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# Non-linear dynamics of classical one-dimensional antiferromagnets

H J Mikeska
Institut für Theoretische Physik, University of Hannover, Hannover, Germany

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**Abstract.** Solutions are presented to the non-linear equations of motion of classical antiferromagnetic chains in a continuum description. Results have been obtained for, in addition to isotropic exchange, various combinations of single-ion anisotropies (Ising and *xy*-like) and external magnetic fields (supporting and breaking the anisotropy). Among the solutions are both sine-Gordon solitons, representing antiferromagnetic domain walls, and pulse solitons with continuously varying amplitude. Solitons in the *xy* antiferromagnet in a symmetry-breaking external field are discussed with respect to their observability in TMMC. They are found to contribute two different central peaks to the dynamical structure factor.

## 1. Introduction

The problem of treating the time development of a macroscopically large number of spins coupled by mutual exchange interactions is essentially non-linear. Nevertheless, the dynamics of spin systems have almost exclusively been treated in linearising approximations, admitting only small deviations from thermal-equilibrium configurations. It is only recently that one has been able to investigate some aspects of the full non-linear equations of motion in more detail. Progress has been possible by restricting the general problem to a treatment of a one-dimensional array of spins; furthermore a classical continuum approximation has frequently been introduced. These restrictions lead to well defined models, which include essential aspects of the non-linearity and which may be investigated without further approximations.

Investigating this type of model, the isotropic Heisenberg ferromagnet with a possible external magnetic field has been found to possess pulse-like finite-amplitude solutions (pulse solitons) in addition to the well known spin waves or magnons (Nakamura and Sasada 1974, Tjon and Wright 1977); this has been generalised to include an easy-axis anisotropy (Long and Bishop 1979). In addition it has been shown that the isotropic Heisenberg ferromagnet is completely integrable, magnons and pulse solitons exhausting the spectrum (Takhtajan 1977, Fogedby 1979). As a second example the *xy* ferromagnet in a symmetry-breaking external field (i.e. a field in the easy plane) has been shown under certain provisions to be equivalent to the sine-Gordon (SG) chain (Mikeska 1978). The SG chain is the prototype of solvable non-linear field theories; it is completely integrable, its spectrum being exhausted by solitons (kinks), breathers and small oscillations (magnons) (Fadeev and Takhtajan 1974). There is an important difference between the various types of finite-amplitude solutions: solitons exhibit an energy gap and are topologically stable, whereas pulse solitons and breathers do not exhibit an energy gap and may be continuously deformed to localised small-amplitude solutions.

In this paper we will present results on the non-linear dynamics of antiferromagnetic chains in the classical continuum approximation. From a physical point of view, the continuum approximation has to be regarded as a low-temperature approximation. In an antiferromagnet this implies nearly perfect local antialignment of spins. This will allow us to reduce the number of degrees of freedom to be treated non-linearly from four to two. The continuum approximation and the resultant equations of motion will be given in § 2. In the following sections we will consider various combinations of external magnetic fields and single-ion anisotropies: an Ising-like anisotropy with a possible staggered field (§ 3), an $xy$-like anisotropy and/or an external field in the $z$ direction (§ 4) and an $xy$-like anisotropy with a symmetry-breaking field in the $xy$ plane (§ 5). Solutions to the full non-linear equations of motion will be obtained and discussed in these cases; both solitons and pulse solitons will be encountered.

The thermodynamic significance of these finite-amplitude solutions is clearly an important subject. However, it is only for the SG chain that results have been obtained on the contributions of solitons to the partition function (Gupta and Sutherland 1976, Currie *et al* 1977, 1979) and to dynamic correlation functions by both analytical (Mikeska 1978) and numerical (Stoll *et al* 1979) methods. The analytical approaches follow the work of Krumhansl and Schrieffer (1975) on the $\Phi^4$ system, which also exhibits soliton solutions; an analogous treatment of the thermodynamic significance of pulse solitons and breathers is inhibited owing to the absence of an energy gap. We will draw on previous work to discuss how soliton solutions in the antiferromagnetic chain show up in dynamic correlation functions, whereas the contribution of pulse solitons is the subject of work being done at present. The restriction to one-dimensional systems is not only of advantage for theoretical progress, but is also of experimental interest. The predictions on the $xy$ ferromagnet in a symmetry-breaking field have turned out to be relevant for neutron scattering experiments on $CsNiF_3$ (Kjems and Steiner 1978). We expect that the results of this paper, as far as the $xy$ antiferromagnet is concerned, may be useful for interpreting analogous experiments on the one-dimensional antiferromagnet TMMC. Therefore, in § 5, we will also discuss in some detail the consequences of our results for inelastic neutron scattering experiments on TMMC in an external field in its $xy$ plane.

## 2. Model, continuum approximation and equations of motion

In this paper we will be concerned with one-dimensional magnetic systems with antiferromagnetic nearest-neighbour exchange $J < 0$ and single-ion anisotropy $A(S^z)^2$ in external (ordinary and staggered) magnetic fields as described by the Hamiltonian

$$\mathscr{H} = -J\sum_n \boldsymbol{S}_n \boldsymbol{S}_{n+1} + A\sum_n (S_n^z)^2 - g\mu_{\mathrm{B}}\boldsymbol{B}\sum_n \boldsymbol{S}_n - g\mu_{\mathrm{B}}\boldsymbol{B}_S\sum_n (-1)^n \boldsymbol{S}_n. \tag{2.1}$$

Corresponding to the two possible signs of $A$ (2.1) can cover two types of anisotropy: an easy-plane ($xy$-like) anisotropy for $A > 0$ and an easy-axis (Ising-like) anisotropy for $A < 0$. The $xy$-like symmetry is supported, owing to the spin flop effect, by a magnetic field $\boldsymbol{B}$ in the $z$ direction, whereas it is further broken by a magnetic field in the $xy$ plane. The Ising-like symmetry will be considered together with a staggered field in the $z$ direction.

At low temperatures a slow variation of the classical spin vectors in space is expected. A continuum approximation which is adapted to these slow variations is performed in the following way: we introduce two continuously varying spin vectors $\boldsymbol{S}_{\text{even}}(z,t)$ and $\boldsymbol{S}_{\text{odd}}(z,t)$ and parametrise them in terms of four fields $\Theta(z,t)$, $\Phi(z,t)$, $\theta(z,t)$, $\phi(z,t)$

$$\left\{\begin{matrix}\boldsymbol{S}_{\text{even}}(z,t)\\ \boldsymbol{S}_{\text{odd}}(z,t)\end{matrix}\right\} = \pm S(\sin(\Theta\pm\theta)\cos(\Phi\pm\phi), \sin(\Theta\pm\theta)\sin(\Phi\pm\phi), \cos(\Theta\pm\theta)). \tag{2.2}$$

$\boldsymbol{S}_{\text{even}}$ ($\boldsymbol{S}_{\text{odd}}$) will be used to describe the spins at even (odd) lattice sites. $(\boldsymbol{S}_{\text{even}} + \boldsymbol{S}_{\text{odd}})/2$ is the local magnetisation, whereas $(\boldsymbol{S}_{\text{even}} - \boldsymbol{S}_{\text{odd}})/2$ is the local sublattice magnetisation. We will assume in the following that the magnetic field is small, $g\mu_{\text{B}}B/JS \ll 1$, which is true for all reasonable values of the magnetic field in the cases of practical interest. Then at low temperatures the local spin structure will be very close to antiferromagnetic. Deviations from the antiferromagnetic alignment occur owing to small spatial variations and to small values of the local magnetisation. In terms of the fields introduced above a continuum approximation for small magnetic fields therefore implies an expansion according to ($a$ is the lattice constant):

$$(a\partial/\partial z) \ll 1, \qquad \theta \ll 1, \qquad \sin\Theta\phi \ll 1, \tag{2.3}$$

whereas the important non-linearities related to the dominating antiferromagnetic exchange will be included fully, since no restrictions on the values of $\Theta$ and $\Phi$ are made. Applying this continuum approximation to the Hamiltonian given in (2.1) we obtain

$$\mathscr{H} = \text{constant} + \tfrac{1}{2}|J|S^2 \int \mathrm{d}z[h_{\text{exc}}(z) + h_{\text{aniso}}(z) + h_{\text{Zeeman}}(z)] \tag{2.4}$$

$$h_{\text{exc}} = (\partial\Theta/\partial z)^2 + 4\theta^2 + \sin^2\Theta[(\partial\Phi/\partial z)^2 + 4\phi^2] \tag{2.5}$$

$$h_{\text{aniso}} = \kappa[\cos^2\Theta + \theta^2(1 - 2\cos^2\Theta)] \tag{2.6}$$

$$h_{\text{Zeeman}} = 2b_z\sin\Theta\theta - 2b_x(\cos\Theta\cos\Phi\theta - \sin\Theta\sin\Phi\phi) - 2b_{Sz}\cos\Theta \tag{2.7}$$

where we have used the lattice constant $a$ as unit of length and have introduced the notation

$$\kappa = 2A/|J|, \qquad b_\alpha = g\mu_{\text{B}}B_\alpha/|J|S. \tag{2.8}$$

The equations of motion can be obtained either directly by applying the continuum approximation to the equations of motion on the discrete lattice or from the Hamiltonian (2.4)–(2.7) using the following Poisson brackets:

$$\begin{aligned}&\{\cos\Theta(z)\cos\theta(z), \phi(z')\} = -\{\sin\Theta(z)\sin\theta(z), \Phi(z')\} = (a/S)\,\delta(z-z')\\ &\{\sin\Theta(z)\sin\theta(z), \phi(z')\} = \{\cos\Theta(z)\cos\theta(z), \Phi(z')\} = 0\\ &\{\Theta(z), \theta(z')\} = \{\Phi(z), \phi(z')\} = 0.\end{aligned} \tag{2.9}$$

These Poisson brackets are derived from the fundamental Poisson bracket

$$\{S_n^z, \Phi_{n'}\} = \delta_{nn'} \tag{2.10}$$

for the polar representation of a spin vector (Villain 1974). The resulting equations of motion are

$$\partial\Theta/\partial t = 4\phi\sin\Theta + b_x\sin\Phi \tag{2.11}$$

$$\partial\Phi/\partial t = -(4\theta/\sin\Theta) - \kappa\theta\sin\Theta - b_z + b_x\cos\Phi\cot\Theta \tag{2.12}$$

$$\partial\theta/\partial t = -4\phi\theta\cos\Theta - 2\cos\Theta\,\partial\Phi/\partial z\,\partial\Theta/\partial z - \sin\Theta\,\partial^2\Phi/\partial z^2 + b_x\cos\Phi\phi \tag{2.13}$$

$$\frac{\partial\phi}{\partial t} = 4\theta^2\frac{\cos\Theta}{\sin^2\Theta} - \cos\Theta\left[4\phi^2 + \left(\frac{\partial\Phi}{\partial z}\right)^2\right] + \frac{1}{\sin\Theta}\frac{\partial^2\Theta}{\partial z^2} + \kappa\cos\Theta(1 - \tfrac{1}{2}\theta^2)$$
$$- b_x\left(\phi\sin\Phi\cot\Theta + \theta\frac{\cos\Phi}{\sin^2\Theta}\right) - b_S \tag{2.14}$$

where we have used $(|J|S)^{-1}$ as unit of time. We will discuss solutions to these coupled non-linear equations in the following sections. To conclude this section we want to point out how the ordinary antiferromagnetic spin-wave solution ($b_x = b_z = 0$, $\kappa = 0$) is obtained from equations (2.11)–(2.14): Use $b_S \neq 0$ to establish a preferred direction and linearise in $\Theta$ (looking for small-amplitude oscillations) to obtain a solution with $\phi = 0$, constant values for $\Theta$ and $\theta$ and

$$\Phi = kz - \omega t, \qquad 4\theta = \omega\Theta, \qquad \omega^2 = c^2(k^2 + b_S). \tag{2.15}$$

Here

$$c = 2|J|Sa \tag{2.16}$$

is the long-wavelength spin-wave velocity ($c = 2$ in our dimensionless units).

## 3. Soliton solutions in Ising-like antiferromagnetic chains

We will now investigate localised finite amplitude solutions to the equations of motion in the case $\kappa = -|\kappa| < 0$, $b_S \neq 0$, $b_x = b_z = 0$. We start by investigating solutions to equations (2.11)–(2.14), which depend on $s = z - ut$, assuming only $b_x = 0$. Then it is easy to obtain from (2.11) and (2.13) the following integral:

$$\sin^2\Theta\,\mathrm{d}\Phi/\mathrm{d}s - u\theta\sin\Theta = c_1. \tag{3.1}$$

Using this result, the equations of motion reduce to

$$(1 - u^2/c^2)\,\mathrm{d}^2\Theta/\mathrm{d}s^2 = F(\Theta) \tag{3.2}$$

$$\theta = \frac{1}{\sin\Theta}\frac{\sin^2\Theta\, b_z - uc_1}{u^2 - 4 - \kappa\sin^2\Theta} \tag{3.3}$$

$$\phi = -\frac{u}{4\sin\Theta}\frac{\mathrm{d}\Theta}{\mathrm{d}s}. \tag{3.4}$$

The general expression for $F(\Theta)$ is too long to be given here; it always allows one analytical integration, whereas the second integration would have to be performed numerically in the general case $\kappa \neq 0$ and $b_z \neq 0$. $\theta$ and $\phi$ can then be found from equations (3.3) and (3.4) and one more integration is necessary to obtain $\Phi$ from equation (3.1).

We now consider the case $b_z = 0$, $\kappa < 0$ and/or $b_S > 0$, i.e. an antiferromagnet with Ising symmetry, which allows a complete analytical treatment. The boundary condition at infinity is $\Theta = 0$, which from equations (3.1) and (3.3) leads to $c_1 = 0$, $\theta = o$, $\Phi =$

constant. Equation (3.2) now reads

$$(1 - u^2/c^2)\,\mathrm{d}^2\Theta/\mathrm{d}s^2 = \tfrac{1}{2}|\kappa|\sin 2\Theta + b_S \sin\Theta. \tag{3.5}$$

The more conventional form of this equation, with the LHS replaced by $\partial^2\Theta/\partial z^2 - (1/c^2)\partial^2\Theta/\partial t^2$ may be obtained directly from equations (2.11) to (2.14) when one makes use of the fact that $\theta = 0$ leads to a consistent solution. The general case $|\kappa| \neq 0$ and $b_S \neq 0$ is thus equivalent to a double SG equation, whereas for $\kappa = 0$ one has a SG equation for the polar angle $\Theta$ with mass parameter $m^2 = b_S$. The antiferromagnet in a staggered field is therefore quite different from the corresponding case of a ferromagnet in a magnetic field (Long and Bishop 1979). The antiferromagnet can be mapped to a SG equation, which is well known (see e.g. Barone *et al* 1971) to have stable soliton solutions with an energy gap and breather solutions, whereas in the ferromagnetic case topologically unstable pulse solitons are found, which share many properties with breathers.

For $b_S = 0$, on the other hand, equation (3.5) reduces to a SG equation for $2\Theta$ with mass parameter $m^2 = |\kappa|$. The soliton solutions to this equation have a rest energy of $2|J|S^2|\kappa|^{1/2}$ as found by using the solution in (2.4). The soliton solution in this case is physically a (moving) domain wall which mediates between the two degenerate ordered configurations of an Ising antiferromagnet. These domain walls contribute to the dynamic structure factor a central peak, which will be discussed in some detail in § 5 in a slightly different physical context.

## 4. Soliton solutions in *xy*-like antiferromagnetic chains

In this section we will consider localised non-linear excitations in the case when the spins are essentially confined to the $xy$ plane. This situation occurs both with a magnetic field in the $z$ direction, $b_z \neq 0$, and with a positive single-ion anisotropy $\kappa > 0$. The equilibrium configuration at infinity then is the spin-flopped state with

$$\sin\Theta = 1, \qquad \theta = b_z/(4+\kappa), \qquad \mathrm{d}\Phi/\mathrm{d}s = 0. \tag{4.1}$$

Since we continue to assume $b_x = 0$, equations (3.1)–(3.4) may be used again, the different boundary condition at infinity now leading to

$$c_1 = ub_z/(4+\kappa). \tag{4.2}$$

Instead of giving the rather complicated complete expression for $F(\Theta)$ as introduced in (3.2) we consider the two limiting cases

$\kappa > 0, b_z = 0$

$$F(\Theta) = -\tfrac{1}{2}\kappa\sin 2\Theta \tag{4.3}$$

$\kappa = 0, b_z \neq 0$

$$F(\Theta) = \frac{b_z^2}{4}\,\frac{u^2/c^2 - \sin^4\Theta}{1 - u^2/c^2}\,\frac{\cos\Theta}{\sin^3\Theta}. \tag{4.4}$$

For small anisotropies $\kappa \ll 4$ and small velocities $u \ll c$ the complete expression actually is the sum of these limiting expressions. One therefore observes that the magnetic field would have to fulfil $b_z \gg 2\kappa^{1/2}$ in order to dominate the single-ion anisotropy at least for slowly moving solutions. Even for the rather small anisotropy encountered in TMMC ($\kappa \approx 10^{-2}$) this is a condition practically impossible to meet.

We now discuss the solutions following from the expressions for $F(\Theta)$ given above. Using equation (4.3) in (3.2), a SG equation is obtained for the variable $\pi - 2\Theta$ with mass parameter $m^2 = \kappa$ The soliton solution to this equation is

$$\cos\Theta(z,t) = \operatorname{sech}\gamma\kappa^{1/2}(z - ut - z_0)$$
$$\Phi(z,t) = \Phi_0 + \tfrac{1}{2}\pi\,\mathrm{sign}(z - ut - z_0) \tag{4.5}$$

with $\gamma = (1 - u^2/c^2)^{-1/2}$. The corresponding energy is $2|J|S^2\gamma\kappa^{1/2}$. This solution describes a change in the direction of the sublattice magnetisation by $\pi$. It can be considered as a local domain wall, superimposed on the short-range order which extends over $|J|/T$ lattice sites and which is limited by small-amplitude fluctuations in the $xy$ plane (Villain 1974).

We now turn to the case $b_z \neq 0$, $\kappa = 0$. Using $F(\Theta)$ from equation (4.4), equation (3.2) can be integrated to give

$$\cos\Theta(z,t) = (1 - u^2/c^2)^{1/2}\operatorname{sech}\xi$$
$$\Phi(z,t) = \Phi_0 + \tan^{-1}[(c/\gamma u)\operatorname{tgh}\xi]$$
$$\theta(z,t) = \tfrac{1}{4}b_z\operatorname{sech}\xi[1 + (u^2/c^2)\operatorname{cosech}\xi]^{1/2}$$
$$\phi(z,t) = (ub_z/4c)\sinh\xi[u^2/c^2 + \sinh^2\xi]^{-1} \tag{4.6}$$

where $\xi = \frac{1}{2}\gamma b_z(z - ut - z_0)$. The energy of this solution is given by

$$E = b_z(1 - u^2/c^2)^{1/2}|J|S^2. \tag{4.7}$$

The physical content of this solution can be described in the following way. As one proceeds along the chain, the sublattice magnetisation moves out of the easy plane up to a maximum angle $\pi/2 - \Theta_{\max}$ and returns to the easy plane with an orientation differing in azimuthal angle from the original one by $2\Delta\Phi$. From equation (4.6) one obtains $\sin\Delta\Phi = (1 - u^2/c^2)^{1/2}$. It is easy to see that energy $E$, maximum $z$-component $\cos\Theta_{\max}$ and spatial extension $2/\gamma b_z$ are all proportional to $\sin\Delta\Phi$. These solutions again are rather similar to the pulse solitons of the Heisenberg ferromagnet. It is interesting to note that in the present case the transition from the topologically unstable pulse soliton solutions, equations (4.6), to the SG soliton solution of equations (4.5) can be followed explicitly by varying $b_z/2\kappa^{1/2}$, if one allows for one numerical integration.

At present we can only speculate about the thermodynamic significance of these non-linear excitations. We expect that random jumps of the orientation of the sublattice magnetisation in the $xy$ plane will lead to a central peak in the dynamic structure factor which, however, will merely increase the contribution from quasi-spin-waves at small wavevector and frequency. This question is investigated in more detail at present.

## 5. Soliton solutions in antiferromagnetic chains with broken $xy$ symmetry

In this section we will consider an antiferromagnetic chain with an easy-plane single-ion anisotropy $\kappa > 0$ in a magnetic field in the easy plane, $b_x \neq 0$. At low temperatures, $T \ll (\kappa|J|/2)^{1/2}$, the spins are confined to the $xy$ plane, whereas the spin flop effect further forces the sublattice magnetisation into the $y$ direction. We want to analyse this situation, which is to some extent comparable to the easy-plane ferromagnet in a symmetry-breaking field, with a particular view to applications to TMMC. This material is an excellent one-dimensional antiferromagnet with a small easy-plane anisotropy of probably dipolar origin which, however, can be simulated by a single-ion anisotropy with $\kappa \approx 0{\cdot}03$ (Hone and Pires 1977, Heilmann *et al* 1979).

Owing to the confinement to the $xy$ plane, our equations of motion can be further linearised about $\Theta = \pi/2$. We introduce $\Theta_S = \pi/2 - \Theta$ and linearise equations (2.11) and (2.12) in $\Theta_S$ to obtain (note that $b_x \ll 1$ has also been assumed)

$$\partial\Theta_S/\partial t = -4\phi - b_x \sin\Phi \tag{5.1}$$

$$\partial\Phi/\partial t = -(4+\kappa)\,\theta. \tag{5.2}$$

Before discussing the remaining equations of motion, it is instructive to consider the Hamiltonian density following from equations (2.4)–(2.7) after using the equations above to eliminate $\theta$ and $\phi$:

$$h(z) = h_\Theta(z) + h_\Phi(z) + h^{(4)}(z) \tag{5.3}$$

$$h_\Theta(z) = \tfrac{1}{2}|J|S^2\left[\frac{1}{c^2}\left(\frac{\partial\Theta_S}{\partial t}\right)^2 + \kappa\Theta_S^2\right] \tag{5.4}$$

$$h_\Phi(z) = \tfrac{1}{2}|J|S^2\left[\frac{1}{c_t^2}\left(\frac{\partial\Phi}{\partial t}\right)^2 + \left(\frac{\partial\Phi}{\partial z}\right)^2 - \tfrac{1}{4}b_x^2\sin^2\Phi\right] \tag{5.5}$$

with $c = 2, c_t = (4+\kappa)^{1/2}$. $h^{(4)}(z)$ contains terms of fourth order in $\Theta_S$ and terms coupling $\Phi$ and $\Theta_S$, such as $b_x^2\,\Theta_S^2\cos^2\Phi$. Neglecting this higher-order coupling in a first approximation one has two decoupled modes: an out-of-plane harmonic oscillator (variable $\Theta_S$) and an in-plane SG system (variable $2\Phi - \pi$); this is seen most clearly by writing $h_\Phi$ in the more conventional way, using $\Psi = 2\Phi - \pi$

$$h_\Phi(z) = \tfrac{1}{8}|J|S^2\left[\frac{1}{c_t^2}\left(\frac{\partial\Psi}{\partial t}\right)^2 + \left(\frac{\partial\Psi}{\partial z}\right)^2 + \frac{b_x^2}{2}(\cos\Psi - 1)\right]. \tag{5.6}$$

The dynamics of the in-plane degree of freedom is therefore equivalent to the dynamics of a SG system with mass parameter $m = b_x/2$ and with the energy scale set by $\tfrac{1}{4}|J|S^2$. The equation of motion for $\Psi$ then is

$$\frac{\partial^2\Psi}{\partial z^2} - \frac{1}{c_t^2}\frac{\partial^2\Psi}{\partial t^2} = m^2\sin\Psi. \tag{5.7}$$

It can of course also be obtained directly from equations (2.13) and (2.14) by linearising in $\Theta_S$ and using (5.1) and (5.2). It should be noted that the coupling $h^{(4)}(z)$ enters into the Hamiltonian density on the same order as does the space dependence of $\Theta_S$. This means that the coupling will be important for the small-wavevector dispersion of the out-of-plane mode. This holds true also without a magnetic field and should not be neglected in an interpretation of the recent neutron scattering results concerning these modes in TMMC (Heilmann *et al* 1979).

The remainder of this section will be devoted to the dynamic properties of the in-plane degree of freedom, which can be discussed in terms of solitons and spin waves as has been done for the one-dimensional $xy$ ferromagnet in a field (Mikeska 1978). The density of solitons is determined by the parameters of the SG equation as before. A soliton in the antiferromagnetic chain, however, induces a change from 0 to $2\pi$ in the variable $2\Phi - \pi$, i.e. a change in $\Phi$ from $\pi/2$ to $-\pi/2$. A soliton in this case thus is an antiferromagnetic domain wall, mediating between the energetically most favourable spin-flopped states at $\Phi = \pm\pi/2$.

We now discuss the soliton contributions to spin correlation functions. They are different from the results for the $xy$ ferromagnetic chain owing to the difference between the spin orientation angle $\Phi$ and the sine-Gordon variable $2\Phi - \pi$. For the longitudinal (with respect to $B$) correlation function

$$\langle S_n^x(t)\, S_0^x(0)\rangle = (-1)^n \langle \cos \Phi_n(t) \cos \Phi_0(0)\rangle$$

the difference is only a minor one. The variation of the longitudinal spin component due to a soliton with velocity $u$ is given by

$$\cos \Phi(z, t) = \operatorname{sech}[m(1 - u^2/c_t^2)^{-1/2}(z - ut - z_0)] \tag{5.8}$$

and correlations are introduced by one soliton moving from the spin at $z = 0$ to the spin located at $z$ within the time $t$. The calculation of the resulting dynamic structure factor is equivalent to the one for the $xy$ ferromagnet (Mikeska 1978, giving the result

$$S^{xx}(q, \omega) = (\beta/2c_t q) \exp(-8\beta m) \exp(-4\beta m\omega^2/c_t^2 q^2)\, 16/(\cosh Q)^2 \tag{5.9}$$

where $Q = \pi q/2m$ and $q$ is now measured with respect to the antiferromagnetic Bragg point. The temperature $T = \beta^{-1}$ is measured in units of $\frac{1}{4}|J|S^2$.

The transverse spin-correlation function

$$\langle S_n^y(t)\, S_0^y(0)\rangle = (-1)^n \langle \sin \Phi_n(t) \sin \Phi_0(0)\rangle$$

is, however, different, since the variation of $\sin \Phi$ due to a soliton is given by

$$\sin \Phi(z, t) = \pm \tanh[m(1 - u^2/c_t^2)^{-1/2}(z - ut - z_0)]. \tag{5.10}$$

A passing soliton switches the domain orientation of the spin-flopped state and long-range correlations present without domain walls are diminished by the random passing of solitons. In an approximate description on a length scale large compared with the soliton extension $1/m$ we can replace $(-1)^n \sin \Phi(n, t)$ by a domain variable $\sigma(z, t) = \pm 1$. The $xy$-antiferromagnet in a symmetry-breaking field is thus equivalent to an Ising system as far as its transverse correlations are concerned. This reduction of symmetry of an antiferromagnet in a magnetic field was first noticed by Villain and Loveluck (1977). The correlation function in this case can be calculated using the method of Krumhansl and Schrieffer (1975), who investigated the $\Phi^4$ system, which also has Ising symmetry. This method leads to

$$\langle \sigma(z, t)\, \sigma(0, 0)\rangle = \exp[-2N(z, t)] \tag{5.11}$$

$N(z, t)$ being an average number of solitons (and antisolitons) at $t = 0$, consisting of two contributions: (i) the number of solitons between 0 and $z$, which will not pass $z$ in the time interval between 0 and $t$; (ii) the number of solitons outside the range from 0 to $z$, which will pass $z$ in the time interval between 0 and $t$. In the classical (Boltzmann) approximation one obtains

$$N(z, t) = 2n\, u_{\text{th}} t f(z/u_{\text{th}} t) \tag{5.12}$$

with

$$f(y) = \pi^{-1/2} e^{-y^2} + 2y\pi^{-1/2} \int_0^y dz\, e^{-z^2}$$

$$n = 4m(\beta m/\pi)^{1/2} \exp(-8\beta m)$$

$$u_{\text{th}} = c_t (4\beta m)^{-1/2}.$$

For a rough analytic discussion one can use the approximation

$$N(z, t) \approx 2n(\pi^{-1/2} u_{\text{th}}t + z) \tag{5.13}$$

which is correct for $x/u_{\text{th}}t$ both large and small compared with 1. This approximation leads to the following result for the transverse dynamic structure factor:

$$S^{yy}(q, \omega) = \frac{1}{\pi^2} \frac{\Gamma_{\text{D}}}{\omega^2 + \Gamma_{\text{D}}^2} \frac{\Gamma_S}{q^2 + \Gamma_S^2} \tag{5.14}$$

$$\Gamma_{\text{D}} = 4nc_t(4\pi\beta m)^{-1/2}, \qquad \Gamma_S = 4n.$$

It has to be considered as a broadening of the antiferromagnetic Bragg point (induced by the ordering of the $y$ component of spin owing to the field in the $x$ direction) due to the presence of moving domain walls. It should be noted that in contrast to equation (5.9) the widths $\Gamma_S$ and $\Gamma_{\text{D}}$ are proportional to the soliton density.

A central peak in an antiferromagnetic chain originating, from the broadening of a Bragg point, has already been considered by Villain (1975) for anisotropy-dominated $S = \frac{1}{2}$ chains. In contrast to the situation considered here, where the domain wall can be treated in the continuum approximation owing to $b_x \ll 1$, a large anisotropy implies an extreme localisation of the domain wall to essentially one single bond.

If the anisotropy is sufficiently small, it may happen that the magnetic-field-induced easy plane is more favourable than the anisotropy-induced easy plane. Then the domain wall will imply a movement of the spin vector in the $yz$ plane instead of the $xy$ plane. This would merely interchange the role of the $z$ and $x$ components of the spins. From §4 we estimate the corresponding soliton energy to be $2\kappa^{1/2}|J|S^2$ as compared with $2b_x|J|S^2$ in the case considered above. Thus for $b_x \ll \kappa$ the treatment given above can be expected to be correct.

Using values of the parameters appropriate for TMMC, $|J|S^2 \approx 130\,\text{K}$, $\kappa \approx 0{\cdot}03$, one finds that it should be possible to observe the central peaks given in equations (5.9) and (5.14) in neutron scattering experiments below 10 K. For a temperature of 8 K and a magnetic field of 60 kG values of $\Gamma_S \approx 0{\cdot}01\ \pi/a$ and $\Gamma_{\text{D}} \approx 2\,\text{K}$ are obtained for the transverse central peak, whereas the longitudinal central peak should have about half of the intensity but be otherwise quite comparable with the central peak observed in $CsNiF_3$ (Kjems and Steiner 1978).

## 6. Conclusions

We have investigated the non-linear dynamics of classical antiferromagnetic chains at low temperatures ($T \ll |J|S^2$) and small magnetic fields ($g\mu_{\text{B}}B \ll |J|S$). We have found that for several combinations of single-ion anisotropy and magnetic field an equivalence can be established between the antiferromagnetic chain and SG equations with soliton solutions which are either complete turns ($2\pi$ solitons) or domain walls ($\pi$ solitons) in the sublattice magnetisation.

Complete turns occur for an isotropic antiferromagnet in a staggered field. Domain walls mediating between fixed easy directions for the sublattice magnetisation are encountered for an easy-axis single-ion anisotropy as well as for an easy-plane single-ion anisotropy combined with a magnetic field in the $xy$ plane. In the latter case the magnetic field actually reduces the symmetry further from $xy$ to Ising like. For an easy-plane single-ion anisotropy without magnetic field a domain-wall solution is found which changes the direction of the sublattice magnetisation by $\pi$, although there is no easy axis in the now isotropic $xy$ plane; rather the domain wall will start at an angle in the $xy$ plane which floats owing to the accumulating effect of small oscillations.

If an easy plane is realised owing to a magnetic field via the spin-flop effect, a different type of finite-amplitude solutions occurs: the sublattice magnetisation then performs jumps of varying angle in the easy plane, which join continuously to localised small-amplitude solutions and correspond to the pulse soliton solutions of the isotropic Heisenberg chain. However, the antiferromagnetic chain with both easy-plane anisotropy and magnetic field offers a so-far unique possibility to investigate a crossover from SG solitons to pulse solitons by varying $\kappa^{1/2}/b_z$.

We have not considered the question whether the classical antiferromagnetic chain is a completely integrable system as is the classical ferromagnetic chain. The fact that it can be shown to be equivalent to a SG system would suggest that this is true, but it remains a challenge to prove this suggestion and, in particular, to see, whether it is true for arbitrary ratios $\kappa^{1/2}/b_z$.

The thermodynamic significance of the finite-amplitude solutions has been discussed in detail for an easy-plane antiferromagnet in a symmetry-breaking field, with a particular view on applications to the one-dimensional antiferromagnet TMMC. We find that the domain wall aspect of these solutions should be observable as a very narrow central peak in the correlation function of spin components perpendicular to the field, whereas the soliton aspects will lead to a broader central peak in the longitudinal correlation function. Both central peaks should be observable in inelastic neutron scattering experiments.

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*Note added in proof.* After submission of this paper I received preprints by Boucher, Regnault, Rossat-Mignot, Renard, Bouillot and Stirling, by Leung, Hone, Mills, Riseborough and Trullinger and by Maki, which are also concerned with the non-linear dynamics of antiferromagnetic chains. The results of the neutron scattering experiments on TMMC of Boucher *et al* (*Solid St. Commun.* to be published) are in nearly quantitative agreement with our results. Leung *et al* and Maki present theoretical work on the $xy$-like antiferromagnet which differs in approach from this paper but leads to similar results.

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