10) into eq.(3) we find for the static soliton energy

$$E_s^0 = 2JS^2 \sqrt{2b} \left[1 + \frac{(p+1)}{\sqrt{p}} \tan^{-1} \sqrt{p} \right] \quad (11)$$

If the parameter p is **negative** we have the following cases

- a) $-1 < p < 0$. The solution is still given by eq. (10) and we have a moving π soliton.
- b) $p = -1$. We have a $\pi/2$ soliton given by

$$\tan \phi = \exp(-m\xi). \quad (12)$$

- c) $p < -1$. We have

$$\tanh \phi = |1 + p|^{-1/2} \operatorname{sech}(m\xi) \quad (13)$$

and the values of ϕ at $\xi \rightarrow +\infty$ and $\xi \rightarrow -\infty$ coincide ($\phi \rightarrow 0$ when $\xi \rightarrow \pm\infty$).

If $b = 0$ eq.(7) becomes

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$$\frac{d^2\phi}{d\xi^2} - 2r \sin^3 \phi \cos \phi , \quad (14)$$

with

$$r = 2\beta_2(1 - u^2/c^2) .$$

The solution of this equation is

$$\tan \phi = (\xi\sqrt{r})^{-1} , \quad (15)$$

a 180-degree algebraic soliton in which the spins approach their equilibrium values according to a power law instead of doing it exponentially as in the other cases considered here. The energy of this soliton is given by

$$E_s^0 = JS^2\pi\sqrt{2\beta_2} . \quad (16)$$

Taking $p = 0$ in eq. (7) we get the well-studied sine-Gordon model.

Since we have considered only a limited type of solution in which the angle θ is constant and equal to $\pi/2$ (the case of $\phi = 0$ can be analyzed in a similar way), it is therefore necessary to investigate the stability of this solution with respect to departure of the soliton from the corresponding plane. For simplicity we will take $B_i = 0$ ($i = 1, 2, 3$) and write

$$\theta(x, y, z, t) = \pi/2 + s(x, y, z) \exp(i\omega_1 t) , \quad (17)$$

$$\phi(x, y, z, t) = \phi_{\text{sol}}(z) + r(x, y, z) \exp(i\omega_2 t) , \quad (18)$$

Substitution of (17) and (18) into (4) and (5) and linearization in s and r leads to the following eigenvalue equations

$$\frac{d^2 r}{dz^2} + \alpha \left(\frac{d^2 r}{dx^2} + \frac{d^2 r}{dy^2} \right) + \frac{\omega_1^2}{c^2} r = 2b(1 - 2\text{sech}^2 \sqrt{2bz}) r , \quad (19)$$

$$\frac{d^2 s}{dz^2} + \alpha \left(\frac{d^2 s}{dx^2} + \frac{d^2 s}{dy^2} \right) + \frac{\tilde{\omega}_1^2}{c^2} s = 2b(1 - 2\text{sech}^2 \sqrt{2bz}) s , \quad (20)$$

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where $\tilde{\omega}_1^2 = \omega_1^2 - 2(6 - b)c^2$.

The dispersion relation is determined by the behavior far from the soliton centre. We find

$$\omega_1^2(\vec{q}) = (2\delta + q_z^2 + \alpha q_\perp^2)c^2, \quad (21)$$

$$\omega_2^2(\vec{q}) = (2b + q_z^2 + \alpha q_\perp^2)c^2,$$

where $\vec{q}_\perp = \vec{i}q_x + \vec{j}q_y$. Eqs. (19) and (20) have the form of a Schrödinger equation with a known complete set of eigenfunctions⁸. Eq. (19) possesses a bound-state solution with

$$\omega_{1b} = \sqrt{\alpha}q_\perp c, \quad (22)$$

and (20) a bound-state with

$$\omega_{2b}^2 = \omega_b^2 + \alpha q_\perp^2 c^2, \quad (23)$$

where

$$\omega_b^2 = 2(\delta - b)c^2. \quad (24)$$

Eq.(24) shows that the type I soliton is stable if $b < 6$ and is unstable in the contrary case. Investigation of the stability of type II soliton proceeds similarly and leads to the condition $6 < b$. Thus the soliton is stable which corresponds to the smaller value of the anisotropy parameter: only one of the two types of soliton can exist. To conclude we see that the spectrum of an antiferromagnet supporting solitons **contains** four magnon modes, two with wave functions

$$f_q = \frac{(q/\sqrt{2b} + i \tanh \sqrt{2bz})}{[2\pi(1 + q^2/2b)]^{1/2}} e^{i\vec{q}\cdot\vec{r}} \quad (25)$$

and frequencies given by eq.(21), corresponding to intrachain excitations and two with wave functions

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$$f_{q\perp} = \frac{(2b)^{1/4}}{\sqrt{2}} \operatorname{sech}(\sqrt{2b}z) e^{i\vec{q}_1 \cdot \vec{r}_\perp}, \quad (26)$$

(where $\vec{r}_\perp = x\vec{i} + y\vec{j}$) having frequencies given by eqs.(22) and (23) and corresponding to excitations localized on the soliton.

3. Dynamics of a canted aniferromagnet

We will now include a Dzyaloshinskii-Moriya term in our Hamiltonian. Such a term is important in order to explain experimental data on the polymer⁶ $\{\text{Co}[(\text{C}_4\text{H}_9)_2\text{PO}_2]_2\}_x$. So we will write a term

$$2JD\vec{i} \cdot \sum_n \vec{S}_n \times \vec{S}_{n+1}, \quad (27)$$

in our Hamiltonian (1) and for simplicity take $B_i = 0$, ($i = 1, 2, 3$) and $J' = 0$. The equation of motion for a type I soliton will then become

$$\frac{\partial^2 \phi}{\partial z^2} - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = 2\tilde{b} \sin \phi \cos \phi \quad (28)$$

where $\tilde{b} = b - D^2$. Eq. (28) is the sine-Gordon equation with solution

$$\phi = 2 \tan^{-1} \exp(-\sqrt{2\tilde{b}}\xi) \quad (29)$$

In what follows it is important, in this case, to know the value of the coordinate v . We have, solving the general equations of motion including the term given by eq. (27)

$$v = 2D \tanh(\sqrt{2\tilde{b}}\xi) + u \frac{\sqrt{2\tilde{b}}}{4JS} \operatorname{sech}(\sqrt{2\tilde{b}}\xi) \quad (30)$$

The solutions obtained above describe the motion of a soliton without allowance for dissipation and a driving force. As a driving force one usually uses an external magnetic field \vec{H} , applied in such a way that because of the magnetic Zeeman energy in a length z ,

$$E_m = -2gu_B \vec{m} \cdot \vec{H} z \quad (31)$$

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with

$$\vec{m} = (\vec{S}_1 + \vec{S}_2)/2 , \quad (32)$$

one of the homogeneous regions of the magnetic chain that are separated by the soliton (that in which $\vec{m} \cdot \vec{H} > 0$ becomes energetically advantageous as compared with the other ($\vec{m} \cdot \vec{H} < 0$). Then there acts on the soliton a force \vec{F}_m that is directed toward the less advantageous region. The moving soliton is also subject to a retarding force $F_d(u)$, produced by various dissipative processes and dependent on the soliton velocity u . At a certain value of u equilibrium occurs, $F_m = F_d(u)$, and the soliton motion becomes stationary.

We shall treat the motion of the soliton under the assumption that both the damping constant a and the driving field H are small in comparison with the characteristic quantities of the problem. In this case it may be supposed that the soliton structure is the same as for $H = a = 0$ and is described by the formulas obtained above. Then from

$$F_m = 2gu_B S \vec{H} \cdot \Delta \vec{m} , \quad (33)$$

letting $H // Oz$, which leads to

$$\Delta m_z = m_z(+\infty) - m_z(-\infty) ,$$

and using the fact that for a type I soliton $m_z = -v$, we obtain from eq. (30)

$$Am_z = 4D . \quad (34)$$

Thus

$$F_m = 8gu_b S H D \quad (35)$$

The magnetic force vanishes in the absence of the Dzyaloshinskii-Moriya term.

The damping force can be calculated using the relation

$$F_d = -\frac{1}{u} \frac{dE}{dt} . \quad (36)$$

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From ref. (4) we have

$$\frac{dE}{dt} = \frac{2\alpha}{c} \int_{-\infty}^{\infty} \left(\frac{\partial \phi}{\partial t} \right)^2 dz , \quad (37)$$

where dissipative effects are taken in account via a Gilbert term

$$i\hbar \dot{\vec{S}} = [\vec{S}, \mathcal{H}] - i\hbar(4J\alpha)\vec{S} \times \dot{\vec{S}} . \quad (38)$$

Using eq.(29) we obtain

$$F_d = \frac{4\alpha}{c} \left(\frac{2\tilde{b}}{1 - u^2/c^2} \right)^{1/2} u . \quad (39)$$

The velocity u of the stationary motion of the soliton is found from the condition $F_m = F_d(u)$. We obtain

$$u = \frac{hc}{\sqrt{h^2 + \alpha^2}} , \quad (40)$$

with $h = 2gu_B SDH/\sqrt{2\tilde{b}}$. As we can see, if D or H vanishes we have $u = 0$ and if $\alpha = 0$ we have $u(H) = c$. When $D \neq 0$ it is possible to control the motion of the soliton by means of an external magnetic field.

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Resumo

Estudamos excitações não lineares em um antiferromagneto de Heisenberg unidimensional clássico anisotrópico, com a inclusão de termos de anisotropia de quarta ordem, interação **entre** cadeias e um termo de Moriya-Dzyaloshinskii.