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QUANTUM SOLITONS AND THE HALDANE PHASE IN ANTIFERROMAGNETIC SPIN CHAINS[1]

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We discuss the relevance of solitons for the present understanding of antiferromagnetic spin chains. For anisotropic $S = 1$ chains, the energies connected with soliton propagation and binding are shown to determine the quantum phase transitions of these models, in particular the Néel-Haldane transition. Restriction to the soliton subspace allows a formulation of the Haldane ground state, which in its simplest form is of molecular field type and which can be improved upon by including correlations.

1. Introduction

The investigation of elementary excitations in magnetic chain systems has been a topic of intense experimental and theoretical research for many years. In addition to wavelike excitations (or magnons), localized excitations have been postulated theoretically and verified experimentally in great detail in the last twenty years. These localized excitations have become to be characterized as solitons; actually, from a physical point of view, magnetic solitons are more commomly (and often more appropriately) known under the name of domain walls. Most of this theoretical work was based on a classical treatment of spin dynamics, aiming in particular at an understanding of experiments in TMMC ($S = \frac{5}{2}$) and in $CsNiF_3$ [1]. In recent years, however, interest in the genuine quantum analog of classical magnetic solitons has grown in parallel with general progress in the theoretical understanding of one-dimensional quantum spin systems. The purpose of this contribution is to describe the role of quantum solitons in spin chains with $S = \frac{1}{2}$ and $S = 1$ defined by the hamiltonian

$$H = \sum_n [(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + \epsilon S_n^z S_{n+1}^z] + d \sum_n (S_n^z)^2 \qquad (1)$$

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After shortly reviewing the present understanding of the role of solitons for the $S = \frac{1}{2}$ Heisenberg antiferromagnetic chain (xxz chain, for $S = \frac{1}{2}$ the parameter d is irrelevant) we will mainly focus on $S = 1$ Heisenberg antiferromagnetic chains. These have received widespread interest since Haldane's conjecture [2] that they behave essentially different from $S = \frac{1}{2}$ chains: Antiferromagnetic $S = 1$ Heisenberg chains are conjectured to be characterized by an energy gap and exponentially decaying correlations (instead of a linear spectrum and algebraicly decaying correlations for $S = \frac{1}{2}$). This conjecture has so far not been rigorously proven but very convincing evidence exists from theoretical, numerical and experimental investigations (for a review see [3]) that a Haldane phase with the conjectured properties exists.

In this contribution we will describe results showing that also for the Haldane phenomenon quantum solitons are the essential degrees of freedom to be considered, in agreement with the original approach of Haldane [2]. We only give the essence of the physical arguments and some results of the calculations and refer to ref. [4] for more details.

2. S = $\frac{1}{2}$ chains

We start by giving a short survey of the present understanding of elementary excitations in the $S = \frac{1}{2}$ xyz-chain. In principle, all information of interest for this problem is available from the exact solution via the Bethe ansatz. In early interpretations of the information extracted from the Bethe ansatz equations low-lying excited states were described in close analogy with classical spin-wave excitations, all the more since the dispersion law for the $S = \frac{1}{2}$ isotropic Heisenberg antiferromagnet

$$\omega(q) = \tfrac{1}{2}\pi|\sin q| \qquad (2)$$

differs from the classical dispersion law only by a factor of $\frac{1}{2}\pi$. It was not before 1981 that Faddeev and Takhtajan [5] pointed out that experimentally accessible excitations actually are composed from two basic particles, each with the dispersion law of eq. (2.1). A given wave vector q can be realized by various combinations of wave vectors of the two particles and a two particle excitation continuum results. The basic particles are properly interpreted as quantum solitons. The existence of this two-particle continuum has recently been experimentally verified by inelastic neutron scattering experiments on the material $KCuF_3$ [6].

From a physical point of view, this picture can be understood, when we start from the Ising limit of the xxz-model, i.e. $\epsilon \to \infty$ in eq. (1.1).

Then we have as ground states the two degenerate Néel states and the conventional way to introduce excited states is to apply $S_n^+(S_n^-)$ raising (lowering) one spin to create a local excitation with energy ϵ. There is, however, the possibility of an excitation with energy $\frac{1}{2}\epsilon$, by turning around all spins after a given site n. The first mechanism breaks two bonds and develops into a spin wave when one goes away from the Ising limit whereas the second mechanism breaks one bond and is nothing but a domain wall. It is obvious that a spin wave excitation can be considered as composed of two domain wall excitations and this is what Faddeev and Takhtajan [5] have shown to be true not

only in the Ising limit but generally, including the isotropic limit. For small transverse interactions this can be verified by simple perturbation theory and easily shown to be in agreement with the exact Bethe ansatz results. Thus the formally complete results from the Bethe ansatz and the physical picture provided by the perturbation approach have combined to give the final interpretation of the dynamics of the $S = \frac{1}{2}$ chain in terms of solitons.

The simplest realization of this picture is actually in the anisotropic xy model, where the Bethe ansatz solution reduces to a solution in terms of free fermions [7]. Here the elementary excitations can be explicitly described by soliton creation and annihilation operators which are fermions [8].

3. S = 1 chains

We start our description of the Haldane condensation in antiferromagnetic S=1 chains by describing its essential features in physical terms, starting from the Ising limit. This discussion shows in principle, why solitons are relevant for this phenomenon; it also reveals differences and similarities to the case of $S = \frac{1}{2}$ chains. The ground state in the Ising limit is the doubly degenerate Néel ground state; the lowest excited states lose the binding energy of two bonds and come in three types, which all have energy 2ϵ above the ground state:

(i) when a a spin raising or lowering operator $S^{\pm}$ at site n is applied to the ground state, we obtain spin deviation states which after linear combination of all sites become spin wave states.

(ii) when we turn around all spins to the right of some site n, either directly or with one site with $S_n^z = 0$ in between, we obtain soliton states. Obviously, two adjacent solitons are identical to two adjacent spin deviations, both are created from the ground state applying the operator $S_n^+ S_{n+1}^-$. The energy of such a configuration with two adjacent zeros is 3ϵ and therefore lower than the total energy of two separated solitons ($\Delta E = 4\epsilon$) and we conclude that there exists a binding energy for soliton excitations.

When we move away from the Ising limit, the essential point to be discussed is the influence of the transverse interaction

$$H_{transv} = \tfrac{1}{2}\sum_n (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+)$$

H_{transv} connects states obtained by raising resp. lowering spin projections at adjacent sites with respect to an initial state. It is easily seen that H_{transv} directly connects soliton states of the first type (one intermediate site with $S_n^z = 0$) at adjacent sites, whereas spin deviation states at adjacent sites and solitons of the second type are separated by an energy barrier. This means that the transverse interaction will be more effective in lowering the energy by delocalization for soliton states than for spin deviation, resp. spin wave states. Thus we conclude that these soliton states will be the

most important ones for an understanding of the behaviour of the antiferromagnetic chain upon its approach to the isotropic limit.

The importance of the soliton states of the first type has first been realized in the work of Gomez-Santos [9], who called this soliton-type nonlocal excitation above the Néel state a spin zero defect (SZD). The basic characteristic of such a state, in contrast to the other low energy excitations is comprehensively described by the statement that antiferromagnetic order appears to continue across the site(s) with $S_n^z = 0$. Stated otherwise, if we cross out all zeros, states with only soliton excitations will have perfect Néel order on the remaining sites. This type of order has become to be called hidden order or string order.

In the real spin chain an odd number of solitons destroys long range antiferromagnetic order. Thus the following picture of the ground state of the antiferromagnetic chain develops when the strength of the transverse interaction ϵ is gradually decreased from ∞: Quantum fluctuations mix preferably SZD's or soliton excitations into the ground state. For large values of ϵ these will be bound due to the binding energy discussed above and long range antiferromagnetic order will persist. For sufficiently small values of ϵ the energy gain from the mobility of a single soliton (lowering in energy due to delocalization over the whole chain) due to the transverse interaction will be large enough to overcome the binding energy - then soliton pairs dissociate and the system undergoes a phase transition to a phase characterized by a ground state without long range antiferromagnetic order, the Haldane phase. For $S = 1$ this dissociation of solitons occurs in the anisotropic region, for a value of $\epsilon = \epsilon_c > 1$.

A quantitative treatment of the quantum phase diagram in the $S = 1$ antiferromagentic chain makes extensive use of the concept of hidden order. Hidden order has been first introduced by den Nijs and Rommelse [10] in the context of surface roughening transitions. A quantitative measure of this hidden order is introduced by defining the operator of the so called string order parameter [11]:

$$T_n^\alpha = \exp(i\pi \sum_{p=1}^{n-1} S_p^\alpha)\, S_n^\alpha \tag{3}$$

The antiferromagnetic order in the Néel phase and the hidden order in the Haldane phase, which we have discussed above, are related to the z-component of this operator. The most important quantity to characterize the Haldane phase, however, is the transverse component T^x and the corresponding string correlation functions.

Hidden order also becomes apparent in the model of Affleck et al (AKLT) [12] for an antiferromagnetic $S = 1$ chain. This chain has an exactly solvable ground state, which possesses all characteristics of the ground state of a Haldane phase. The Hamiltonian of this model is

$$H = \sum_n \vec{S}_n \vec{S}_{n+1} - \beta(\vec{S}_n \vec{S}_{n+1})^2 \tag{4}$$

with $\beta = -\frac{1}{3}$, i.e. it has biquadratic exchange in addition to the standard Heisenberg model. The exact ground state for this Hamiltonian has been given explicitly by AKLT as valence bond state. This ground state has only components with perfect hidden order and has been shown to have a finite correlation length, $\xi = 1/\ln 3$ and a gap in the excitation spectrum. To make the hidden order more transparent a nonlocal unitary transformation has been introduced by Kennedy and Tasaki [13], which transforms a state with perfect hidden order into a ferromagnetic state.

When this unitary tranformation is applied to the AKLT ground state, a factorized state results. In an alternative formulation this state is formulated as a matrix product [14], which avoids to introduce the unitary tranformation. A factorized state is the basic characteristic of a molecular field approximation and we interpret the result for the AKLT model saying that in this limit a molecular field formulation of the Haldane ground state exists. The existence of this representation is obscured by the fact that it does not become apparent before the nonlocal unitary is applied, on the other hand it can be used as starting point to formulate a molecular field approach to the Néel and Haldane phases also for realistic hamiltonians such as given in eq. (1.1). This has first been done by Kennedy and Tasaki [13] and discussed in some more detail by the author [4]. Here we only give a short list of the results:

(i) The phase diagram of the antiferromagnetic $S = 1$ chain with single site and exchange anisotropy is obtained in a qualitatively satisfying way, exhibiting the Néel-, Haldane- and large-D phases. Quantitative agreement with numerical results is not expected and is actually rather poor.

(ii) Spin correlations can be calculated and are found to exhibit Néel order in the Néel phase and exponential decay in the Haldane phase. For $d = \epsilon$ the longitudinal correlation length vanishes, which indicates a switching of the correlation function from antiferromagentic to ferromagnetic behaviour.

(iii) The behaviour of the string correlation functions allows to characterize uniquely the different phases. In particular the Haldane phase is characterized by the fact that only in this phase the transverse string correlation function is nonvanishing. Appropriate expectation values of the string operators allow to define order parameters in the usual sense. In the Haldane phase both the longitudinal and the transverse component can take two equivalent values; this broken symmetry corresponds to four equivalent ground states in this phase. Close to the phase boundaries the string operator averages are characterized by a square root behaviour as is characteristic for a molecular field type approach.

(iv) Wavefunctions of excited states can be easily written down as domain walls mediating between the different equivalent groundstates. Linear combination of these domain wall states as required by translational invariance leads to states which in the limit of the AKLT model can be identified with the states discussed by Knabe [15] and Arovas et al [16]. In this molecular field type approach these excited states can be discussed in the whole phase diagram: Entering the Haldane phase from the Néel phase the lowest excited state is at $k = \pi$; when the strength of the single ion anisotropy is increased, the minimum of the excitation energy shifts to $k = 0$ [17]. This behaviour, predicted by this approach, has not been investigated in real or computer experiments so far.

(v) A convincing justification of the conjecture that the low-lying excited states are of the domain wall character just described can be obtained using numerical methods: For the isotropic antiferromagnetic $S = 1$ chain with up to 18 spins we have calculated energies and wavefunctions of low-lying excited states [18]. ¿From the wavefunctions we find as numerical result that the string correlation function for the lowest excited state changes sign when the distance along the chain is varied. This is in complete agreement with the analytical result [17]

$$\langle T^{z,z}(n)\rangle = a^4(1-\frac{2n}{N}) \qquad \text{for} \quad S^z_{tot} = \pm 1 \tag{5}$$

$$\langle T^{x,x}(n)\rangle = 2\,a^2\,b^2(1-\frac{2n}{N}) \qquad \text{for} \quad S^z_{tot} = 0 \tag{6}$$

following from assuming the domain wall character for this state as described above and thus verifies this assumption. Analogous results are obtained for higher excited states.

We would like to emphasize once more that these domain walls should be considered as 'second order' solitons: They are constructed to describe a localized transition between two equivalent ground states which themselves have soliton character in the original spin space.

The basic characteristic of the approach described so far is that spins at different sites are assumed uncorrelated after the unitary transformation has been applied. There are two approaches which go beyond this factorization but keep the physically motivated restriction to take into account spin zero defect states only:

(i) The general state with longitudinal string order, i.e. the state which has only components in the subspace of spin zero defect states, can be mapped to a $S = \frac{1}{2}$ chain [19]. The resulting hamiltonian is that of an xyz chain in an external magnetic field. Its eigenstates can be discussed exactly for some combinations of the $S = 1$ parameters. The resulting picture is in qualitative agreement with that obtained from the molecular field type approach and improves on it qualitatively. Details can be found in ref. [19].

(ii) In generalization of the uncorrelated wave function of the simplest approach we can include correlations over a finite number of sites in a cluster approximation and perform a variational calculation as has been done by Mikeska and Verrucchi [20]. Including correlations of three neighbouring sites, this leads to a phase diagram which is surprisingly close to the one obtained by numerical methods. In addition, this approach allows to follow the dissociation of bound solitons as the fundamental instability mechanism for the formation of the Haldane phase.

4. Conclusions

We have discussed the relevamce of solitons for the present understanding of antiferromagnetic spin chains. For the $S = \frac{1}{2}$ xxz-chain the basic elementary excitations are solitons (spinons), two solitons combine to form a magnon. In $S = 1$ chains the soliton (domain wall with respect to antiferromagnetic order) is the relevant excitation

owing to its high mobility as compared to the spin deviations. In the Néel phase solitons are bound and the phase transition to the Haldane phase is determined by the dissociation of these soliton pairs. A qualitatively correct and technically simple treatment is obtained restricting oneself to the subspace which has only excited states of the soliton type. These states have in common the appearance of (hidden) string order, the nonvanishing of transverse string order is the unique characteristic of the Haldane phase. After applying the nonlocal unitary tranformation of Kennedy and Tasaki [13] the simplest approximation to the Haldane ground state is a factorizing state. We have discussed how to obtain improved results by using an effective $S = \frac{1}{2}$ model and by taking into account correlations in a cluster expansion. The elemantary excitations in the Haldane phase are described as domain walls in the string order.

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