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Abstract. We have studied nonlinear excitations of a quasi-one-dimensional anisotropic Heisenberg model subject to an external magnetic field. We have particularly been interested in the situation where the Zeeman energy can be varied continuously as a function of the parameter r. Taking the continuum limit, we have been able to show that this magnetic system can be mapped approximately onto the one-dimensional deformable sine–Gordon model at extremely low temperatures. Two classes of implicit soliton solutions that depend on r are presented and the total density of kinks and antikinks are calculated at low temperatures.

Nonlinear excitations in quasi-one-dimensional (1D) magnetic systems have received much theoretical, experimental and computational attention in recent years, primarily ferromagnetic easy-plane, or $S = 1/2$ systems [1–10]. However, the applicability of an idealized concept to real physical systems for the understanding of soliton properties is limited, since it is unlikely that physical condensed matter will be exactly described by potentials with defined shapes. In those systems, the shape of nonlinear one-site potential may deviate considerably from that attributed to the local potential. It is established that under variation of some physical parameters such as the temperature and pressure, some physical systems may undergo changes which are either shape distortion, variations of crystalline structures or conformational changes. For example, in solid hydrogen halides under pressure, as pressure is increased, the central barrier reduces rapidly until a critical pressure has been reached and the system has undergone a phase transition to symmetric phase [11]. On the other hand, using pseudopotential band-structure results, it has been shown that the electrostatic energy of a unit point charge located in Si along the (111) direction can be described by deformable double-well potentials [12–14]. This electrostatic energy has its minimum at the tetrahedral interstitial site whereas the hexagonal site is a saddle point [13]. Volume effects in perovskite-type oxides can also lead to deformable double-well potentials. For example, for $KTaO_3$, the set of total-energy curves over independent displacements of individual atoms along (111) and (001) directions have been obtained for a sequence of volumes [15]. The displacement of Ta occurs in an even more anisotropic potential well, the shape of which apparently indicates considerable phonon frequency softening below the experimental volume as well as the tendency to go off centre, forming a ferroelectric structure for larger volumes. The dynamical behaviour of a sine–Gordon (sG) soliton in the presence of external perturbations has been discussed by Fogel *et al* [16, 17], where they concluded that sG solitons in many respects behave as deformable classical particles whose dynamics are governed by Newton's law. An interesting problem to be studied is the possibility of the formation of deformable coherent structures in quasi-1D ferromagnets.

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The purpose of this paper is to present briefly the deformable-spin model Hamiltonian. We analyse this model based on the standard field theoretical techniques and identify solitary-wave solutions.

The system we consider is described by the Hamiltonian

$$H = -J\sum_n \vec{S}_n\vec{S}_{n+1} + A\sum_n \left(S_n^z\right)^2 + g\mu_B\vec{B}\sum_n \frac{(1-r)^2(1-\vec{S}_n)}{1+r^2+2r\vec{S}_n} \tag{1}$$

where the first term represents the isotropic ferromagnetic Heisenberg exchange interaction between neighbouring spins denoted by the vectors $\vec{S}_n$ and $\vec{S}_{n+1}$ with exchange constant $J > 0$. The second term represents the easy-plane (xy) anisotropy energy with $A > 0$ and the last term represents the deformable Zeeman energy of the spins in an external magnetic field ($B^x = B$) perpendicular to the chain axis (Z). g and μ_B are the Landé g-factor and the Bohr magneton, respectively. The shape parameter r varies in the range $-1 < r < 1$ as previously introduced by Remoissenet and Peyrard [18, 19]. When $r = 0$, we recover the familiar Zeeman energy. The introduction of this new term yields new features, and in particular the existence of deformable domain-wall structures.

Since we are going to treat the problem classically, at sufficiently low temperatures ($T \ll (AJ)^{1/2}$) [1], we introduce at this level the classical approximation in the sense that, neglecting quantum effects ($A/JS(S+1) \ll 4\pi^2$) [20], we treat the spin as an ordinary vector of length S specified by two polar angles θ and ϕ. In spherical coordinates $\vec{S}_n$ is written as

$$\vec{S}_n = S(\sin\theta_n\cos\phi_n, \sin\theta_n\sin\phi, \cos\theta_n) \tag{2}$$

where $0 \leqslant \theta_n \leqslant \pi$ is the excursion angle of the magnetization from the (S^x, S^y) plane, and $0 \leqslant \phi_n \leqslant 2\pi$ represents the azimuthal angle of $\vec{S}_n$ in the (S^x, S^y) plane. The spin dynamics is described by the usual undamped Bloch equation. In the continuum approximation, and keeping terms up to second order in lattice spacing a over wavelength $\lambda \geqslant 2\pi a(2A/J)^{-1/2}$, we obtain the following partial differential equation

$$\begin{aligned}\overline{h}\phi_t\sin\theta = {} & JSa^2(\theta_{ZZ}\sin\theta - \phi_Z^2\sin\theta\cos\theta) + 2A\sin\theta\cos\theta \\ & + g\mu_B B\frac{(1-r^2)^2\cos\theta\cos\phi}{(1+r^2+2rS\sin\theta\cos\phi)^2}\end{aligned} \tag{3a}$$

$$-\overline{h}\theta_t = JSa^2(\phi_{ZZ}\sin\theta + 2\phi_Z\theta_Z\cos\theta) - g\mu_B B\frac{(1-r^2)^2\sin\phi}{(1+r^2+2rS\sin\theta\cos\phi)^2}. \tag{3b}$$

Here, subscripts denote differentiation and Z is the position on the chain. For magnetic fields $JS/g\mu_B B \gg 1$, equations (3*a*) and (3*b*) can be reduced to the deformable sG equation

$$\phi_{tt} - C_0^2\phi_{ZZ} + \omega_0^2\left(1-r^2\right)^2\frac{\sin\phi}{(1+r^22r\cos\phi)^2} = 0 \tag{4a}$$

$$\theta = (\overline{h}/2AS)\phi_t \tag{4b}$$

where

$$C_0^2 = 2AJS^2a^2/\overline{h}^2 \qquad \omega_0^2 = 2Ag\mu_B BS/\overline{h}^2. \tag{4c}$$

The constant C_0 is the characteristic velocity and ω_0 the characteristic frequency of the spin system. In this derivation we highlight certain aspects that are also found in the investigation of the previous works [1, 5]. Before proceeding with further analysis of this problem, it is useful to see that the last term in equation (4*a*) is precisely the first derivative with respect to ϕ, that is $(\partial V_{RP}(\phi, r)/\partial\phi)$, of the Remoissenet–Peyrard (RP) potential

$$V_{RP}(\phi, r) = (1-r)^2\frac{1-\cos\phi}{1+r^2+2r\cos\phi} \qquad |r| < 1. \tag{4d}$$

When $r = 0$, the RP potential reduces to the sG potential. The deformable sG equation has solutions in the form of large-amplitude travelling waves (kinks), low-amplitude linear modes (spin waves or magnons) and breathers [18, 19]. Our recent results based on the RP potential have shown that the dependence of the diffusion coefficient of adsorbates in metallic substrates on the deformability parameter r can explain the gaps observed on existing measurements [21]. The critical nucleus has been studied and the nucleation rate of kink–antikink pairs has been determined at low temperatures and in the limit of strong damping [22]. The two families of implicit kink solutions with v given in terms of the moving coordinates $s = x - vt$ are travelling-wave rotations of the spins through 2π within the easy plane, with the spin tilting out of the easy plane being proportional to the kink translation velocity $0 \leqslant v < C_0$, and are described as [18, 19]

$$\frac{\gamma S}{d^{(1)}} = \mathrm{sgn}(\phi - \pi)\left\{\frac{(1-\alpha^2)^{1/2}}{\alpha}\tan^{-1}\left[\frac{(1-\alpha^2)^{1/2}}{[\alpha^2 + \tan^2(\phi/2)]^{1/2}}\right] + \tanh^{-1}\left\{\frac{\alpha}{[\alpha^2 + \tan^2(\phi/2)]^{1/2}}\right\}\right\} \tag{5a}$$

with the rest energy

$$E_S^{(1)} = 8A'C_0\omega_0\alpha(1-\alpha^2)^{-1/2}\tan^{-1}\left[\frac{(1-\alpha^2)^{1/2}}{\alpha}\right] \tag{5b}$$

for $-1 < r \leqslant 0$, and

$$\frac{\gamma S}{d^{(2)}} = \mathrm{sgn}(\pi - \phi)\left\{(1-\alpha^2)^{1/2}\tanh^{-1}\left[\frac{(1-\alpha^2)^{1/2}}{[1 + \alpha^2\tan^2(\phi/2)]^{1/2}}\right] - \tanh^{-1}\frac{1}{[\alpha^2 + \tan^2(\phi/2)]^{1/2}}\right\} \tag{6a}$$

with the rest energy

$$E_S^{(2)} = 8A'C_0\omega_0\alpha(1-\alpha^2)^{-1/2}\tanh^{-1}[(1-\alpha^2)^{1/2}] \tag{6b}$$

for $0 \leqslant r < 1$, with

$$\alpha = \frac{1-|r|}{1+|r|} \qquad d^{(1)} = d_0\alpha \qquad d^{(2)} = d_0/\alpha \tag{7a}$$

$$d_0 = C_0/\omega_0 \qquad A' = \overline{h}^2/2Aa \qquad \gamma = (1 - v^2/C_0^2)^{-1/2}. \tag{7b}$$

This rotation occurs over a characteristic length $d^{(j)} (j = 1, 2)$ which are the 'pseudokink widths', determined by the applied field (for velocities $v \ll C_0$), and the shape parameter r. The antikink solutions are obtained by replacing ϕ by $(2\pi - \phi)$ in equations (5a) and (6a). For $r = 0$, equations (5) and (6) reduce to the usual sG kink. When r tends to 1, $d^{(2)}$ tends to infinity. On the other hand, when r decreases and tends to -1, $d^{(1)}$ tends to zero. Thus, the kink extension is not only determined by the characteristic length scale d_0, but also by the curvature of the minima of the potential. The deformable sG equation has the low-amplitude periodic wave solutions of the form $\phi = \phi_q \cos(qZ - \omega_q t)$ corresponding to small oscillations of the spin vector around one of the ground states which form a continuous spectrum characterized by the dispersion

$$\omega_q^2 = \omega_r^2 + C_0^2 q^2 \qquad \omega_r = \left(\frac{1-r}{1+r}\right)\omega_0 \tag{8}$$

where ω_r is a characteristic frequency of oscillations of an isolated spin vector at the bottom of the substrate potential well ($\phi = 2\pi n$, n integer) and q, the wavevector. The magnitude of ϕ_q is required to be infinitesimally small especially in the cases where $r \to -1$ (potential with a sharp bottom) [19]. Breather solitons, which can be viewed as soliton–antisoliton bound states, have been observed in numerical simulations by Peyrard and Remoissenet [19]. Considering kink–antikink collisions, in the case of sharp potential wells ($r < 0$) leading to narrow kinks, for $r = -0.8$, with $v = \pm 0.1\ C_0$, the two waves cannot separate from each other and they form a stable breather mode. On the other hand, considering the case of the potential wells with a flat bottom ($r > 0$), for very small value of $r (r = 0.15)$, the two waves form a breather mode.

At low temperatures, the total density of kinks and antikinks is given by [23]

$$n_{k-\bar{k}}^{tot(j)} = n_0^{(j)} \left(1 - 2B^{(j)} n_0^{(j)}\right) \tag{9}$$

with

$$n_0^{(j)} = \frac{2}{d^{(j)}} \left(\frac{2}{\pi}\right)^{1/2} \left(8\sqrt{m^*}\tilde{C}^{(j)}\right)^{1/2} \exp\left[-\beta E_S^{(j)}\right] \tag{10a}$$

$$B^{(j)} = d^{(j)} \ln\left(32\gamma\sqrt{m^*}\tilde{C}^{(j)}\right) \tag{10b}$$

$$\tilde{C}^{(1)} = \exp\left\{\left[2(1-\alpha^2)^{1/2}/\alpha\right] \tan^{-1}\left[(1-\alpha^2)^{1/2}/\alpha\right]\right\} \alpha \tag{11a}$$

$$\tilde{C}^{(2)} = \exp\left\{\left[-2(1-\alpha^2)^{1/2}\right] \tanh^{-1}\left[(1-\alpha^2)^{1/2}\right]\right\} /\alpha \tag{11b}$$

where $n_0^{(j)}$ are the total density of kinks and antikinks within the ideal gas approximation and $\gamma = 1.7810\ldots$ is Euler's constant. The coefficients $B^{(j)}$ are the logarithmic temperature dependence, which are attributed to the exponential decay of the interaction potential between soliton at large distances.The temperature-dependent parameter $m^* = A'^2 C_0^2 \omega_0^2 \beta^2$ plays the role of an effective mass of a particle, where $\beta = 1/k_B T$, k_B being the Boltzmann constant, T the temperature.

We focus our attention on the archetypical example of a 1D ferromagnet $CsNiF_3$, where 1D ordering appears in the temperature range $3 \leqslant T \leqslant 16$ K [24], and whose Hamiltonian can be described by equation (1). Our preliminary study presented in this paper must be pursued in order to relate the obtained theoretical results with the experimental data for $CsNiF_3$. Specifically, although effects of deformability of the medium are expected to become significant, for example in the physical properties of localized waves, Pini and Rettori [25] have demonstrated the inadequacy of the classical approximation for $CsNiF_3$, since the exact numerical transfer matrix data strongly disagree with the experimental results for magnetization, specific heat, susceptibility and static spin-correlation functions. They, consequently, suggested necessity of a quantum treatment. The problem has already been addressed in the latter context by Cuccoli *et al* [26] using the pure-quantum self-consistent harmonic approximation [27]. Nevertheless, interesting discussions by Cuccoli *et al* [26] have shown how Hamiltonian (1), with $r = 0$, using the Weyl symbol, can be approximated by the simpler planar model and by the sine–Gordon model. Again, our study reveals many interesting features of the magnetic systems such as the case of Fe/Cr(211) superlattices which is isomorphic to a classical two-sublattice, uniaxial, antiferromagnet [28, 29]. Recent study by Trallori [30] shows the equivalence between the magnetic model and a Frenkel–Kontorova-type model with an additional second-harmonic contribution to the sinusoidal potential, while the Remoissenet–Peyrard potential contains more than two harmonics [18].

However, for the particle-like properties of solitons, the stability appears to be a necessary condition. These problems are under consideration and will be published in a future work.

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