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LETTER TO THE EDITOR

Solitons in an order-parameter-preserving antiferromagnet

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Abstract. Introducing the Dyson–Maleev transformation and the coherent state *ansatz*, we obtain two partial differential equations of motion with non-linear coupling in an order-parameter-preserving antiferromagnet (OPP-AFM). These equations are reduced to a single non-linear Schrödinger equation by using the method of multiple scales combined with the long-wavelength approximation. The single-soliton solution and the two-soliton bound-state solution are obtained using the inverse-scattering transformation. These results show that soliton-like magnon localization and two-magnon bound states in the FCC-AFM compound CeAs are possible. The possibility of observing a gap soliton in this system are also discussed.

Recently Mikeska and Steiner have reviewed the solitary excitations in one-dimensional magnets [1]. Bell *et al* [2] examined the nature of two-magnon excitations in the alternating bond ferromagnetic $s = \frac{1}{2}$ spin chain using two different methods: a direct analytic approach considered as a generalization of the Bethe *ansatz* for the uniform chain and a scaling approach introduced by Southern *et al* [3]. Huang *et al* [4–7] have published the two-parameter theory of solitons in magnetic systems. Their aim is to study the excitations of the alternating antiferromagnetic chain. Soliton-like excitations in antiferromagnetic chains with rotational symmetry in spin space with respect to the z axis have been discussed. Monte Carlo calculations for the easy-plane antiferromagnet have been performed by Gaulin and Collins [8, 9]. When the planar symmetry of antiferromagnetic chain systems such as TMMC is further broken, a large variety of soliton-like phenomena are found; this situation is among the best investigated soliton phenomenologies both theoretically and experimentally. The possibility of finding a pair of bound solitons in TMMC was investigated theoretically and experimentally. Recent experiments indeed show the existence of such soliton pairs below T_N [10]. In TMMC, a very good description of the experiments could be obtained using sine–Gordon theory for such complicated effects as the cross over from longitudinal to transverse solitons at high magnetic field and the breakdown of the ballistic movements of solitons upon a very small doping of the chain. In TMMC, a detailed investigation of the single-soliton properties such as the soliton shape was not yet possible because of the weakness of the corresponding signal in the inelastic neutron spectrum. As in $CsNiF_3$ a study of the solitons in the large-density limit would be interesting, too. Further experimental, theoretical and computational efforts should now aim at the investigation of details of these soliton-bearing systems, trying to establish a more quantitative picture.

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Ferromagnets are described by an order parameter which is a conserved quantity and the excitation spectrum which is quadratic in the wave vector $|k|$. Conventional antiferromagnets described by the Heisenberg Hamiltonian are characterized by a non-conserved order parameter, staggered magnetization, and a spin wave spectrum linear in the wave vector $|k|$. An order-parameter-preserving antiferromagnetic (OPP-AFM) Hamiltonian is defined on a bipartite lattice in any dimension and Néel states taken as the exact ground states [11–13]. Neutron scattering experiments suggest that the FCC-AFM compound CeAs could be the first example of an OPP-AFM where the order parameter is not exactly conserved but is almost conserved [14, 15]. The OPP-AFM Hamiltonian is unitarily related to that of a ferromagnet and hence has an excitation spectrum quadratic in the wave vector $|k|$. In the presence of an external magnetic field, the Hamiltonian of an OPP-AFM is no longer unitarily connected to that of the ferromagnet in a magnetic field and the excitation spectrum is expected to be different. The effect of the external field is to remove the degeneracy in the excitation spectrum and open a gap. Bose deduced an exact expression for the excitation spectrum of one-dimensional OPP-AFMs in the presence of an external magnetic field and generalized this result to three dimensions by considering the FCC-AFM compound CeAs which has been cited as the first example of an OPP-AFM [13–15].

In this letter, we will employ the Dyson–Maleev transformation and the coherent state *ansatz*, and investigate the single-soliton solution and the two-soliton bound-state solution in an OPP-AFM by using the method of multiple scales. The aim of this letter is to show that the approach developed above is self-consistent and systematic. Our approach may be a good method of investigating ferromagnetic and antiferromagnetic chains.

The frame of this letter is as follows. We first employ the Dyson–Maleev transformation and the coherent state *ansatz*, and obtain two parallel differential equations of motion with non-linear coupling. We then use the method of multiple scales combined with the long-wavelength approximation, and reduce these equations of motion into an envelope-function equation. Next, we investigate the single-soliton solution and the two-soliton bound-state solution in an OPP-AFM by using the inverse-scattering transformation. Finally we present the discussion.

The Hamiltonian describing an OPP-AFM in the external magnetic field is given by [11–13]

$$H = \sum_{\langle ij\rangle}\Big[J_{ij}S_i^z s_j^z - \tfrac{1}{2}\Delta_{ij}(S_i^+S_j^+ + S_i^-S_j^-)\Big] - h\sum_i S_i^z \tag{1}$$

where J_{ij} and Δ_{ij} are the exchange integrals for spins located at sites i, j of the lattice and h is the magnitude of the external magnetic field.

For antiferromagnets composed of two interpenetrating sublattices A and B, we introduce the Dyson–Maleev transformation by giving a correspondence between any operator A in the Hilbert space of the spin system and an operator $\tilde{A}$ in the boson Hilbert space [16, 17]

$$S_i^+ - (2S)^{1/2}\Big(1 - a_i^\dagger a_i/2S\Big) \qquad S_i^- = (2S)^{1/2}a_i^\dagger \qquad S_i^z = S - a_i^\dagger a_i \qquad \text{for } i\in A \tag{2a}$$

$$S_j^+ = (2S)^{1/2} b_j^+ \left(1 - b_j^+ b_j / 2S\right) \qquad S_j^- = (2S)^{1/2} b_j \qquad S_j^z = -S + b_j^+ b_j$$
$$\text{for } j \in B \tag{2b}$$

and get the boson Hamiltonian

$$H = \sum_{\langle ij \rangle} \Big[(SJ_{ij} + h) a_i^+ a_i + SJ_{ij} b_j^+ b_j - S\Delta_{ij} (a_i b_j^+ + a_i^+ b_j) - J_{ij} a_i^+ a_i b_j^+ b_j + \tfrac{1}{2} \Delta_{ij} (a_i b_j^{+2} b_j + a_i^+ a_i^2 b_j^+) - (1/S4) \Delta_{ij} a_i^+ a_i^2 b_j^+ b_j \Big] \tag{3}$$

where $a_i(a_i^+)$ and $b_j(b_j^+)$ are boson annihilation (creation) operators associated with the A and B sublattices, S is the magnitude of spin operators and the symbol $\langle ij \rangle$ denotes the sum over nearest-neighbour pairs.

We employ the coherent state *ansatz* for the eigenfunction $\Psi(t)$ of H:

$$\Psi(t) = \exp\left[-\tfrac{1}{2} \left(\sum_i |\alpha_i(t)|^2 + \sum_j |\beta_j(t)|^2 \right) \right] \exp\left[\sum_i \alpha_i(t) a_i^+ + \sum_j \beta_j(t) b_j^+ \right] |0\rangle \tag{4}$$

where $|0\rangle$ is the vacuum state of the boson system, and set up the time-dependent variational principle [18, 19]

$$\delta \int \mathrm{d}t \; \langle \Psi(t) | \mathrm{i}\hbar \frac{\partial}{\partial t} - H | \Psi(t) \rangle = 0. \tag{5}$$

The coherent state representation $\langle \Psi(t) | H | \Psi(t) \rangle$ of H in equation (5) is identical to equation (3) with $a_i(a_i^+)$, $b_j(b_j^+)$ replaced by $\alpha_i(\alpha_i^*)$, $\beta_j(\beta_j^*)$ for all i and j. Then, the variational principle yields the following equations of motion for the values of α_i and β_j:

$$\mathrm{i}\hbar (\mathrm{d}/\mathrm{d}t) \alpha_i = (SJ + h)\alpha_i - S\Delta(\beta_j + \beta_{j-1}) - J\alpha_i(|\beta_j|^2 + |\beta_{j-1}|^2) + \tfrac{1}{2}\Delta\alpha_i^2(\beta_j + \beta_{j-1})^* - (1/4S)\Delta\alpha_i^2(|\beta_j|^2\beta_j^* + |\beta_{j-1}|^2\beta_{j-1}^*) \tag{6a}$$

$$\mathrm{i}\hbar (\mathrm{d}/\mathrm{d}t) \beta_j = SJ\beta_j - S\Delta(\alpha_i + \alpha_{i+1}) - J\beta_j(|\alpha_i|^2 + |\alpha_{i+1}|^2) + \tfrac{1}{2}\Delta(|\alpha_i|^2\alpha_i + |\alpha_{i+1}|^2\alpha_{i+1}) + \Delta|\beta_j|^2(\alpha_i + \alpha_{i+1}) - (1/2S)\Delta|\beta_j|^2(|\alpha_i|^2\alpha_i + |\alpha_{i+1}|^2\alpha_{i+1}) \tag{6b}$$

where we consider the system described by the Hamiltonian (1) containing only nearest-neighbour interactions and with $J_{ij} = J$, $\Delta_{ij} = \Delta$ for all spin pairs. Although equations (6) have been transformed to c-number equations, it is very difficult to solve them because of their non-linearity and discreteness. If we assume that a typical wavelength of the solitons $\lambda_0 \gg 2d_0$, where d_0 is the lattice constant, then we may take the continuum approximation

$$\begin{aligned}
&\alpha_i(t) \to \Psi_1(x,t) \\
&\alpha_{i+1}(t) \to \Psi_1 + \eta\Psi_{1x} + (1/2!)\eta^2\Psi_{1xx} \\
&\qquad\qquad + (1/3!)\eta^3\Psi_{1xxx} + \mathrm{O}(\eta^4)
\end{aligned} \tag{7a}$$

$$\begin{aligned}
&\beta_j(t) \to \Psi_2(x,t) \\
&\beta_{j-1}(t) \to \Psi_2 - \eta\Psi_{2x} + (1/2!)\eta^2\Psi_{2xx} \\
&\qquad\qquad - (1/3!)\eta^3\Psi_{2xxx} + \mathrm{O}(\eta^4)
\end{aligned} \tag{7b}$$

where $\eta = 2d_0/\lambda_0$ is a small dimensionless parameter. In this paper, we only consider the case $\mathrm{O}(\eta^2)$. Retaining terms in equation (6) to $\mathrm{O}(\eta^2)$, we have

$$\begin{aligned}
\mathrm{i}\hbar\Psi_{1t} = {} & (SJ+h)\Psi_1 - S\Delta\left(2\Psi_2 - \eta\Psi_{2x} + \tfrac{1}{2}\eta^2\Psi_{2xx}\right) - 2J\Psi_1|\Psi_2|^2 + \Delta\Psi_1^2\Psi_2^* \\
& - (1/2S)\Delta\Psi_1^2|\Psi_2|^2\Psi_2^*
\end{aligned} \tag{8a}$$

$$\begin{aligned}
\mathrm{i}\hbar\Psi_{2t} = {} & SJ\Psi_2 - S\Delta\left(2\Psi_1 + \eta\Psi_{1x} + \tfrac{1}{2}\eta^2\Psi_{1xx}\right) - 2J\Psi_2|\Psi_1|^2 + 2\Delta\Psi_1|\Psi_2|^2 \\
& + \Delta|\Psi_1|^2\Psi_1 - (1/S)\Delta\Psi_1|\Psi_1|^2|\Psi_2|^2.
\end{aligned} \tag{8b}$$

It is very difficult to solve equations (8) exactly because they are non-linear and coupled. To find the solution of slowly varying components of Ψ_1 and Ψ_2, we use the method of multiple scales [20, 21] to reduce equations (8) to another non-linear equation which can be solved exactly. This general technique calls in the present problem for the introduction of different length scales $x_j = \mu^j x$ and time scales $t_j = \mu^j t (\mu \ll 1, j = 0, 1, 2, \ldots)$. It is important that in the subsequent discussion these new variables are considered to be independent. Under this condition, the first spatial and temporal derivatives can be written as

$$\begin{aligned}
\partial/\partial t &= \partial/\partial t_0 + \mu\partial/\partial t_1 + \mu^2\partial/\partial t_2 + \ldots \\
\partial/\partial x &= \partial/\partial x_0 + \mu\partial/\partial x_1 + \mu^2\partial/\partial x_2 + \ldots
\end{aligned} \tag{9}$$

from which expressions for higher derivatives follow straightforwardly. Similarly, the quantities Ψ_1 and Ψ_2 are written as expansions

$$\begin{aligned}
\Psi_1 &= \mu\Psi_1^{(1)} + \mu^2\Psi_1^{(2)} + \mu^3\Psi_1^{(3)} + \ldots \\
\Psi_2 &= \mu\Psi_2^{(1)} + \mu^2\Psi_2^{(2)} + \mu^3\Psi_2^{(3)} + \ldots
\end{aligned} \tag{10}$$

where $\Psi_1^{(j)}$, $\Psi_2^{(j)}$ are functions of all x_j and t_j (j = 1, 2, 3, ...), but these arguments will not be written explicitly. Equation (10) is now substituted into equations (8) and terms with equal powers of μ are collected. This substitution results in equations for $\Psi_1^{(j)}$, $\Psi_2^{(j)}$ as follows:

$$(\mathrm{i}\hbar\partial/\partial t_0 - \omega_k)\Psi_k^{(j)} + L_k\Psi_l^{(j)} = \beta_k^{(j)} \tag{11a}$$

$$\omega_k = SJ + \delta_1 h \qquad \delta_1 = \begin{cases} 1 & k = 1 \\ 0 & k = 2 \end{cases} \tag{11b}$$

$$L_k = 2S\Delta + S\eta\Delta\delta_2\partial/\partial x_0 + \tfrac{1}{2}S\eta^2\Delta\partial^2/\partial x_0^2 \qquad \delta_2 = \begin{cases} -1 & k = 1 \\ 1 & k = 2 \end{cases} \tag{11c}$$

$$\beta_k^{(1)} = 0 \tag{11d}$$

$$\beta_k^{(2)} = -\mathrm{i}\hbar(\partial/\partial t_1)\Psi_k^{(1)} + \delta_3 S\eta\Delta(\partial/\partial x_1)\Psi_l^{(1)} - S\eta^2\Delta(\partial^2/\partial x_0\partial x_1)\Psi_l^1$$
$$\delta_3 = \begin{cases} 1 & k = 1 \\ -1 & k = 2 \end{cases} \tag{11e}$$

$$\beta_k^{(3)} = -\mathrm{i}\hbar\Big[(\partial/\partial t_1)\Psi_k^{(2)} + (\partial/\partial t_2)\Psi_k^{(1)}\Big] + \delta_4 S\eta\Delta\Big[(\partial/\partial x_1)\Psi_l^{(2)}$$
$$+ (\partial/\partial x_2)\Psi_l^{(1)}\Big] - \tfrac{1}{2}S\eta^2\Delta\Big[2(\partial^2/\partial x_0\partial x_1)\Psi_l^{(2)} + 2(\partial^2/\partial x_0\partial x_2)\Psi_l^{(1)}$$
$$+(\partial^2/\partial x_1^2)\Psi_l^{(1)}\Big] - 2J\Psi_k^{(1)}|\Psi_l^{(1)}|^2 + \Delta\Big[\delta_5|\Psi_k^{(1)}|^2\Psi_l^{(1)*} + 2\delta_6|\Psi_k^{(1)}|^2\Psi_l^{(1)} + \delta_6|\Psi_l^{(1)}|^2\Psi_l^{(1)}\Big]$$
$$\delta_4 = \begin{cases} 1 & k = 1 \\ -1 & k = 2 \end{cases} \qquad \delta_5 = \begin{cases} 1 & k = 1 \\ 0 & k=2 \end{cases} \qquad \delta_6 = \begin{cases} 0 & k = 1 \\ 1 & k = 2 \end{cases} \tag{11f}$$

where $k, l = 1, 2$; $k \neq l$; $j = 1, 2, 3, \ldots$. We obtain the equations of $\Psi_1^{(3)}$ and $\Psi_2^{(3)}$ for $j = 3$

$$(\mathrm{i}\hbar\partial/\partial t_0 - \omega_1)(\mathrm{i}\hbar\partial/\partial t_0 - \omega_2)\Psi_1^{(3)} - L_1L_2\Psi_1^{(3)} = -(2\omega - \omega_1 - \omega_2)$$
$$\times \Big[\mathrm{i}(\partial/\partial t_2)A^{(1)}$$
$$+ \tfrac{1}{2}\omega''(k)(\partial^2/\partial\xi^2)A^{(1)} + \lambda|A^{(1)}|^2A^{(1)}\Big]\exp[\mathrm{i}(kx_0 - \omega t_0)] \tag{12a}$$

$$\lambda = [\Delta/(\omega - \omega_1 - \omega_2)]\Big\{4(\omega - \omega_1) + [(2\omega - \omega_1 - \omega_2)/(\omega - \omega_2)](r + r^*)$$
$$+ 4(\omega - \omega_1)\Big[A_1^{(2)}(\omega - \omega_2)^2 + A_2^{(2)}(\omega - \omega_1)^2\Big]\Big/\Delta(\omega - \omega_2)^2\Big\} \tag{12b}$$

$$(\mathrm{i}\hbar\partial/\partial t_0 - \omega_2)\Psi_2^{(3)} + L_2\Psi_1^{(3)} = \beta_2^{(3)} \tag{12c}$$

and demand the coefficient of $\exp[\mathrm{i}(kx_0 - \omega t_0)]$ be zero in order to apply perturbation theory. The force function $A^{(1)}$ will be evolved according to the equation

$$\mathrm{i}(\partial/\partial t_2)A^{(1)} + \tfrac{1}{2}\omega''(k)(\partial^2/\partial\xi^2)A^{(1)} + \lambda|A^{(1)}|^2A^{(1)} = 0. \tag{13}$$

Equation (13) is the non-linear Schrödinger equation which belongs to the completely integrable system and can be solved exactly by the inverse-scattering transformation [20, 21].

The single-soliton solution is

$$A^{(1)} = (1/\mu)\left(\omega''(k)c_0^2/\lambda\right)^{1/2} \sec \left[\!\left[c_0\{x - [c_g + c\omega''(k)]\}t - x_0 \right]\!\right] \times \exp\left\{ i[(k+c)x - \Omega t] - \phi_0 \right\} \tag{14a}$$

$$\Omega = \omega + c_g c + \tfrac{1}{2}(c^2 - c_0^2)\omega''(k) \tag{14b}$$

where $\xi = \mu(x - c_g t)$ and c, c_0, x_0, ϕ_0 are integration constants. Equations (14) are a wave packet travelling to the right with velocity $c_g + 2\tau k$.

If c is set to be zero, equation (14b) becomes

$$\Omega = \omega - \tfrac{1}{2}c_0^2\omega''(k) \tag{15a}$$

at $k = 0$ or $\pi/2d_0(c_g = 0)$. For the acoustic branch and the optical branch, we see that

$$\begin{aligned}
\Omega_{\max}(k=0) &= \omega_{\max} - \tfrac{1}{2}c_0^2\omega''_{\max} > \omega_{\max} \\
\Omega_{-\max}(k=\pi/2d) &= \omega_{-\max} - \tfrac{1}{2}c_0^2\omega''_{-\max} > \omega_{-\max} \\
\Omega_{\min}(k=\pi/2d) &= \omega_{\min} - \tfrac{1}{2}c_0^2\omega''_{\min} < \omega_{\min} \\
\Omega_{-\min}(k=0) &= \omega_{-\min} - \tfrac{1}{2}c_0^2\omega''_{-\min} < \omega_{-\min}
\end{aligned} \tag{15b}$$

so the soliton frequencies have four values, which enter into the frequency gap of the linear dispersion curve of the system and denote the non-linear localized modes of the chain. This shows the possibility of observing a gap soliton in an OPP-AFM. Bose found that a gap of magnitude $2h$ opens up in the excitation spectrum at $k = \pi/2$ for the one-dimensional chain, and so on for the three-dimensional chain [12, 13]. Our approach provides the same conclusion.

Using the inverse-scattering transformation, we can obtain the two-soliton bound-state solution

$$\begin{aligned}
A^{(1)} = (1/\mu)(\omega''(k)/\lambda)^{1/2}\Big\{&(c_2^2 - c_1^2)/(c_1^2 + c_2^2) - 2c_1c_2[\tanh c_1(x - c_g t + x_0) \\
&\times \tanh c_1(x - c_g t - x_0) - \sec c_1(x - c_g t + x_0) \\
&\times \sec c_2(x - c_g t - x_0) \cos \tfrac{1}{2}(c_1^2 - c_2^2)\omega''(k)]\Big\} \\
&\times \left[\!\left[c_1 \sec c_1(x - c_g t + x_0) \exp\{-i[\omega - k_1^2\omega''(k)]t\} \right.\right. \\
&\left.\left. - c_2 \sec c_2(x - c_g t - x_0) \exp\{-i[\omega - k_2^2\omega''(k)t]\} \right]\!\right]
\end{aligned} \tag{16}$$

where c_1, c_2 are integration constants. Equation (16) represents two bound solitons which move to the right with velocity c_g. If $c_g = 0$, equation (16) becomes the localized two-soliton bound state in which one soliton vibrates around the equilibrium position $x = -x_0$ with frequency $\omega - c_1^2\omega''(k)/2$ and the other around $x = x_0$ with frequency $\omega - c_2^2\omega''(k)/2$. They may be called two-magnon bound states of an OPP-AFM. If $k = 0$ or $\lambda_0/2d_0$, equation (16) represents the two-gap-soliton bound state of an OPP-AFM.

Introducing the Dyson–Maleev transformation and the coherent state *ansatz*, we have investigated the single-soliton solution and the two-soliton bound-state solution in an OPP-AFM by using the method of multiple scales combined with the long-wavelength approximation. Huang *et al* have published the two-parameter theory of solitons in magnetic systems [4–7]. Kapor *et al* [22] demonstrated the inconsistency of the two-parameter theory. For studying the soliton in ferromagnets and antiferromagnets, the approach which has been developed in this letter is self-consistent and systematic.

For the OPP-AFM and other AFMs, we obtain the equations of motion by employing the Dyson–Maleev transformation and the coherent state *ansatz*. Although there are more than one equations of motion with non-linear coupling, it is very difficult to solve them; the method of multiple scales used here can reduce these equations to a single equation, for example, the non-linear Schrödinger equation in this paper. This equation plays an important role in many non-linear phenomena and its properties have been widely studied. The single-soliton solution and two-soliton bound-state solution are obtained by the inverse-scattering transformation. These results show that soliton-like magnon localization and two-magnon bound states in an OPP-AFM are possible. The possibility of observing a gap soliton in this system is also discussed.

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