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On the compressible Heisenberg chain

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Abstract. It is shown via the coherent state formalism for magnetic and elastic states that small-amplitude non-linear excitations of the magnetic modes induce solitary wave excitations of the elastic modes.

The study of the effect of non-linear magnetic excitations on the elastic modes in the compressible Heisenberg chain [1] has attracted increasing interest during this decade. In [2] the complete integrability of the compressible Heisenberg chain in the continuum limit was shown and it was concluded that magnetic solitons lead to kink-like excitations of the elastic degree of freedom. In [3] the classical continuum limit was investigated and the equations of motion deduced. On the ground of these equations, the existence of magnetic solitary waves, coupled with simultaneous travelling deformations of the lattice, was proved [4]. Deficiencies of the approach in [2] were discussed in [5]. Equations of motion have also been deduced [6] using the method of functional integration. The influence of spin–phonon interaction on the soliton creation in the compressible Heisenberg chain has been considered using the Glauber representation of coheren spin states [7] in the limit of small spin-wave densities, thereby demonstrating that solitonic excitations are dominated by non-linear effects arising from spin–spin interaction.

To investigate the general dependence of the non-linear excitations on the internal parameters, we have used the coherent state representation for the spin and elastic states of the compressible Heisenberg chain in the continuum limit. We have deduced and solved the low-amplitude non-linear equations of motion describing simultaneously the dynamics of the spins and of the magnetic ions.

The Hamiltonian describing the compressible chain is

$$\mathcal{H} = \mathcal{H}_{\rm mag} + \mathcal{H}_{\rm ph} + \mathcal{H}_{\rm int} \tag{1}$$

where $\mathcal{H}_{\rm mag}$ represents the magnetic degrees of freedom and has the form

$$\mathcal{H}_{\rm mag} = -\frac{J}{2}\sum_{n,\delta=\pm a} \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+\delta} - D\sum_n (S_n^z)^2 - g\mu_{\rm B}H\sum_n S_n^z \tag{2}$$

with J the nearest-neighbour exchange interaction, a the lattice parameter, g the g-factor, $\mu_{\rm B}$ the Bohr magneton and H the intensity of an external magnetic field applied

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in the z direction; $D > 0$ is the anisotropy parameter which tends to keep the spin $\boldsymbol{S}_n$ on site n parallel to the field.

$\mathcal{H}_{\text{ph}}$ represents the elastic modes and is given by

$$\mathcal{H}_{\text{ph}} = \sum_n \frac{p_n^2}{2m} + \frac{k}{2} \sum_{n,\delta=\pm a} (q_{n+\delta} - q_n)^2 \tag{3}$$

with q_n the displacement from the equilibrium position of the magnetic ion at site n in the absence of spin–phonon interaction; m is the mass and k is the elastic constant. p_n are the corresponding moments.

The last term $\mathcal{H}_{\text{int}}$ represents the first-order coupling between magnetic and elastic modes and takes the form

$$\mathcal{H}_{\text{int}} = -\lambda \sum_{n,\delta=\pm a} (q_{n+\delta} - q_n)\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+\delta} \tag{4}$$

where $\lambda \equiv \partial J/\partial x$ is the exchange striction parameter.

On the basis of a long-wavelength limit emerges the possibility of writing Hamiltonians (2)–(4) in the more tractable forms

$$\mathcal{H}_{\text{mag}} = -\tfrac{1}{2}J \int \mathrm{d}x \{\tfrac{1}{2}[S^{\dagger}(x)S^{-\prime\prime}(x) + S^{-}(x)S^{\dagger\prime\prime}(x)] + S^{z}(x)S^{z\prime\prime}(x)\}$$
$$- D \int \mathrm{d}x\, [S^{z}(x)]^2 - h \int \mathrm{d}x\, S^{z}(x) - \tfrac{1}{2}NJS^2 \tag{5}$$

$$\mathcal{H}_{\text{ph}} = \int \mathrm{d}x \frac{p(x)^2}{2m} + k \int \mathrm{d}x\, [q'(x)]^2 \tag{6}$$

$$\mathcal{H}_{\text{int}} = -2\lambda \int \mathrm{d}x\, q'(x)\{\tfrac{1}{2}[S^{\dagger}(x)S^{-\prime}(x) + S^{-}(x)S^{\dagger\prime}(x)]$$
$$+ S^{z}(x)S^{z\prime}(x)\} - \lambda S^2 \int \mathrm{d}x\, q''(x) \tag{7}$$

where $h = g\mu_{\text{B}}H_0$ and the chain direction is the x axis. Throughout this paper the prime denotes $\partial/\partial x$. The distance a between the spins defines the length unit.

The ground-state ($T = 0$) configuration of this system corresponds to all the spins aligned in the z axis direction and the ions in their equilibrium positions. To study non-linear excitations of the coupled system, we consider non-linear excitations of the magnetic modes, performing a third-order Holstein–Primakoff transformation of the spin operators

$$\begin{aligned} S^{\dagger}(x) &= \sqrt{2S}[1 - a^{\dagger}(x)a(x)/4S]a(x) \\ S^{-}(x) &= \sqrt{2S}a^{\dagger}(x)[1 - a^{\dagger}(x)a(x)/4S] \\ S^{z}(x) &= S - a^{\dagger}(x)a(x). \end{aligned} \tag{8}$$

For the operators $p(x)$ and $q(x)$, we take the usual representation

$$p(x) = \mathrm{i}\sqrt{m\omega/2}(b^{\dagger}(x) - b(x)) \qquad q(x) = (1/\sqrt{2m\omega})[b^{\dagger}(x) + b(x)] \tag{9}$$

with $\omega = \sqrt{k/m}$.

The time dependence of the annihilation operators $b(x)$ and $a(x)$ are given by ($\hbar = 1$)

$$i\dot{b}(x,t) = [b(x,t), \mathcal{H}] \qquad i\dot{a}(x,t) = [a(x,t), \mathcal{H}] \tag{10}$$

where dots denote $\partial/\partial t$.

Replacing equations (8) and (9) in the Hamiltonian (1), and keeping terms to the fourth order in the bosonic operators, we get from equation (10) the following system of two non-linear differential equations:

$$i\dot{b} = -(\omega/2)(b^\dagger - b) - (k/m\omega)(b^{\dagger\prime\prime} + b'') + (\lambda/\sqrt{m\omega})(a^\dagger a'' - a^{\dagger\prime\prime} a) \tag{11}$$

$$i\dot{a} = -(J/2)(2Sa' + a^{\dagger\prime} a^2 + 2a^{\dagger\prime} a' a - a^\dagger a'^2) + [D(2S-1) + h]a - 2Da^\dagger a^2 - (\lambda/\sqrt{2m\omega}[(b^{\dagger\prime\prime} + b'')a + 2(b^{\dagger\prime} + b')a']. \tag{12}$$

We define now the state of the chain by

$$|\alpha\beta\rangle = \prod_x |\alpha(x)\beta(x)\rangle \tag{13}$$

where

$$|\alpha(x)\beta(x)\rangle = \exp\{-[|\alpha(x)|^2 + |\beta(x)|^2]/2\} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\alpha(x)^n \beta(x)^m}{\sqrt{n!m!}} |n\rangle |m\rangle. \tag{14}$$

These states are eigenstates of the operator b with eigenvalue β. A semi-classical approach allows us to consider that the projections of the spins can be continuously distributed along the z axis; these states are then eigenstates of the operator a with eigenvalue α. So we write

$$b(x)|\alpha\beta\rangle = \beta(x)|\alpha\beta\rangle \qquad a(x)|\alpha\beta\rangle = \alpha(x)|\alpha\beta\rangle. \tag{15}$$

For the system in the state $|\alpha\beta\rangle$, we can find the equations for the averages $\langle\alpha\beta|\dot{b}|\alpha\beta\rangle$ and $\langle\alpha\beta|\dot{a}|\alpha\beta\rangle$ using equations (11) and (12). From this, we obtain

$$\ddot{\beta}^* + \ddot{\beta} = (k\sqrt{2m\omega}/m)(\beta^{*\prime\prime} + \beta'') + (2\lambda\sqrt{2m\omega}/m\omega)\frac{\partial}{\partial t}[\mathrm{Im}(\alpha^* \alpha'')] \tag{16}$$

$$i\dot{\alpha} = -(J/2)(2S\alpha'' + \alpha^{*\prime\prime}\alpha^2 + 2|\alpha'|^2\alpha - \alpha^*\alpha'^2) + [D(2S-1) + h]\alpha - 2D|\alpha|^2\alpha - (\lambda/\sqrt{2m\omega})[(\beta^{*\prime\prime} + \beta'')\alpha + 2(\beta^{*\prime} + \beta')\alpha']. \tag{17}$$

For $\lambda = 0$, equation (16) corresponds to a sound wave equation with $q(x,t) = 0$ as a particular solution, and equation (17) is the non-linear differential equation for the magnetic modes [8].

We shall consider the case of permanent-form travelling-wave solutions assuming the magnetic and the lattice excitations travelling at the same speed v; so we define $\xi \equiv x + vt$. For the border conditions, we choose $q(\pm\infty) = 0$, $q'(\pm\infty) = 0$, $\alpha(\pm\infty) = 0$ and $\alpha'(\pm\infty) = 0$.

From equations (16) and (17), we can obtain

$$q'(\xi) = [2\lambda v/\omega(mv^2 - k)]\,\mathrm{Im}[\alpha^*(\xi)\alpha''(\xi)] \tag{18}$$

and

$$i v\alpha'(\xi) = (J/2)[2S\alpha''(\xi) + \alpha^{*\prime\prime}(\xi)\alpha^2(\xi)] + (J/2)[2|\alpha'(\xi)|^2\alpha(\xi) - \alpha^*(\xi)\alpha'^2(\xi)] - [D(2S-1)+h]\alpha(\xi) + 2D|\alpha(\xi)|^2\alpha(\xi) - \Lambda\{\mathrm{Im}[\alpha^*(\xi)\alpha''(\xi)]'\alpha(\xi) + 2\mathrm{Im}[\alpha^*(\xi)\alpha''(\xi)]\alpha'(\xi)\} \qquad (19)$$

where $\Lambda \equiv [2\lambda^2 v/\omega(k - mv^2)]$.

Defining the real functions $\rho(\xi)$ and $\varphi(\xi)$ through $\alpha(\xi) \equiv \rho(\xi)\exp[-i\varphi(\xi)]$, we obtain from equation (19), after comparing real and imaginary parts, the following system of two non-linear differential equations:

$$v\rho' = JS(2\rho'\varphi' + \rho\varphi'') + (J/2)[\rho^2(2\rho'\varphi' + \rho\varphi'') + 2\rho^2\rho'\varphi'] - 2\Lambda\rho^2\varphi'(2\rho'\varphi' + \rho\varphi'') \qquad (20)$$

$$v\rho\varphi' = JS(\rho'' - \rho\varphi'^2) + (J/2)(\rho^2\rho'' + \rho\rho'^2 + 2\rho^3\varphi'^2) - [D(2S-1)+h] + 2D\rho^3 - \Lambda(6\rho\rho'^2\varphi' + 3\rho^2\rho'\varphi'' + 2\rho^2\rho''\varphi' + \rho^3\varphi'''). \qquad (21)$$

The corresponding boundary conditions are now $\rho(\pm\infty) = 0$, $\rho'(\pm\infty) = 0$ and we can integrate (20) once to obtain

$$\Lambda\rho^2\varphi'^2 - J(S + \rho^2/2)\,\varphi' + v/2 = 0. \qquad (22)$$

For the case where $\Lambda \neq 0$, we obtain from (21) and (22) the following equation for $\rho(\xi)$:

$$JS\,\rho'' - 7\gamma\rho^3\rho'^2 - A\rho - B\rho\rho'^2 - C\rho^2\rho'' - E\rho^3 - 2\gamma\rho^4\rho'' = 0 \qquad (23)$$

where we have made the definitions: $A = v\mu/2\Lambda + JS\mu^2/4\Lambda^2 + D(2S-1) + h$; $B = 3\mu - J/2$; $C = \mu - J/2$; $E = v\gamma/2\Lambda + JS\mu\gamma/2\Lambda^2 - J\mu^2/4\Lambda^2 - 2D$; $\gamma = \Lambda v(\Lambda v - J^2S)/4J^3S^4$; $\mu = [J^2S(2S-1) + 2\Lambda v]/4JS^2$.

Now defining $F(\rho) \equiv \rho'^2$ we obtain from (23)

$$(JS - C\rho^2 - 2\gamma\rho^4)\,\mathrm{d}F(\rho)/\mathrm{d}\rho - 2(7\gamma\rho^3 + B\rho)\,F(\rho) - 2A\rho - 2E\rho^3 = 0. \qquad (24)$$

Boundary conditions and the fact that $F(\rho) = F(-\rho)$ allow us to expand, to the fourth order:

$$F(\rho) = a_2\rho^2 - a_4\rho^4. \qquad (25)$$

Using (25) in (24) we find $a_2 = A/JS$ and $a_4 = -(4\mu + E - J)/2JS$; and finally:

$$\rho(\xi) = \sqrt{a_2/a_4}\,\mathrm{sech}\,(\sqrt{a_2}\,\xi). \qquad (26)$$

For $\varphi(\xi)$ we obtain

$$\varphi(\xi) = (1/2\Lambda)[\mu\xi + (\gamma\sqrt{a_2}/a_4)\tanh(\sqrt{a_2}\,\xi)]. \qquad (27)$$

Using these results in (18) we find

$$q(\xi) = -(\mu a_2/2\Lambda a_4)\tanh(\sqrt{a_2}\,\xi)\,\mathrm{sech}\,(\sqrt{a_2}\,\xi). \qquad (28)$$

The equivalent relations for the magnetic modes are, to the third order in ρ:

$$\langle S_x(\xi)\rangle = \sqrt{2S}\,(1 - \rho^2(\xi)/4S)\,\rho(\xi)\cos\varphi(\xi)$$
$$\langle S_y(\xi)\rangle = \sqrt{2S}\,(1 - \rho^2(\xi)/4S)\,\rho(\xi)\sin\varphi(\xi) \qquad (29)$$
$$\langle S_z(\xi)\rangle = S - \rho^2(\xi).$$

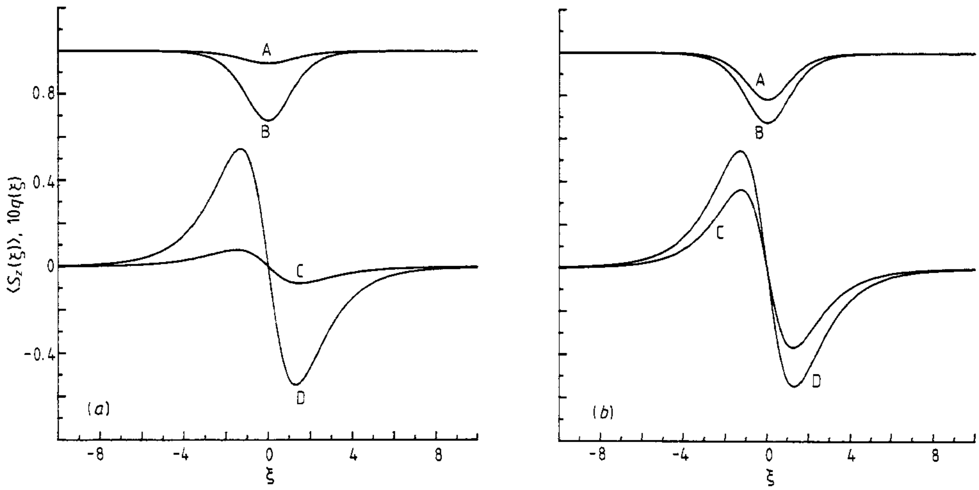

Figure 1. (*a*) Dependences of $\langle S_z(\xi)\rangle$ and $q(\xi)$ on λ ($k=2$, $v=1$, $m=1$, $d=0.01$ and $h=0.01$): curve A, $\langle S_z(\xi)\rangle$ for $\lambda=2$; Curve B, $\langle S_z(\xi)\rangle$ for $\lambda=1$; curve C, $10q(\xi)$ for $\lambda=2$; curve D, $10q(\xi)$ for $\lambda=1$. (*b*) Dependences of $\langle S_z(\xi)\rangle$ and $q(\xi)$ on v ($k=2$, $\lambda=1$, $m=1$, $d=0.001$ and $h=0.01$): curve A, $\langle S_z(\xi)\rangle$ for $v=1.5$; curve B, $\langle S_z(\xi)\rangle$ for $v=1$; curve C, $10q(\xi)$ for $v=1.5$; curve D, $10q(\xi)$ for $v=1$.

Equations (28) and (29) describe completely the magnetic and acoustic solitary waves which are characterised by the five parameters $k, v, \lambda, d \equiv D/J$ and m. In the following, we scale energies in J, taking $J=1$.

We show first in figures 1(*a*) and 1(*b*) the dependences of $\langle S_z(\xi)\rangle$ and $q(\xi)$ on λ and v, respectively. For both magnitudes the amplitude decreases with increasing λ and increasing v, and a close relation between the amplitudes and widths of the coupled

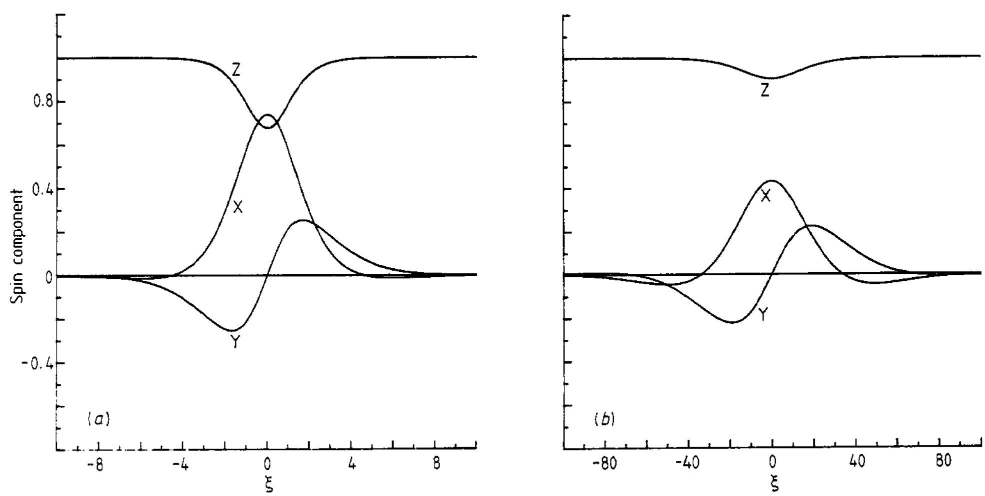

Figure 2. (*a*) Spin components for $\lambda=1$ and $v=1$ ($k=2$, $m=1$, $d=0.01$ and $h=0.01$): curve X, $\langle S_x(\xi)\rangle$; curve Y, $\langle S_y(\xi)\rangle$; curve Z, $\langle S_z(\xi)\rangle$. (*b*) Spin components for $\lambda=20$ and $v=0.01$ ($k=2$, $m=1$, $d=0.01$ and $h=0.01$): curve X, $\langle S_x(\xi)\rangle$; curve Y, $\langle S_y(\xi)\rangle$; curve Z, $\langle S_z(\xi)\rangle$.

solitary waves. We also find an upper limit for the velocity and a lower limit for the striction constant; between these limits, no solitary wave solutions are predicted with this theory. Moreover, it is possible to have small-amplitude solutions for very small velocities only for large coupling. Equations (26)–(28) also predict sharper and narrower curves for increasing h, d and k.

The structure of the magnetic solitary waves becomes particularly transparent in figure 2. The presence of a localised tilt mode in the direction of propagation should be noted.

In conclusion, we have shown via the formalism of coherent states in which non-linear magnetic excitations in the compressible Heisenberg chain induce non-linear excitations of the elastic modes. This approach may be adequate for investigating the compressible easy-plane Heisenberg chain; the results of the first calculations demonstrate that, in the case of extreme anisotropy, no induced non-linear elastic mode is present.

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