

Excitations for the one-dimensional $S = 1$ pseudo-Heisenberg antiferromagnetic chain

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ABSTRACT

We are interested in the anisotropic $S=1$ antiferromagnetic chain. System of particles with an arbitrary spin is described directly from the first principles, based on the symmetry law. The ground state of the one-dimensional $S=1$ pseudo-Heisenberg antiferromagnet with single-ion anisotropy is calculated. Excitations of the chain in the form of nonlinear spin waves and, in particular, the possibility of a soliton solution is considered.

Keywords: Pseudo-Heisenberg Hamiltonian; Antiferromagnetic Spin-1 Chain; Soliton Excitations

1. INTRODUCTION

We investigate an anisotropic $S=1$ antiferromagnetic chain. Interest in one-dimensional $S=1$ antiferromagnets is traced back to the works concerned with Bose-Einstein condensates of alkali atomic system with arbitrary spin [1] from one hand and to the original work by Haldane [2,3] from other hand. In the case of spin-1 Bose gas with antiferromagnetic interaction like ^{23}Na , it has been pointed out [4] that as the magnetic field gradient is reduced the single condensate involves toward an angular momentum eigenstate, which becomes a spin singlet as the magnetic field is reduced to zero. The singlet state has a “fragmented” structure which bears no resemblance to single condensate state. The part of the Hamiltonian that describes the interaction between the boson particles with angular momentum $s=1$ [5] has a Heisenberg form, but in general case assumes to the Hamiltonian has a polynomial form: $V = \sum_{n=0}^{n=s} C_n (\vec{S}_1 \cdot \vec{S}_2)^n$, where the operators \vec{S}_1 and \vec{S}_2 the spins of atom 1 and 2, respectively, C_n is a linear combination of the s -scattering interaction constants, S – the maximal

total spin of two particles. It was emphasized there that “for bosons (or fermions), the symmetry implies that only even (or odd) S terms appear in V .” Contrary to this statement, it is shown in [6] that both the even and the odd S -values in the interaction Hamiltonian are possible for the both fermionic and bosonic systems in the spin representation, concerned to the symmetry of the coordinate part of wave function. The polynomial form of the interaction is very useful for the description of the symmetric (antisymmetric) states in the spin representation, but the general form of the interaction of Hamiltonian was not found in reference [5].

By analyzing the presence of topological terms in effective-field theories for one-dimensional antiferromagnets, Haldane conjectured that integer-spin chains display a ground state with exponentially decaying spin-spin correlations and a gapped excitation spectrum—properties markedly different from those displayed by the exactly solvable $S=1/2$ chain. Despite early controversy, this so-called “Haldane conjecture” is now supported by solid numerical and experimental evidences [7]. The single-ion anisotropy is relevant in accounting for the magnetic properties of a number of compounds: CsNiCl_3 (weak axial anisotropy), $\text{NENP} [\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2]\text{ClO}_4$ (weak axial anisotropy), CsFeBr_3 , $\text{NENC} [\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{Ni}(\text{CN})_4]$, and $\text{DTN} [\text{NiCl}_2-4\text{SC}(\text{NH}_2)_2]$ (strong planar anisotropy) [7]. Haldane^{3,4} has analyzed the isotropic point. The intermediate phase was investigated by studying an extended $S=1$ model with biquadratic interactions,

$$H_{AKLT} = J \sum_i \left[\vec{S}_i \cdot \vec{S}_{i+1} + \beta (\vec{S}_i \cdot \vec{S}_{i+1})^2 \right] \quad (1)$$

Affleck, Kennedy, Lieb, and Tasaki (AKLT) [8] showed that this Hamiltonian is exactly solvable at $\beta=1/3$, where it displays a simple valence-bond solid (VBS) ground state with gapped excitations. Since the ground state at $\beta=0$ has been shown [3] to exhibit long-ranged string correlations and is adiabatically connected to the ground state at $\beta=1/3$ (see, e.g., [9]), one

concludes that the Haldane phase has a VBS character. In contrary to this position, it was shown by E. Orlenko [10], that neither $\beta=1/3$, nor $-\beta=0$ could appear in the **Eq.1**, the constant only possible here for such system is $\beta=1$. The interest in Haldane-type phases exhibiting long-range string correlations has been renewed and proposals for investigating string order in cold atomic systems have recently been made [11,12]. The investigation of string order in cold atomic system has been made in reference [10]. Here the ground state of a set of particles with spins $j=1$ and $j=2$ were obtained and nonlinear magnetic phenomena in the set of particles with $j=1$ were considered. The presence of nonlinear terms in the Hamiltonian of a system may give rise to nonlinear spin waves in atomic systems with the spin $j=1$ and, in particular, to a soliton.

Analyzing excited states above the Néel ground state, following den Nijs and Rommelse¹³, it is interpreted the spin $S=1$ chain as a diluted system of a pseudospin $S=1/2$ pseudoparticles; sites with spin projections $S_z=\pm 1$ as being occupied by spin-half particles with pseudospin components $S_z=\pm 1/2$ and sites with $S_z=0$ as being empty (occupied by “holes”). Using this language, the Néel ground state is equivalent to an “undoped” antiferromagnet, and for small positive values of D/J , the low-lying excited states lie in the “one-hole sector” (containing one site with $S_z=0$). The situation is reminiscent of spin-charge separation in one-dimensional fermionic systems where a hole doped into the system fractionalizes into “holon” and “spinon” constituents. Unlike den Nijs and Rommelse’s artificial interpretation the $S=1$ chain as a diluted system of $S=1/2$ pseudoparticles; we show that the system of particles with an arbitrary spin can be described directly from the first principles, based on symmetry law.

The theoretical description of the spin ordering in the antiferromagnetic $S=1$ - chain requires a new form of the model Hamiltonian. The universal Hamiltonian of the exchange interaction for the system of particles with an arbitrary spin is developed here from the first principles. In this paper, we are interested in improving on previous estimates for ground state of the one-dimensional $S=1$ pseudo-Heisenberg antiferromagnet with single-ion anisotropy. Additionally, we obtain results for the excitations in the form of nonlinear spin waves and, in particular, the possibility of a soliton solution is considered. We will show that the soliton is stable if the nonpoint potential varies slowly within the soliton length. For the one-dimensional $S=1$ spin system, we will arrive at the pattern of nonlinear magnetic vortices that transform into macroscopic vortices of a magnetic field in a system and bring the phase separation.

2. MAGNETIC ORDERING IN THE ONEDIMENSIONAL CHAIN OF IONS WITH $S=1$ SPINS

2.1. Pseudo-Heisenberg Hamiltonian of the Exchange Interaction for the Chain of Particles with $s=1$

In the simplest case of the chain of ions with two-particle interaction, the Hamiltonian in the coordinate representation can be written as follows:

$$\hat{H}(1, \dots, N) = \sum_i \hat{H}(i, i+1) \quad (2)$$

where the numbers of particles are $1, \dots, i, i+1, \dots, N$. The Hamiltonian $\hat{H}(i, i+1)$ describing pair interaction can be represented as a sum of noninteracting particle Hamiltonians $\hat{h}(i) + \hat{h}(j) = \hat{H}^0(i, j)$ and the pair interaction operator $\hat{V}(i, j)$.

The first order correction of the total energy of a two-particle system is

$$E^{(1)} = K \pm A, \quad (3)$$

where K is the direct input and A is the exchange input to the energy correction, and sign \pm is corresponded with the symmetry of coordinate part of wave function.

The total wave function of two bosons is a product of the coordinate-dependent part and $X_{s/a}(i, i+1)$ a spin part of the same permutation symmetry.

$$\Psi_s(i, i+1) = \Phi_{s/a}(i, i+1) \cdot X_{s/a}(i, i+1) \quad (4)$$

In other words, the factor ± 1 for the exchange input **Eq.3** depended of the symmetry of the spatial part corresponds to the determined spin part symmetry of the wave function. The symmetry of the spin part of the two particle system is connected with the total spin S because of the symmetry of the Clebsch-Gordan coefficients. In the case $s_1=s_2=s$ is:

$$C_{s, s_1z, s, s_2z}^{SS_z} = (-1)^{2s-S} C_{s, s_2z, s, s_1z}^{SS_z}, \quad (5)$$

where the two particle spin function is represented in the form

$$|S, S_z; s_1, s_2\rangle = \sum_{s_1z+s_2z=S_z} C_{s_1s_1z, s_2s_2z}^{SS_z} |s_1, s_{1z}\rangle |s_2, s_{2z}\rangle \quad (6)$$

The vectors of the spin states of particles number 1 and number 2 are $|s_1, s_{1z}\rangle$ and $|s_2, s_{2z}\rangle$.

The permutation operator $\hat{P}_{s,s}$ acting on the spin state **Eq.6** gives the eigenvalue $(-1)^S$, because of the two particle spin functions are symmetric or antisymmetric with respect to particle permutation. It can be seen from **Eq.6** for Clebsch-Gordan coefficients.

Then we will change the factor ± 1 in **Eq.4** by the permutation operator \hat{P}_{s_1, s_2} in the spin representation:

$$\hat{E}^{(1)} = K + A \cdot \hat{P}_{s_1, s_2}, \quad (7)$$

Then the Hamiltonian of the chain taken into account

pair interactions and acting on spin functions, can be presented as

$$\hat{H}_{\text{int}} = \sum_i (K_{i,i+1} + A_{i,i+1} \hat{P}_{s_i, s_{i+1}}). \quad (8)$$

For obtaining the permutation operator in the spin representation the following condition is used:

$$\hat{P}_{s_1, s_2} |S, S_z; s_1, s_2\rangle = (-1)^S |S, S_z; s_1, s_2\rangle. \quad (9)$$

The permutation operator can be presented in the form of a polynomial expansion as

$$\hat{P}_{s_1, s_2} = c_{2s} (\hat{s}_1 \cdot \hat{s}_2)^{2s} + c_{2s-1} (\hat{s}_1 \cdot \hat{s}_2)^{2s-1} + \dots + c_1 (\hat{s}_1 \cdot \hat{s}_2) + c_0. \quad (10)$$

Here the number of free coefficients c_n is equal to the number of possible eigenvalues of the scalar product operator. The eigenvalue of the scalar product $\hat{s}_1 \cdot \hat{s}_2$ operator depends on the value of total spin S :

$$\overline{\hat{s}_1 \cdot \hat{s}_2} = \frac{1}{2} (\overline{S^2} - 2s^2) = \frac{1}{2} (S(S+1) - 2s(s+1)). \quad (11)$$

In the case $s_1 = s_2 = 1$, the total spin of the two particle system has three eigenvalues $S=2, 1, 0$.

The free coefficients c_n can be determined from the system of three linear equations resulting from **Eq.10**. This system has only one, unique solution with determinate coefficients:

$c_0 = -1, c_1 = c_2 = 1$. Then, the permutation operator for the two particle system in the case $s_1 = s_2 = 1$ has the form:

$$\hat{P}_{s_1, s_2} = (\hat{s}_1 \cdot \hat{s}_2)^2 + (\hat{s}_1 \cdot \hat{s}_2) - 1, \quad (12)$$

and the Hamiltonian of N particles with $s = 1$ interacting in pairs can be represented in the form:

$$\hat{H}_{\text{int}} = \sum_i \left[K_{i,i+1} + A_{i,i+1} \left\{ (\hat{s}_i \cdot \hat{s}_{i+1})^2 + \hat{s}_i \cdot \hat{s}_{i+1} - 1 \right\} \right]. \quad (13)$$

This Hamiltonian of the exchange interaction has a biquadratic term, which gives rise for the nonlinear phenomena in the $S=1$ antiferromagnetic chain.

2.2. Ground State of the $S=1$ Chain

Unlike the $s=1/2$ system of particle, the total spin Σ of the system with $s=1$ spins is not a good quantum number because it does not commute with the Hamiltonian **Eq.13** $[\hat{H}_{\text{int}}, \Sigma^2] \neq 0$. The Hamiltonian **Eq.14** can be rewritten in the form, where $\hat{S}_{i,i+1}^2 = (\hat{s}_i + \hat{s}_{i+1})^2$ is the two-particles spin operator, with indices i and $i+1$ denoting the particles numbers:

$$\hat{H}_{\text{int}} = K \frac{N}{2} + \sum_i A_{i,i+1} \left\{ \left(\frac{1}{2} (\hat{S}_{i,i+1}^2 - 2\hat{s}_i^2) \right)^2 + \frac{1}{2} (\hat{S}_{i,i+1}^2 - 2\hat{s}_i^2) - 1 \right\}. \quad (14)$$

First of all we calculate the exchange energy $E_{i,i+1}^{\text{exc}}$ of ions couple as a function of couple spin S . It will be equal to

$$E_{i,i+1}^{\text{exc}} = A_{i,i+1} \left\{ \left(\frac{1}{2} (S(S+1) - 2s(s+1)) \right)^2 + \frac{1}{2} (S(S+1) - 2s(s+1)) - 1 \right\}. \quad (15)$$

Let us consider the spin of ion's couple as an integer variable, then the new integer variable x can be written as

$$x = \frac{1}{2} (S(S+1) - 2s(s+1)), \quad (16)$$

where x varies in the $[-2, 1]$.

Then the exchange energy $E_{i,i+1}^{\text{exc}}$ of ions couple can be presented as a function of x

$$E_{i,i+1}^{\text{exc}}(x) = A_{i,i+1} (x^2 + x - 1). \quad (17)$$

Here the lowest energy value is achieved at $x=-0.5$, which corresponds the spin $S=1.3$, close to the physically available total spin of couple $S=1$. This state is anti-symmetric and stable with respect to the small fluctuations from the equilibrium. Then we come to conclusion, that the most preferable value of the total couple spin is $S=1$. Then we can present the Hamiltonian of whole chain as the perturbation expansion in the following schema, which conserves the spin anti-symmetry of whole chain:

$$\hat{H}_{\text{int}} \approx K \frac{N}{2} + \sum_{i=1, N/2} A_{i,i+1} \langle \bullet_i \bullet_{i+1} \rangle + \sum_{q=1, N/4} A_{q,q+1}^{(1)} \langle \langle \bullet \bullet \rangle_q \langle \bullet \bullet \rangle_{q+1} \rangle + \dots, \quad (18)$$

where symbolic expressions mean for neighbour ions

$$A_{i,i+1} \langle \bullet_i \bullet_{i+1} \rangle = A_{i,i+1} \left\{ (\hat{s}_i \cdot \hat{s}_{i+1})^2 + \hat{s}_i \cdot \hat{s}_{i+1} - 1 \right\} \quad \text{and}$$

$$A_{q,q+1}^{(1)} \langle \langle \bullet \bullet \rangle_q \langle \bullet \bullet \rangle_{q+1} \rangle = A_{q,q+1}^{(1)} \left\{ (\hat{s}_q \cdot \hat{s}_{q+1})^2 + \hat{s}_q \cdot \hat{s}_{q+1} - 1 \right\}$$

for the neighbour couple of ions with the first renormalized constant of the exchange interaction $A_{q,q+1}^{(1)}$ and the total couple's spin

$$\hat{s}_{q-\frac{i}{2}} = \hat{s}_i + \hat{s}_{i+1}, \quad \hat{s}_{q+\frac{i+2}{2}} = \hat{s}_{i+2} + \hat{s}_{i+3}.$$

Because of these constants $A_{q,q+1}^{(n)}$ are equal for each couple in the chain, it is possible to find the energy of the system in the representation of S spin of couples. Because of each term of this expansion corresponds to the most preferable spin $S_{q,q+1}=1$ anti-symmetric state, then the total spin of whole chain Σ will be also equal to 1, ($\Sigma=1$)

which corresponds to anti-symmetric state. It is a anti-ferromagnetic state, because of the averaged spin pro ion is reduced to zero as Σ/N . In this case the total energy of the chain can be written as follows:

$$E_{int} \approx K \frac{N}{2} + \frac{N}{2} \left(-\frac{1}{2} \right) \left(A^{(0)} + \frac{A^{(1)}}{2} + \dots + \frac{A^{(\nu)}}{2^\nu} \right). \tag{19}$$

We assume, that the renormalized exchange parameter of the k step $A^{(k)}$ is connected with the $k-1$ approximation exchange parameter $A^{(k-1)}$ as follows:

$$A^{(k)} \approx A^{(k-1)} \exp \left(-\frac{b}{a_B} \right), \tag{20}$$

where a_B – is Bohr’s radius, b - is the constant of lattice. Then the total energy of the basic anti-symmetric state of infinite length chain for each ion will be

$$\frac{E_{int}}{N} \approx \frac{K}{2} + \frac{1}{2} \left(-\frac{1}{2} \right) \sum_{\nu} \frac{A^{(\nu)}}{2^\nu} = \frac{1}{2} \left(K - A^{(0)} \sum_{\nu} \frac{e^{-\frac{b}{a_B \nu}}}{2^\nu} \right) = \left(\frac{1}{2} K - A^{(0)} \frac{1}{2 - \exp(-\frac{b}{a_B})} \right) \tag{21}$$

It is easy to see that the exchange interaction plays more important role for the long chains than for the short and brings to the system a strong long order correlation.

3. SPIN DARK-BRIGHT SOLITON

Let us consider the anisotropic spin-1 antiferromagnetic chain that preserves ground state **Eq.21** of the system. The Hamiltonian of the system that takes into account only exchange interaction is taken in the form of **Eq.14**. Then, assuming that the interaction takes place with the nearest neighbors in the chain, we can set the spin of a pair of atoms to be equal to $S=1$ and the eigenvalue of the operator $\widehat{s}_i \cdot \widehat{s}_{i+1}$, to $\widehat{s}_i \cdot \widehat{s}_{i+1} = -1$. If a spin k in a chain of atoms is flipped, the operator of the excitation energy can be written in the form:

$$\widehat{V} = \widehat{H}_{int} - E_0 = A \{ \widehat{s}_{k-1} \widehat{s}_k + \widehat{s}_k \widehat{s}_{k+1} + (\widehat{s}_{k-1} \widehat{s}_k)^2 + (\widehat{s}_k \widehat{s}_{k+1})^2 - 2 \{ (-1)^2 s_k^4 + (-1)^2 s_k^4 \} \}, \tag{22}$$

where (considering the flip of a single spin k) $E_0 = A \sum_i \{ (-1)^2 s_i^4 + (-1)^2 s_i^2 - 1 \}$.

In the semi-classical continuous approximation of magnetic moment eigenvalues, the magnetic moment of an atom may be represented by a function that smoothly varies with distance. Then, the spin $k \pm 1$ can be ex-

panded as

$$\bar{s}_{k\pm 1} = \bar{s}_k \pm b \frac{\partial \bar{s}_k}{\partial x} + \frac{b^2}{2} \frac{\partial^2 \bar{s}_k}{\partial x^2}, \tag{23}$$

where b is the constant of the lattice. After the substitution of the above expansion into **Eq.22**, the excitation energy becomes

$$\widehat{V} = 2A \left\{ s_k^2 \left(2 + b^2 \left(\frac{\partial \bar{s}_k}{\partial x} \right)^2 + \frac{b^4}{4} \left(\frac{\partial^2 \bar{s}_k}{\partial x^2} \right)^2 \right) + \frac{b^2}{2} (1 + 2s_k^2) \bar{s}_k \cdot \frac{\partial^2 \bar{s}_k}{\partial x^2} \right\}. \tag{24}$$

On the other hand, in the approximation of an effective field H^* produced by all spins of the system, the excitation energy of the system can be defined as the energy of interaction of each of the spins with this field:

$$V = g \mu_0 \bar{s}_k \cdot \bar{H}^*. \tag{25}$$

Then, each of the spins precesses (in accordance with the Bloch theorem) in the effective magnetic field

$$\frac{\partial \bar{m}}{\partial t} = \frac{e}{Mc} [\bar{H}^* \times \bar{m}]$$

$$\bar{H}^* = \frac{A}{g \mu_0} \left\{ \bar{s}_k \left(2 + b^2 \left(\frac{\partial \bar{s}_k}{\partial x} \right)^2 + \frac{b^4}{4} \left(\frac{\partial^2 \bar{s}_k}{\partial x^2} \right)^2 \right) + \frac{b^2}{2} (1 + 2s_k^2) \frac{\partial^2 \bar{s}_k}{\partial x^2} \right\}. \tag{26}$$

Applying **Eq.24** to the components of the magnetic moment vector $m = \text{sg} \mu_0$ and assuming $m_z \gg m_x, m_y$, one can rewrite **Eq.26** in the cyclic coordinate system:

$$\dot{m}_+ = -i \frac{Ab^2}{\hbar} \left[\frac{\partial^2 m_+}{\partial x^2} + \left(\frac{m_+^2}{b^2 g^2 \mu_0^2} - \frac{4(m_-^2)}{b^2 g^2 \mu_0^2} \right) m_+ \right];$$

$$\dot{m}_- = -\frac{Ab^2}{\hbar} i \left[\frac{\partial^2 m_-}{\partial x^2} + \left(\frac{m_-^2}{b^2 g^2 \mu_0^2} - \frac{4m_+^2}{b^2 g^2 \mu_0^2} - \Delta \right) m_- \right]; \tag{27}$$

where $m_{\pm} = m_x \pm im_y, \Delta = \frac{A}{(g \mu_0)^2} b$.

The equation obtained is similar to that for a dark-bright soliton [14-16]. Following [14], we represent a solution in the form

$$m_- = \sqrt{\frac{m_0^2 ka}{2}} e^{i\Omega t} e^{ixktg\alpha} \text{sech} \{ k(x - q(t)) \},$$

$$m_+ = \sqrt{Aa^3} (i \sin \alpha + \cos \alpha \tanh \{ k[x - q(t)] \}) \tag{28}$$

Here, $1/k$ is the soliton length, $m_z = m_0$,

$$k = \frac{1}{a} \left\{ \sqrt{\frac{4m_0^2}{g^2 \mu_0^2} \cos^2 \alpha + \left(\frac{m_0^2}{4g^2 \mu_0^2} \right)^2} - \frac{m_0^2}{4g^2 \mu_0^2} \right\},$$

$$\Omega = \frac{A}{\hbar} \left(1 - \frac{tg^2 \alpha}{2}\right) (ka)^2 - \Delta$$

is the precession frequency with regard to the shift, and

$$q(t) = q(0) + kt \frac{Aa^2}{\hbar} tg \alpha$$

is the soliton coordinate.

Such integrable systems in which the free energy is conserved are known as Manakov equations [17]. The higher the velocity of a soliton, the lower the free energy of system [17]; therefore, the soliton is formally unstable (it is accelerated). However, the effect of other excitations (solitary or ordinary spin waves), which is disregarded here, does not cause dissipation [17]. With an additional inhomogeneous potential added to **Eq.26**, the system becomes nonintegrable, allowing for the nontrivial interaction of a soliton with the environment. Nevertheless, if the interaction potential varies slowly within the scale of the soliton length k^{-1} , the variations (propagations) in the soliton and potential correlate and the free energy can be treated as an adiabatic invariant in this case [15,16]. Thus, for the spin system considered above, we will arrive at the pattern of nonlinear magnetic vortices that transform into macroscopic vortices of a magnetic field in a antiferromagnetic chain system. It is important to note that we analyzed the case when only one spin was flipped. Considering the flip of two, three, etc. spins, we will generate a set of solitons with different frequencies $\Omega_1, \Omega_2, \dots, \Omega_n$ that differ in the exchange interaction constants.

4. CONCLUSIONS

The universal form of the exchange interaction Hamiltonian of the system of particles with an arbitrary spin in the spin representation is developed from the first principles. The Hamiltonian described the antiferromagnetic S1-chain contains the biquadratic term with determined coefficient. The ground state energy of the chain is more dependent from the exchange interaction in the case of a long chain. The exchange interaction makes such system antiferromagnetic and strong long-order correlated. The presence of biquadratic term in the Hamiltonian of the system gives rise to nonlinear spin waves in the chain and, in particular, to a soliton. The soliton is stable if the nonpoint potential varies slowly within the soliton length. For the one-dimensional S=1 spin system, we will arrive at the pattern of nonlinear magnetic vortices that bring the phase separation.

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