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Solitons in the anisotropic xy chain: semiclassical treatment of quantum effects

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Abstract. We have investigated soliton solutions and their contribution to the specific heat for the anisotropic xy chain in the classical and semiclassical approximation. The soliton solutions, which can be given analytically for the discrete classical chain, are shown to be stable. In the continuum approximation the classical system is equivalent to the sine–Gordon model. The energy of the moving soliton is determined up to second order in the soliton velocity. In the semiclassical approximation the magnetic chain with spin S is equivalent to a quantum sine–Gordon chain with coupling constant $g^2 = [32/S(S+1)]^{1/2}$. Using the magnon phase shift in the presence of a dilute gas of solitons we have calculated the specific heat. We find that the semiclassical approximation reasonably describes the transition from the classical limit to the $S = \frac{1}{2}$ model as solved exactly by Lieb, Schultz and Mattis.

1. Introduction

The low-temperature dynamics of one-dimensional magnetic systems has attracted considerable attention in recent years. The model systems mainly investigated are planar ferro- or antiferromagnets such as $CsNiF_3$ and TMMC with an external magnetic field breaking the rotational symmetry in the xy plane.

These systems support soliton-like excitations (domain walls), which give rise to new observable phenomena such as the presence of a central peak in inelastic neutron scattering data, an additional linewidth in resonance experiments and an additional maximum in the magnetic specific heat as a function of temperature or magnetic field.

Qualitative agreement with experimental data has been obtained by mapping the spin chain approximately to the classical sine–Gordon (SG) chain, assuming the continuum approximation as well as an ideally strong planar anisotropy (Mikeska 1978, 1980). For a more quantitative treatment corrections to these approximations have to be considered and, among these, quantum corrections have turned out to be most important for an understanding of the soliton contribution to the specific heat (Mikeska and Frahm 1986, Fogedby *et al* 1986).

Quantum corrections to soliton effects in magnetic chain systems have so far been discussed mainly in the semiclassical approximation, i.e. in an expansion in $1/S$, and the validity of these approximations remains untested. In an effort to study the importance of quantum effects with varying spin magnitude S and to test the validity of the semiclassical approximation we consider in the present paper non-linear excitations in the anisotropic xy model defined by the Hamiltonian

$$H = -J \sum [(1+\gamma) S_n^x S_{n+1}^x + (1-\gamma) S_n^y S_{n+1}^y]. \tag{1.1}$$

For $\gamma \neq 0$ this model has two degenerate ground states (e.g. $S_n^x = \pm S$ in the classical limit for $J > 0$) and supports soliton-like excitations mediating between them. When compared with the familiar models describing $CsNiF_3$ or TMMC, the exchange anisotropy thus replaces the magnetic field as the source of symmetry breaking, and planar behaviour is favoured by the absence of exchange in the z direction rather than by single-ion anisotropy. The model (1.1) has the following interesting properties, which make it particularly well suited for our purpose.

(i) For $S = \frac{1}{2}$ the Hamiltonian can be diagonalised exactly in terms of free fermions and the specific heat can be calculated (Lieb *et al* (1961), referred to as LSM in the following). Using these results the effect of solitons has been explicitly demonstrated for the S^zS^z correlation function (Puga and Beck 1982).

(ii) In the classical limit an exact analytic solution can be given for the static soliton in the discrete chain (Gochev 1983, Granovskiî and Zhedanov 1986). Using spherical coordinates to specify the direction of the classical spin vector,

$$S_n = S(\cos\theta_n \cos\varphi_n, \cos\theta_n \sin\varphi_n, \sin\theta_n) \tag{1.2}$$

this solution is given by

$$\theta_n = 0 \qquad \varphi_n = \pm\tan^{-1}\operatorname{cosech}[q(n+\alpha)] \tag{1.3}$$

with

$$\cosh q = (1+\gamma)/(1-\gamma)$$

and has the energy

$$E_{\text{sol}} = 4\sqrt{\gamma}JS^2. \tag{1.4}$$

The phase α is arbitrary and, quite remarkably for the discrete chain, the energy does not depend on α.

In § 2 of this paper we present results for the soliton properties of the classical approximation to (1.1), discussing in particular the effects of the continuum and planar approximations. In § 3 the semiclassical approach is given—in particular the specific heat is calculated, discussed in terms of its dependence on the spin value S and compared with the exact results for the $S = \frac{1}{2}$ chain. A short summary is given in § 4—our main result is that the semiclassical approximation accounts surprisingly well for the quantum specific heat if the different roles of spin waves in classical and quantum spin chains are appropriately accounted for.

2. Solitons in the classical anisotropic *xy* model

In this section we discuss solitons in the model (1.1) in the classical limit for ferromagnetic coupling ($J > 0$). Using the representation (1.2), the equations of motion are given by

$$\begin{aligned}(\partial/\partial t)\varphi_n = JS\tan\theta_n\{&\cos\theta_{n+1}[(1+\gamma)\cos\varphi_n\cos\varphi_{n+1} + (1-\gamma)\sin\varphi_n\sin\varphi_{n+1}] \\ &+ \cos\theta_{n-1}[(1+\gamma)\cos\varphi_n\cos\varphi_{n-1} + (1-\gamma)\sin\varphi_n\sin\varphi_{n-1}]\} \\ (\partial/\partial t)\theta_n = -JS[&(1+\gamma)(\cos\theta_{n+1}\cos\varphi_{n+1} + \cos\theta_{n-1}\cos\varphi_{n-1})\sin\varphi_n \\ &-(1-\gamma)(\cos\theta_{n+1}\sin\varphi_{n+1} + \cos\theta_{n-1}\sin\varphi_{n-1})\cos\varphi_n].\end{aligned} \tag{2.1}$$

The simplest theoretical approach treats these equations in the continuum limit

($\varphi_n - \varphi_{n+1} \ll 1$) and assumes strong planar behaviour ($\theta_n \ll 1$), motivated by the absence of exchange between the z (out-of-plane) components of spin.

It is convenient to introduce the following parameters:

$$m^2 = 4\gamma \qquad c^2 = 2(JS)^2 \qquad E_0 = \tfrac{1}{4}JS^2 \tag{2.2}$$

and to use the dimensionless variables $\zeta = (m/a)z$ and $\tau = mct$ (a is the lattice constant, which will be set equal to unity in the following).

The continuum approximation in our dimensionless variables corresponds to an expansion up to lowest order in γ. In this order the Hamiltonian (1.1) can be mapped exactly to the sine–Gordon (SG) model:

$$H = 4E_0 m \int \mathrm{d}\varphi \left[\frac{1}{2}\left(\frac{\partial\varphi}{\partial\tau}\right)^2 + \frac{1}{2}\left(\frac{\partial\varphi}{\partial\zeta}\right)^2 + \tfrac{1}{4}(1-\cos 2\varphi)\right]. \tag{2.3}$$

The equations of motion then take the form

$$\partial^2\varphi/\partial\tau^2 - \partial^2\varphi/\partial\zeta^2 = \tfrac{1}{2}\sin 2\varphi \qquad \theta = (m/\surd 2)\partial\varphi/\partial\tau. \tag{2.4}$$

Thus in the simplest theoretical approach the anisotropic xy chain is equivalent to models describing $CsNiF_3$ and TMMC when the appropriate identifications are made for the parameters and the SG variable (2φ in the present case). Thus the well known results for the SG soliton can be taken over for the domain walls in the classical xy model to $O(\gamma)$.

When one wants to go beyond this simplest approach the situation for the various soliton-bearing models becomes different: whereas in the easy-plane chain with single-ion anisotropy A and external magnetic field B out-of-plane corrections are governed by $1/A$ and discreteness corrections are governed by $m \sim B^{1/2}$, in the present model there is only one parameter, γ, which governs both these corrections. Thus, as can be checked explicitly from the equation of motion, it is inevitable to include discreteness effects when one wants to go beyond the SG approximation and to consider out-of-plane corrections. For these reasons we use in the following the exact static soliton solution for the discrete lattice given in (1.3) as a starting point for further investigations. For the classical model we will discuss in the remainder of this section the stability of the solution (1.3) and an approximate treatment for slowly moving solitons.

The stability of the soliton solution (1.3) can be investigated following Magyari and Thomas (1982). Expanding in the deviations:

$$\theta_n \to \varepsilon\theta_n \qquad \varphi_n \to \varphi_n + \varepsilon\psi_n \tag{2.5}$$

from the static soliton leads to stability conditions that are fulfilled if the following eigenvalue equation has no negative eigenvalues:

$$2\cosh(q)\psi_n - (1 + \sinh^2(q)\,\mathrm{sech}^2(qn))(\psi_{n+1} + \psi_{n-1}) = \lambda\psi_n. \tag{2.6}$$

We found that the eigenfunctions and eigenvalues are given by

$$\begin{aligned} &\psi_n^0 = \mathrm{sech}[q(n+\alpha)] && \lambda^0 = 0 \\ &\psi_{n,k} = \mathrm{e}^{ikn}\{a + ib\tanh[q(n+\alpha)]\} && \lambda_k = 2(\cosh(q) - \cos(k)) \\ &a/b = \tan(k)\coth(q). && \end{aligned} \tag{2.7}$$

Thus it follows that (1.3) is a stable solution of the equations of motion. Notice that (2.6) reduces in the continuum limit ($q \ll 1$) to the equivalent problem for the SG model (Rubinstein 1970) and that the eigenfunctions (2.7) then go over to those for the SG system.

The fact that the static soliton satisfies the equations of motion enables us to investigate slowly moving solitons via successive approximations taking the dimensionless velocity $u = v/c$ as a small parameter, following Mikeska and Osano (1982). Therefore we make the following *ansatz* for θ_n and φ_n:

$$\theta_n = \theta_n(s) \qquad \varphi_n = \Phi_n(s) + \psi_n(s) \tag{2.8}$$

Here θ_n and ψ_n are $O(u)$ and $O(u^2)$ respectively, Φ_n is the static soliton solution given in (1.3) and $s = n - vt - n_0$.

Inserting this *ansatz* into the equations of motion gives

$$\theta_n = [-\sqrt{2}uq/2(1+\gamma)]\,\mathrm{sech}(qs)(1 + \sinh^2(q)\,\mathrm{sech}(qs)). \tag{2.9}$$

Thus the kinetic energy up to $O(u^2)$ is given by

$$E_{\mathrm{kin}} = \tfrac{1}{2}u^2\lambda^2\,8E_0 m$$
$$\lambda^2 = \frac{q^2}{2m(1+\gamma)}\sum \mathrm{sech}^2[q(n-vt-n_0)]\{1+\sinh^2(q)\,\mathrm{sech}^2[q(n-vt-n_0)]\}. \tag{2.10}$$

We were not able to evaluate the sum in (2.10) analytically, but numerically we find that replacing it by the corresponding integral is an excellent approximation for $q \leqslant 1$. The numerical calculation gives $\lambda^2 = 1.2514$ for $\gamma = 0.1$. The difference of λ^2 from unity shows the deviation from the 'relativistic' velocity dependence of the continuum SG model.

3. Semiclassical theory of solitons in the anisotropic *xy* model

A semiclassical approach to our model can be formulated in close analogy with the procedure for the easy-plane ferromagnet (Mikeska 1982). Introducing the planar representation of spin operators (Villain 1974) with angle φ and S^z as canonical operators, expanding in S^z and performing the continuum limit, the anisotropic xy model is mapped to the quantum SG chain with the Hamiltonian

$$H = E_0 g^2 \int \mathrm{d}z \left[\frac{1}{2}\left(\frac{\partial\Phi}{\partial z}\right)^2 + \tfrac{1}{2}\pi^2 + \frac{m^2}{g^2}(1-\cos(g\Phi))\right] \tag{3.1}$$

where

$$g^2 = [32/S(S+1)]^{1/2} \qquad E_0 = \tfrac{1}{4}J\hat{S}^2 \qquad m^2 = 4\gamma$$
$$\hat{S}^2 = S(S+1) \qquad \Phi = (2/g)\phi \qquad \pi = (\sqrt{8}/g\hat{S})S^z.$$

The magnitude of the coupling constant g^2 quantitatively describes the quantum character of this theory.

Quantum corrections to the soliton energy up to first order in g^2 are found by considering the difference in zero-point vibrational energy between the vacuum and the one-soliton state, as carried through first for the continuum SG model by Dashen *et al* (1975). In the present case we start from the discrete model which at the same time supplies a physical cut-off (the reciprocal of the lattice constant) allowing us to avoid the renormalisation procedure (see Mikeska 1982) and takes into account correction terms beyond the SG approximation (see § 2). Linearising the equations of motion (2.1) in ϕ_n and θ_n one gets, as the vibration spectrum in the vacuum state,

$$\omega_k^{(0)} = E_0 m g^2 \Omega_k \tag{3.2a}$$

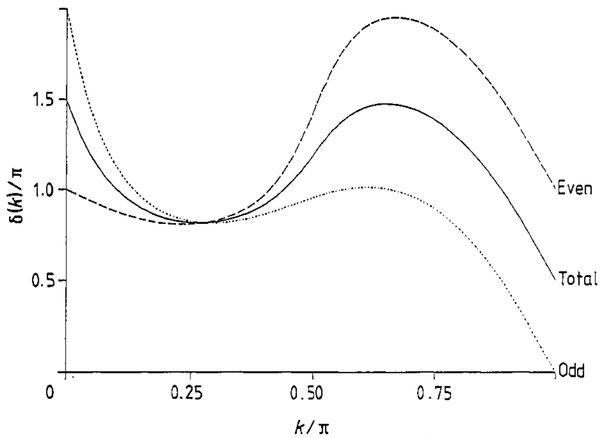

Figure 1. Asymptotic phase shifts δ for the even and odd scattering solutions of (3.3) and the total phase shift $\delta = \frac{1}{2}(\delta_e + \delta_0)$.

$$\Omega_k = (1+\gamma)^{1/2}\left[1 + \frac{4(1-\gamma)}{m^2}\sin^2\left(\frac{k}{2}\right)\right]^{1/2}. \qquad (3.2b)$$

The allowed k-values are given by $Lk = 2\pi n$, where n is an integer such that $-\pi < k \leqslant \pi$ and L is the length of the system.

In order to investigate small vibrations in the one-soliton state, we linearise (2.1) in θ_n and $\psi_n = \Phi_n - \varphi_n$ (Φ_n is given by (1.3)) and obtain the following eigenvalue equation for the frequencies ω (the phase α is set equal to zero):

$$\omega^2\psi_n = 2J\hat{S}^2(1-\gamma^2)(1+\sinh^2(q)\,\mathrm{sech}^2(qn))^{-2}$$
$$\times\,[2\cosh(q)\psi_n - (\psi_{n+1}+\psi_{n-1})(1+\sinh^2(q)\,\mathrm{sech}^2(qn))]. \qquad (3.3)$$

We were not able to solve this eigenvalue problem analytically. Nevertheless we can give a complete discussion of its structure.

(i) There exists one bound state related to translational invariance, which can be given analytically as

$$\psi_{n,\mathrm{b1}} = \mathrm{sech}(qn) \qquad \omega_{\mathrm{b1}} = 0. \qquad (3.4a)$$

(ii) There exists a second bound state, which is found numerically to be given by

$$\omega_{\mathrm{b2}} = E_0 m g^2 \Omega_{\mathrm{b2}} \qquad \Omega_{\mathrm{b2}} = 1.009\,0158 \qquad \text{for } \gamma = 0.1. \qquad (3.4b)$$

(iii) The remaining solutions are scattering solutions $\omega_k = E_0 m g^2 \Omega_k$ with Ω_k given in (3.2b), but the allowed k-values are now given by $Lk + \delta(k) = 2\pi n$ (where $\delta(k)$ is the phase shift of the scattering solutions). Using the fact that (3.3) is invariant under parity transformations we have calculated the phase shifts for the even and odd solutions numerically. The result is shown in figure 1 for $\gamma = 0.1$. Extrapolating the results to $k = 0$ we get $\delta(k=0) = \frac{3}{2}\pi$, which according to Barton (1985) agrees with the existence of two bound states. By analogy with the work of Mikeska (1982) the energy of the static soliton in the semiclassical approximation is given by

$$E_{\mathrm{sol}} = 8E_0 m_{\mathrm{sol}} \qquad (3.5a)$$

$$m_{\mathrm{sol}} = m\left[1 - \frac{g^2}{8}\left(\Omega_{k=0} - \tfrac{1}{2}\Omega_{\mathrm{b2}} + \frac{1}{2\pi}\int_0^{\pi} \mathrm{d}k\,\delta(k)\frac{\partial}{\partial k}\Omega_k\right)\right]. \qquad (3.5b)$$

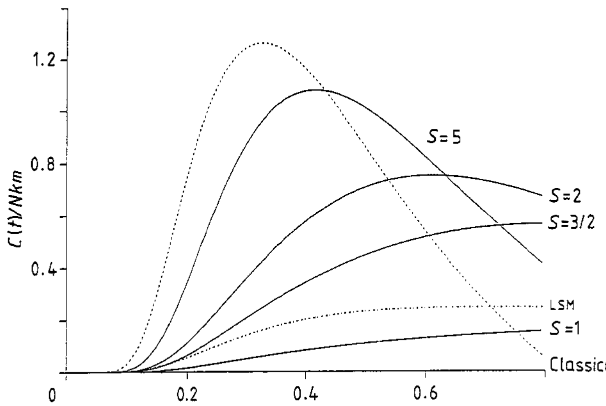

Figure 2. The semiclassical soliton contribution to the specific heat C in units of Nk_Bm ($m = 2\sqrt{\gamma}$ is the classical spin-wave mass) as a function of the temperature $t = k_BT/E_{sol}$ (E_{sol} is the semiclassical soliton energy, equation (3.5)) for different spin lengths S corrected for the spin-wave contribution; see the text. Dotted curve: non-linear part of the exact LSM result; see the text ($m = 2\gamma$ is the spin-wave mass for $S = \frac{1}{2}$, $t = k_BT/E_s$; E_s is the soliton energy; see (3.8)).

Evaluating this result numerically we find that the soliton energy decreases monotonically with decreasing S and decreasing γ. Breakdown of our approximation is indicated by m_{sol} becoming negative which occurs for $S = \frac{1}{2}$ for all γ and for $S = 1$ for $\gamma \leqslant 0.02$; for $S > 1$ the dependence on γ is rather weak except when γ is very small.

This semiclassical approach can be generalised to finite temperatures following Mikeska and Frahm (1986) and Fogedby *et al* (1986). The soliton contribution to the free-energy density is given by ($\beta = (k_BT)^{-1}$)

$$F_{sol} = -\frac{\beta^{-1}}{\pi}\int dp \exp(-\beta\Omega_{sol}) \tag{3.6}$$

with

$$\beta\Omega_{sol} = \beta E_{sol}\left[1+\frac{1}{2}\left(\frac{v}{c}\right)^2\lambda^2\right] - \frac{1}{\pi}\int_0^\pi dk\,\delta(k)\frac{\partial}{\partial k}\ln(1-\exp(-\beta\omega_k))$$
$$+\ln(1-\exp(-\beta\omega_{b2})) - 2\ln(1-\exp(-\beta\omega^{(0)}_{k=0})).$$

The momentum integration can be carried out and the soliton contribution to the free energy and to the specific heat can easily be calculated numerically, using our results for Ω_k and $\delta(k)$. Results for various values of S are shown in figure 2 (the temperature is measured in units of the soliton energy, which depends on S).

In order to get an idea about the quality of the semiclassical approximation we want to compare our results for the specific heat to the exact result for $S = \frac{1}{2}$ as given by LSM. This exact result of course gives the total specific heat, to be compared with the sum of soliton and spin-wave contributions in our semiclassical model. We therefore have to calculate the spin-wave contribution to the specific heat. For spin-wave frequencies $\omega_{sw}(q)$ it is given by

$$C_{sw} = \frac{Nk_B}{4\pi T^2}\int_0^\pi dq\left[\omega_{sw}(q)/\sinh\left(\frac{\beta}{2}\omega_{sw}(q)\right)\right]^2. \tag{3.7}$$

To obtain C_{sw} for $S = \frac{1}{2}$ as reliably as possible we use the spin-wave spectrum from (3.2) with the following renormalised parameters

$$E_0 g^2 = J \qquad m = 2\gamma. \tag{3.8}$$

The values for E_0 and g^2 follow from the exact mapping of the $S = \frac{1}{2}$ *xy* model to the quantum SG chain (Luther 1976, 1980); this mapping gives for the bare mass $m_0 = \sqrt{4\gamma}$, which is modified to the value given above after renormalisation (Coleman 1977, Maki and Takayama 1979). To choose the correct units for the representation of the LSM specific heat we also need the soliton mass m_s in the $S = \frac{1}{2}$ chain. The relation between the renormalised spin-wave mass m and the soliton mass m_s is given by

$$m = 2m_s \sin[(g^2/16)/(1 - g^2/8\pi)]. \tag{3.9}$$

For $g^2 = 4\pi$ this gives $m_s = \gamma J$, in agreement with the energy gap in the LSM excitation spectrum—the exact solution for the excitation spectrum of the quantum system is properly interpreted in terms of solitons only.

In figure 2 we have included a plot of the difference $C_{LSM} - C_{sw}$ (in units of Nk_B), which is the quantity to be compared with the soliton contribution to the specific heat in our semiclassical calculation. The semiclassical result for small values of S approaches this 'exact' (apart from the uncertainties involved in the spin-wave contribution) result surprisingly well: it reproduces both the strong reduction of the classical specific heat and the broadening of this peak, which are clearly seen in quantum results.

4. Summary

We have investigated soliton-like excitations in the anisotropic *xy* chain. Assuming strongly planar behaviour, this system in the continuum limit can be mapped to the SG model in both the classical and semiclassical regime. The coupling constant describing the quantum character of the theory is found to be $g^2 = [32/S(S+1)]^{1/2}$. This appears to be an underestimate, because for $S = \frac{1}{2}$ it amounts to $g^2 \simeq 2\pi$ which is significantly smaller than the value $g^2 = 4\pi$ found by Luther (1976) when mapping the spin-$\frac{1}{2}$ system to the SG chain. The semiclassical calculation of the soliton contribution to the specific heat describes qualitatively the transition from the classical limit to the LSM result for the $S = \frac{1}{2}$ model: the maximum of the classical specific heat is strongly reduced and the sharp peak is broadened due to quantum effects. This supports speculations that a semiclassical calculation of the specific heat may give quantitatively useful results for $S = 1$ also, when higher-order terms in $\hat{S}^{-1}$ are considered. This is the situation of interest for $CsNiF_3$ ($S = 1$); calculations of the specific heat for this material to $O(S^{-2})$ are now in progress (Fogedby *et al* 1989).

The dependence of our results for the specific heat on the spin value S also agrees qualitatively with experimental results (Ramirez and Wolf 1982, 1985, Kopinga *et al* 1984, 1985) in showing that the magnetic specific heat of soliton-bearing quantum spin chains is much smaller than predicted classically. It was noted before that this reduction can only be understood in terms of the combination of quantum corrections and out-of-plane effects (Mikeska and Frahm 1986). This is consistent with the fact that the present result was only obtained by going beyond the continuum quantum SG theory.

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