Solitons in quantum Heisenberg chain

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Received 18 April 1980

Abstract. Using the coherent states method combined with the Schwinger coupled boson representation of the spin operators, it is shown that solitons can propagate in the continuum limit of the quantum ferromagnetic Heisenberg chain. These solitons are solutions of a nonlinear Schrödinger equation similar to that discussed by Lakshmanan for the classical Heisenberg chain. Several characteristics of the soliton, like its momentum, energy, and the number of bosonic excitations involved in the soliton formation, are calculated.

1. Introduction

The classical ferromagnetic Heisenberg chain has been recently studied vigorously from several different points of interest. Numerical (Heller and Blume 1977) and analytical (Reiter and Sjölander 1977, 1980) calculations have revealed a large number of interesting low-temperature properties of that system and its continuum limit has become a convenient probing ground for various modern field-theoretical concepts like solitons, complete integrability, etc.

The nature of the soliton solutions of the equations of motion for the continuous Heisenberg chain (CHC) has been discussed thoroughly by Lakshmanan (1977), Lakshmanan et al (1976), and Takhtajan (1977). Fogedby (1980), has argued that there exists a relation between the soliton solutions of the CHC and the bound magnon states. Zafar Iqbal et al (1979) discussed the possibility of the soliton solutions in the quantum theory of the Heisenberg chain with dipole–dipole interactions taken into account. These interactions lead, in the Holstein–Primakoff representation, to a three-magnon coupling potential which is a constant in the long-wavelength limit.

In this paper we show that even without the dipole–dipole interactions solitons do exist in the quantum Heisenberg chain in its long-wavelength limit. Unlike the Fogedby analysis we begin with a purely quantum picture of the system and then investigate the semi-classical limit of the quantum CHC by means of the coherent-states technique. Our approach is based on the Schwinger coupled-boson representation of the spin operators rather than the conventional Holstein–Primakoff or Dyson–Maleev representations.

§ Research supported in part by Polish Ministry of Science, Higher Education and Technology Grant M.R.I.7.
|| Also in part by US National Bureau of Standards Grant made available via the Maria Skłodowska-Curie Foundation.

0022-3719/80/315741 + 07 $01.50 © 1980 The Institute of Physics 5741
This algebraic method was discussed previously by Liu and Chow (1971) and ourselves (Cieplak and Turski 1976).

This paper is organised as follows. In §2 we introduce an effective Hamiltonian for the quantum Heisenberg chain and derive an equation for a boson field that carries all the information about the \( T = 0 \) dynamics of the system in the long-wavelength limit. In §3 we discuss relations between the semi-classical limit of that equation with the one derived by Lakshmanan (1977) for the classical CHC. In the final section we investigate certain properties of the solitons. These solitons are solutions of the coherent-states representation of the boson field equation of motion. We calculate the energy–momentum relation for the soliton which leads us to the conclusion that solitons do indeed behave as massive particles.

2. The effective quantum Hamiltonian

Consider the Heisenberg Hamiltonian for the ferromagnetic chain with the nearest-neighbour interactions:

\[
H = -(J/\hbar^2) \sum_i S_i \cdot S_{i+1} - (B/\hbar) \sum_i S_i^z,
\]

where \( S_i \) are the spin operators (spin length \( S \)), \( J \) is the exchange constant, \( B \) denotes an external magnetic field measured in units of the Bohr magneton, and \( \hbar \) is the Planck constant. The spin operators can be rigorously expressed in terms of the Schwinger coupled bosons (Schwinger 1965, Mattis 1965) \( a_i \) and \( b_i \) as follows

\[
\begin{align*}
S_i^+ &= \hbar a_i^\dagger b_i \\
S_i^- &= \hbar b_i^\dagger a_i \\
S_i^z &= (\hbar/2)(a_i^\dagger a_i - b_i^\dagger b_i).
\end{align*}
\]

It has been shown by Liu and Chow (1971) and Cieplak and Turski (1976) that the Hamiltonian (2.1) takes the form

\[
H = E_0 + [B + SJ(0)] \sum_q b_q^\dagger b_q - \frac{1}{2N} \sum_{q_1 q_2 q_3} J(q_3 - q_1)(b_{q_1}^\dagger b_{q_2} b_{q_3}^\dagger b_{q_1 + q_2 - q_3}) + a_{q_1}^\dagger b_{q_2}^\dagger b_{q_1} a_{q_1 + q_2 - q_3}
\]

(2.3)

where

\[
\begin{align*}
J(q) &= 2J \cos(ql) \\
a_q &= N^{-1/2} \sum_j \exp(-iqR_j)a_j \\
E_0 &= -NS(B + JS).
\end{align*}
\]

Here \( N \) is the number of lattice sites (labelled by \( R_j \)) and \( l \) is the site spacing. In equation (2.3) use was made of the kinematic condition

\[
a_i^\dagger a_i + b_i^\dagger b_i = 2S
\]

by means of which the 'all-a' terms were eliminated.

In the ground state the spins are aligned (particularly when \( B \neq 0 \)) and no \( b \)-bosons
are present. We can account for the macroscopic occupation of the ground state by the $a$-bosons by means of the Bogoliubov-like transformation

$$ a_q = A_q + (2SN)^{1/2} \delta_{q,0}. \tag{2.8} $$

This leads us to the unitary equivalent form of the Hamiltonian

$$ H = H_0 + H_I + \delta H \tag{2.9} $$

where

$$ H_0 = E_0 + \sum_q e(q)b_q^\dagger b_q - \frac{1}{2N} J(0) \sum_{q_1 q_2 q_3} b_{q_1 - q_2} b_{q_2 - q_3} b_{q_3} b_{q_1} \tag{2.10} $$

$$ H_I = \frac{1}{2N} \sum_{q_1 q_2 q_3} [J(0) - J(q)] b_{q_1 - q_2} b_{q_2 - q_3} b_{q_3} b_{q_1} \tag{2.11} $$

and

$$ \delta H = - \left( \frac{S}{2N} \right)^{1/2} \sum_{q_1 q_2} J(q_1) b_{q_1} b_{q_2} A_{q_2 - q_1} + A_{q_1 - q_2}^\dagger b_{q_2}^\dagger b_{q_1} $$

$$ - \frac{1}{2N} \sum_{q_1 q_2 q_3} J(q_1) A_{q_1 - q_2}^\dagger b_{q_2}^\dagger b_{q_3} A_{q_3 - q_2}. \tag{2.12} $$

In equation (2.10) the spin-wave energy $\epsilon(q)$ is equal to

$$ \epsilon(q) = B + S[J(0) - J(q)]_{q_1 < 1} = B + JS(ql)^2. \tag{2.13} $$

The $\delta H$ part of the Hamiltonian contains the small fluctuations $A_q$ of the boson condensate and therefore can be neglected. These fluctuations carry no energy and merely redistribute the spin quantum numbers. More detailed arguments in favour of dropping the $\delta H$ term were given by Liu and Chow (1971). Our effective Hamiltonian consists then of $H_0$ and $H_I$.

The $b_q$-bosons featuring in the effective Hamiltonian are not the standard magnons used in the theory of magnetism even though their energies, in the harmonic approximation, are equal to those of the magnons. The whole effective Hamiltonian is needed in order to account for the known thermodynamic properties of the Heisenberg system. Indeed, in the three-dimensional case the $H_0$ part of the Hamiltonian leads to the existence of the $b$-boson bound states at small wavevectors (Liu and Chow 1971). One has to include these bound states in the evaluation of the partition function in order to obtain, say, the $T^{3/2}$ dependence of the magnetisation. The Hamiltonian $H_I$ has now to be treated as a perturbation and the $T^2$ correction to the magnetisation follows. At low temperatures ($T = 0$) the effect of $H_I$ can be disregarded and the effective Hamiltonian reduces to $H_0$, given explicit.

It is convenient now to introduce field operators

$$ \Psi(x, t) = N^{-1/2} \sum_q b_q(t) \exp(iqx) = \frac{1}{2\pi\sqrt{N}} \int dq b_q(t) \exp(iqx). \tag{2.14} $$

On calculating the commutator of $\Psi(x, t)$ with $H_0$ we obtain, in the continuum limit $ql \ll 1$, a non-linear Schrödinger equation for the operators $\Psi(x, t)$:

$$ i\hbar \partial_t \Psi(x, t) = (B - SJP\partial_x^2)\Psi(x, t) - J(0)\Psi^\dagger(x, t)\Psi(x, t) \Psi(x, t). \tag{2.15} $$

The three-dimensional version of equation (2.15) was derived for the first time by Liu and Chow (1971).
3. Semi-classical limit

The magnetic field term $B\Psi(x, t)$ in equation (2.15) can be eliminated easily by means of the transformation

$$\Psi(x, t) = \exp(-itB/h)\Phi(x, t), \quad (3.1)$$

or in the momentum space

$$b_{q}(t) = \exp(-itB/h)b_{q}(t). \quad (3.2)$$

The $b_{q}$ operators also satisfy the bosonic commutation relations. The equation for the $\Phi$ field is like equation (2.15) except for the lack of the $B$ term.

Clearly this operator equation is difficult to analyse. We can follow the standard procedure used in quantum optics (Klauder and Sudarshan 1968) or in the theory of superfluidity (Langer 1968, Turski 1972) and look for the semi-classical limit of equation (2.15) using the coherent states for the field $\Phi$. These states, denoted in what follows as $|\tilde{a}\rangle$, are defined by

$$\Phi(x, t)|\tilde{a}\rangle = \tilde{a}(x, t)|\tilde{a}\rangle, \quad (3.3)$$

and they are 'as classical as possible' from all of the quantum states.

On taking the matrix element of equation (2.15) between the coherent states $|\tilde{a}\rangle$ and changing conveniently the units of the field $\tilde{a}(x, t)$ according to

$$\tilde{a}(x, t) = (4t^{2}S)^{1/2}\tilde{a}(x, t), \quad (3.4)$$

we arrive at the $c$-number non-linear Schrödinger equation for the $\alpha(x, t)$ field:

$$i\partial_{t}\alpha(x, t) = -\partial_{x}^{2}\alpha(x, t) - \frac{1}{2}\alpha(x, t)\alpha^{2}(x, t), \quad (3.5)$$

where the time units are also scaled according to

$$\tau = JS^{1/2}/\hbar. \quad (3.6)$$

Equation (3.5) is identical in the form to the Lakshmanan equation for the classical CHC (Lakshmanan 1977). The classical 'wavefunction' in the Lakshmanan theory is of the same dimension as our quantum field $\alpha$. The time scaling equation (3.6) is also identical to the classical one, for the classical limit is defined as $\hbar \to 0$, $S \to \infty$, $KS \to S_{\text{classical}}$ and $J_{\text{classical}} = J/\hbar^{2}$.

Unlike the classical theory, though, our equation (2.15) is only an approximate one, and this should be kept in mind in the interpretation of the results. Let us mention that if Holstein–Primakoff bosons were used instead of Schwinger ones, the non-linear term would involve the second space derivative. In our approach such a term also appears as a higher-order correction stemming from $H_{t}$.

4. The solitons

Equation (3.5) is an example of a completely integrable equation. Using the inverse scattering method one can analyse all of the fast-decaying, at spatial infinity, solutions of equation (3.5). Besides these solutions—solitons—there are some other ones, e.g. finite-amplitude spin waves. Since these waves are unstable and give rise to the Fermi–Pastur–Ulam recurrence (Turski 1979) it follows that some remnants of this phenomenon should also be present in the quantum CHC.
We shall not repeat here all of the soliton solutions of equation (3.5). We restrict ourselves to the analysis of a particular soliton solution given explicitly as

$$x_{\text{soliton}}(x, \tau) = -C \exp(\text{i}Cx/2 \sech[-(C/2)[x - x_0 - C\tau]].$$  \hspace{1cm} (4.1)

Here $C$ is a constant which in our units has the dimension of inverse length and $x_0$ is the initial location of the soliton.

Having the soliton equation (4.1), we can easily calculate the mean number of $B_q$ quanta in the coherent state which correspond to the soliton. A straightforward calculation leads to the expression for $\langle n_q \rangle$:

$$\langle n_q \rangle = \langle \tilde{\alpha}_{\text{soliton}} | B_q^* B_q | \tilde{\alpha}_{\text{soliton}} \rangle = (S!/4)! \tilde{\alpha}_{\text{soliton}}(q, \tau)^2,$$  \hspace{1cm} (4.2)

where

$$\tilde{\alpha}(q, \tau) = \frac{1}{\sqrt{N}} \int dx \exp(-\text{i}qx) \alpha(x, \tau).$$  \hspace{1cm} (4.3)

Setting $x_0 = 0$, for simplicity, we obtain:

$$\langle n_q \rangle = (1/N)! \pi^2 S \sech(q/C - \pi/2)$$  \hspace{1cm} (4.4)

which asserts that the mean number of $B_q$ quanta participating in the soliton is constant in time.

The total number of quanta in the soliton $N^*$, is equal to

$$N^* = \frac{N!}{2\pi} \int dq \langle n_q \rangle = C S.$$  \hspace{1cm} (4.5)

This constant of motion can be also related to the, conserved, angular momentum of the chain $L_z$. Using equations (2.2c), (2.7) and (4.5) we obtain $\langle L_z \rangle = \hbar N^*$, where as in the classical case we have extracted from $L_z$ an (infinite) constant related to the perfect chain ordering.

Analogously as in equation (4.5) we can calculate the momentum carried by excitations forming the soliton.

$$P = \frac{\hbar N!}{2\pi} \int dq \langle n_q \rangle = \hbar C^2 S l/2 = \hbar C N^*/2.$$  \hspace{1cm} (4.6)

Finally, we can calculate the soliton energy by evaluating the mean value of the long-wave-length limit of the Hamiltonian $H_0$ in the state (cf. equation (4.1)). We obtain

$$E = \frac{N!}{2\pi} \int dq \langle n_q \rangle [B + JS(q)l^2] - \frac{J}{l} \int dx \langle \tilde{\alpha}_{\text{soliton}} | \Phi^\dagger(x) \Phi(x) | \tilde{\alpha}_{\text{soliton}} \rangle.$$  \hspace{1cm} (4.7)

In the above we have reinstated the magnetic field $B$; this is legitimate since the numbers of $B_q^*$ and $\phi_q$ quanta are the same. After performing the integration in equation (4.7) we obtain:

$$E = BN^* + \frac{1}{2}JS^2 C^3 l^3 - 2^{-4} JS^2 l^3 \int dx |\alpha_{\text{soliton}}(x)|^4.$$  \hspace{1cm} (4.8)

The last term in equation (4.8) is the energy required to form and keep the soliton together and it amounts to $-JS^2 (Cl)^3 / 6$. The energy $E$ can then be written as

$$E = BN^* + P^2 / 2m^*.$$  \hspace{1cm} (4.9)
This shows clearly that the soliton has particle-like features and that the soliton mass \( m^* \) is equal to
\[
m^* = (3\hbar^2/4J)C = \mu C.
\]

Notice that the soliton mass \( m^* \) depends linearly on its ‘velocity’ \( C \) and the coefficient \( \mu \) is a constant characterising the magnetic structure of the chain.

The above results lead to the conclusion that the solitons can indeed be found in the quantum CHC and that their presence does not require inclusion of the dipole-dipole interactions as in the work of Zafar Iqbal et al (1979). We shall also now compare our results with those obtained by Fogedby (1980). Unlike in Fogedby’s analysis we rely on the quasi-classical limit of a purely quantum system; thus we avoid the well known difficulty with quantisation of a non-linear classical field theory. Working with Schwinger bosons and using the coherent-states technique we obtain a direct counterpart of the classical Lakshmanan equations. This justifies, \textit{a posteriori}, our use of the Liu and Chow arguments in favour of dropping the \( \delta H \) term of the Hamiltonian. The Lakshmanan equations for curvature-torsion variables (Lakshmanan 1977, Turski 1979) can be derived from a Hamiltonian which is identical to that obtained, in the quasi-classical limit, for the fields \( \sigma \) after calculating the matrix elements of the Hamiltonian \( H\sigma \) in the \( |\sigma \rangle \) state. Thus the Lakshmanan equations correspond to the Hartree–like approximation in the quantum case (cf equation (2.15)). It is interesting to note that when a ‘naive’ quantisation of the Lakshmanan equations is performed we obtain quantum theory identical to that described in the present work. What is intriguing in that procedure is that the classical Hamiltonian for the Lakshmanan equation differs from the continuous limit of the conventional classical spin Hamiltonian \( H_{\text{classical}} = -J \sum_{\alpha} S_{\alpha} S_{\alpha+1} \). This difference accounts for the fact that our energy–momentum relation (4.9) differs from Fogedby’s result but in the numerical factor only. Indeed, using the rules \( \hbar J/\hbar^2 = J_{\text{classical}} \), \( \hbar S = S_{\text{classical}} \) we obtain
\[
E = BN^* + \frac{2}{3}(J_{\text{opt}}S_{\text{eff}}/|L|)(\hbar \ell)^2.
\]

Equation (4.11) can now be ‘quantised’ by means of the de Broglie rule, \( P = \hbar \hat{Q} \), and that would give us the spectrum obtained by Fogedby (1980). We do not see the reason why we should do so. Our interpretation of the soliton energy–momentum relation given by equation (4.9) seems to be more physical. The soliton in our case is a particular coherent wave packet consisting of exactly \( N^* \) bose excitations, moving as a whole without changing its shape and therefore behaving as a free, massive, classical particle with mass \( m^* \).

We think that the quantisation of the classical Heisenberg chain via the use of the Lakshmanan variables requires more thorough investigation and we shall return to this problem in a separate publication.

Where our analysis differs from that of Zafar Iqbal et al (1979) and also from Fogedby (1980) is in our use of the Schwinger bosons rather than the Holstein–Primakoff magnons. There is no simple relation between these quanta and our analysis seems to indicate that the Schwinger bosons are more relevant to the investigation of the non-linear effects in the Heisenberg chain. Reiter et al (1979) have shown that most of the results obtained in the asymptotically exact theory of the classical Heisenberg chain can be derived from a properly tailored Holstein–Primakoff procedure. On the other hand there are no indications that solitons play an important role in either thermodynamics or finite (but low) temperature dynamics of the CHC. The understanding of the relations between the Schwinger bosons and the conventional magnons seems therefore to be crucial
before the full physical role of the quantum solitons, discussed in this paper, can be fully explored.

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