Coupled spin-lattice solitary waves in a compressible classical Heisenberg chain

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The equation for solitary waves in the continuum limit of a classical compressible Heisenberg chain is treated rigorously. It is proven that infinitely many coupled spin-lattice solitary waves exist. An explicit formula for the behavior of spin angles and lattice distortion is obtained. As an example of the general behavior, a particular case is worked out explicitly. The motion of spin and lattice coordinates is obtained rigorously in terms of a few well-defined integrals that are calculated numerically. The relevant solitary wave parameters—the speed, spin-precession rate, total energy, and total magnetization—are also obtained rigorously.

Solitary waves are a topic of much current interest. In particular, a lot of work has been devoted to the study of magnetic solitary waves in one-dimensional classical magnets.¹ Much less attention has been paid to the investigation of coupled spin-lattice solitary waves in compressible magnets.

In an earlier paper,² we have derived coupled equations for displacement and spin motion in a continuum version of the compressible classical Heisenberg chain. Assuming solitary-wave solutions, it was possible to decouple the equations for lattice distortions and spins. We argued that the equations did not admit of the very simple solitary waves found by Cieplak and Turski³ in a different—and, in our opinion, wrong²—analysis. However, at that time we were unable to give the solutions to our equations.

An important step forward has been made by Magyari,⁴ who showed how to decouple in a simple way our two equations for the angular spin coordinates. He also obtained solutions in the small coupling limit, but the question of a more general solution remained open. In this paper we will exactly prove the existence of infinitely many solitary waves. Moreover, it will be shown how to obtain the solutions, to almost any desired accuracy, by numerically carrying out a few integrals.

In Ref. 2 we started from the model Hamiltonian⁵

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{\alpha}{2} \sum_{i=1}^{N-1} (x_{i+1} - x_i)^2 - J \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1} - \epsilon \sum_{i=1}^{N-1} (x_{i+1} - x_i) \vec{S}_i \cdot \vec{S}_{i+1} \quad .$$
(1)

Then we took the continuum limit $[x_i \rightarrow \eta(x,t)]$ and $\vec{S}_i \rightarrow \vec{S}(x,t)$ and assumed solitary waves of the form⁶

$$\overline{\mathbf{S}}(x,t) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$
, (2a)

$$\theta(x,t) = \theta(u), \quad \phi(x,t) = \overline{\phi}(u) + \Omega t , \quad (2b)$$

$$\eta(x,t) = \frac{\epsilon}{\alpha} x + f(u) \quad , \tag{2c}$$

$$u = x - ct \quad , \tag{2d}$$

where c is the solitary-wave velocity. With the boundary conditions

$$f'(-\infty) = 0, \ \vec{S}'(-\infty) = 0, \ S^{z}(-\infty) = 1, \ (3)$$

we obtained the equations

$$(mc^2 - \alpha)f' = \frac{\epsilon}{2}(\vec{S}')^2$$
, (4a)

$$A(z'^{2} + y^{2})(1 - z^{2}) + \frac{3}{2}B(z'^{2} + y^{2})^{2} - 2\Omega(1 - z)(1 - z^{2})^{2} = 0 , \quad (4b)$$
$$[A(1 - z^{2}) + B(z'^{2} + y^{2})]y - c(1 - z)(1 - z^{2}) = 0 , \quad (4c)$$

where $A = J + \epsilon^2/\alpha$, $B = \epsilon^2/2(mc^2 - \alpha)$ ($\alpha \neq mc^2$), $z = \cos\theta$, $y = \phi' \sin^2\theta$, and a prime denotes derivation $\partial/\partial u$. Magyari⁴ showed that [Eqs. (4b) and (4c)], with the boundary conditions (3), are equivalent to

$$z'^2 + V(z) = 0 , (5a)$$

$$y = (3c/A)(1-z)/(W+2)$$
, (5b)

where

$$V(z) = (9c^2/A^2)(1-z)^2(W+2)^{-2} + (A/3B)(1-W)(1-z^2)$$
(6a)

$$W = [1 + 12(B\Omega/A^2)(1 - z)]^{1/2} , \qquad (6b)$$

and where the parameters must obey the restrictions

$$c^2 < 4A \Omega$$
 , (7a)

$$A^2 \ge -24B\,\Omega \quad . \tag{7b}$$

In order to have solitary-wave solutions, Magyari argues that there is the supplementary condition that the equation V(z) = 0 must have at least one simple

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$$\pm \left(\frac{A}{12B}\right)^{1/2} (u - u_0)$$

= $\int_{W(u_0)}^{W(u)} dW \frac{W(W+2)}{(W-1)(W+1)^{1/2}Q(W)^{1/2}}$, (8)

where

$$Q(W) = -W^4 - 4W^3 + aW^2 + b(W+1) , \quad (9a)$$

$$a = 24B\,\Omega/A^2 - 3 \quad , \tag{9b}$$

$$b = 4(a+4) - \gamma \quad , \tag{9c}$$

$$\gamma = 27 B c^2 / A^3 \quad . \tag{9d}$$

In the following, we consider only the dynamic case $c \neq 0$. The static case c = 0 has been considered by Magyari.⁴ The conditions (7) then become

$$a > -3$$
 and $0 < \gamma < \frac{9}{2}(a+3)$ if $B > 0$; (10a)

$$-4 \le a < -3$$
 and $0 > \gamma > \frac{9}{2}(a+3)$ if $B < 0$. (10b)

$$1 \le W < (a+4)^{1/2}$$
 if $B > 0$; (11a)

$$(a+4)^{1/2} < W \le 1$$
 if $B < 0$. (11b)

We will now prove that the equation Q(W) = 0has exactly one simple root $W_0 \neq 1$ in the allowed domain (11). It is easily verified that this is equivalent to the existence of one z_0 . From Eqs. (9) and (10), it follows that

$$Q(1) > 0$$
 and $\lim_{w \to \infty} Q(W) = -\infty$ if $B > 0$; (12a)

$$Q(1) < 0 \text{ and } Q(0) > 0 \text{ if } B < 0$$
. (12b)

Hence, in both cases, there is at least one root W_0 in the domain (11). Let us now show that this is the only one. From $Q(W_0) = 0$ it follows that

$$b = W_0^2 \left(W_0^2 + 4 W_0 - a \right) / (W_0 + 1) \quad . \tag{13}$$

Extracting the factor $(W - W_0)$ and choosing $W(0) = W_0$, Eq. (8) becomes

$$\pm (3c/2A\sqrt{|\gamma|})u = \int_{W_0}^W dW \frac{W(W+2)}{(W-1)(W+1)^{1/2}|W-W_0|^{1/2}P(W)^{1/2}}$$
(14)

Here we used Eq. (9d) and the equality $sgn(B) = sgn(W_0 - W)$. We must now investigate how the remaining third-order polynomial

$$P(W) = W^{3} + (W_{0} + 4) W^{2} + (W_{0}^{2} + 4W_{0} - a)[W + W_{0}/(W_{0} + 1)]$$
(15)

behaves in the domain (11). First consider B > 0. Then (9c), (10a), and (13) yield

$$a < a_0 = W_0^2 + 4W_0 + (W_0 + 5)(W_0 + 1)/(2W_0 + 1) \quad .$$
(16)

Now it can be shown that, if (16) is fulfilled, P(W) is strictly positive for $W \ge 1$. It is also easy to show that $W_0^2 - 4 < a_0$, so that it is possible to fulfill (11a) and (16) at the same time. From Eqs. (9d) and (10a) and the explicit expression of B, it follows that

$$a > a_m = 3\left(\frac{\epsilon^2}{A^3m} - 1\right) > -3 \quad . \tag{17}$$

This is compatible with (16) if $a_m < a_0$. Since $a_0 > 9$

for all $W_0 > 1$, this will be fulfilled for physical values of the model parameters. If B < 0, it is trivial that P(W) > 0 if W > 0. This completes the proof of the existence of a unique W_0 compatible with Eq. (11), and at the same time the existence of solitary waves.

Thus we arrive at the following recipe: Choose $W_0 > 0$, $W_0 \neq 1$. Then choose *a* such that $\max(W_0^2 - 4, a_m) < a < a_0$ if $W_0 > 1$, and such that $-4 \leq a < W_0^2 - 4$ if $0 < W_0 < 1$. The local magnetization z(u) then follows from Eq. (14), with

$$W = \left(1 + \frac{a+3}{2}(1-z)\right)^{1/2} .$$
 (18)

Although z cannot be expressed in terms of elementary functions of u, if $W \neq 1$ the integral (14) is readily carried out numerically since the integrand has no singularities except at W_0 , which is removed by a change of integration variable. If $W \rightarrow 1$, the integral diverges logarithmically, assuring the exponential approach of z to 1 as $u \rightarrow \pm \infty$. The behavior of the precession angle ϕ is found from Eqs. (5), (6), and (14) as

$$\phi(u) = \frac{1}{2A}u + \psi(u) , \qquad (19a)$$

$$\psi(u) = \operatorname{sgn}(u) \frac{\sqrt{|\gamma|}}{3} \int_{W(u)}^{W_0} dW \frac{W(W^2 + 3W - a - 1)}{|W - W_0|^{1/2}(W + 1)^{1/2}P(W)^{1/2}(a + 4 - W^2)} . \qquad (19b)$$

Thus, by Eq. (2b), the precession is made up of a constant precession Ωt , a term linear in u and a pure solitary-wave contribution $\psi(u)$. The solitary-wave contribution f(u) to the displacement η is found from Eq. (4a) to be

$$f(u) = \left(\frac{2}{3}\right)^{1/2} \left| \frac{A}{mc^2 - \alpha} \right|^{1/2} \operatorname{sgn}(\epsilon) F(u) , \qquad (20a)$$

$$F(u) = \int_{1}^{W_{0}} g(W) dW + \operatorname{sgn}(u) \int_{W(u)}^{W_{0}} g(W) dW ,$$
(20b)

$$g(W) = \frac{W(W+2)}{|W-W_0|^{1/2}(W+1)^{1/2}P(W)^{1/2}} \quad . \tag{20c}$$

 $\psi(u)$ and F(u), in contradistinction with z(u), can be shown to be kink solitary waves.

As an example, we depict in Fig. 1 the local magnetization (a), the precession angle (b), and the distortion function (c), for the choice of parameters



FIG. 1. (a)-(c) Behavior of the coupled spin-lattice solitary wave as a function of $\nu = (3c/8A)(x-ct)$ for the particular choice of parameters $W_0 = 2$, a = 3: (a) local z magnetization (dots show how $\tanh^2 \nu$ behaves); (b) spin precession around the z axis; (c) lattice expansion. The functions ψ and F are defined in Eqs. (18) and (19).

 $W_0 = 2$, a = 3. Scaling the independent variable u by v = (3c/8A)u, the graphs are independent of the model parameters α , ϵ , J, and m. Therefore the width of the solitary wave is inversely proportional to its speed c. It can be shown that this is a general property of Eqs. (14), (19), and (20). When the solitary wave passes, the spins dip down to $\pi/2$ ($z_0=0$). At the same time and in the same restricted region, the angle ϕ , apart from the constant precession Ωt and the linear term cu/2A, increases by approximately $\pi/3.5$ rad. In the same region the lattice is locally expanded or compressed depending on the sign of ϵ . The results of Fig. 1 are qualitatively characteristic of all solutions to the equations. In Fig. 1(a) it is shown that the local magnetization behaves very much like $tanh^2 \nu$ in this particular case. Magyari's result to order ϵ would yield⁴ tanh²($\sqrt{3/2}\nu$). Therefore it is to be expected that a perturbation approach has to take into account many orders of ϵ to reproduce our result. The velocity c and the constant precession rate Ω of the wave read

$$c^2 = \alpha / (m - 27\epsilon^2/32A^3)$$
, (21a)

$$\Omega = 27c^2/64A \quad . \tag{21b}$$

The total energy reads

$$E = c \left(\frac{0.394 c_H^2}{c^2 - c_H^2} + 2.303 \right) , \qquad (22)$$

where $c_H = (\alpha/m)^{1/2}$ denotes the harmonic lattice frequency. The total magnetization is given by

$$M = \int_{-\infty}^{+\infty} (1-z) \, du = 5.458 \, A/c \quad . \tag{23}$$

In summary, we have shown that the compressible chain described by Hamiltonian (1) bears infinitely many coupled solitary waves of spin and lattice deviations. Equations (5) with the conditions (7) were proven to be completely integrable in terms of solitary waves. By means of simple function analysis we have shown how to find the complete set of solutions in terms of well-defined simple integrals. With the help of an example we have shown the general qualitative behavior of spins and lattice. It was possible to obtain all quantities relevant to the solutions.

Some interesting but probably very difficult questions remain to be answered. Apart from the solutions of the form (2) we have concentrated on in this paper, the general equations resulting from Hamiltonian (1) in the continuum limit [Eqs. (4) of Ref. 2] also have as solutions pure lattice waves and pure spin waves. Are there still other solutions? Also, how are the solitary waves influenced by mutual interactions? In particular, are there multisoliton solutions? It would also be interesting to investigate the quantum-mechanical version of the problem.

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⁶Here we make the same assumption as made for the rigid chain in M. Lakshmanan, Th. W. Ruijgrok, and C. J. Thompson, Physica (Utrecht) 84A, 577 (1976).

⁷This formulation by means of an integral over W has been suggested by E. Magyari (private communication).