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Spontaneous SU(2) symmetry breaking in one-dimensional quantum antiferromagnet*

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Abstract. We present a Bethe Ansatz based investigation of a one-dimensional (1D) Heisenberg spin chain in a real 3D crystal lattice. We have shown that due to an influence of the lattice distortion on a crystalline field of ligands of magnetic ions, a Heisenberg antiferromagnetic spin $S = \frac{1}{2}$ chain is unstable under the appearance of a magnetic anisotropy of the "easy-plane" type. The effects of an external magnetic field and nonzero temperature onto such a phase transition are studied.

PACS. 75.10.Jm Quantized spin models – 75.30.Gw Magnetic anisotropy – 75.80.+q Magnetomechanical and magnetoelectric effects, magnetostriction

Last decade the study of low-temperature behaviour of low dimensional quantum antiferromagnets (AF) has attracted great interest. In particular, several quantum AF have been synthesized in which the interaction of spins along some space direction was 10^2-10^4 times larger than along other directions of the crystal lattice [1,2]. Such magnets usually reveal phase transitions to an ordered (three-dimensional) magnetic state at very low temperatures ($T_c \sim 1$K). However at temperatures between T_c and a characteristic energy of the exchange interaction along this special direction, they usually manifest properties of magnetic 1D chains. In 1D systems quantum fluctuations are usually enhanced due to peculiarities of the density of states. Therefore approximate theoretical methods can give even qualitatively incorrect results for 1D quantum systems. Thus, a theoretical investigation of many-body effects in 1D AF spin chains demands for the use of exact quantum methods like Abelian or non-Abelian bosonization or Bethe ansatz [3].

Among the variety of low-dimensional spin systems studied last decade, the systems with site spins $S = \frac{1}{2}$ have a special place (for instance, ions of Cu^{2+} [1] or V^{4+}) [2]. Besides, magnetic behaviour of rare-earth ions at low temperatures can be described by effective spin-$\frac{1}{2}$ Hamiltonians[1]. It is worthwile to notice that such a description, however, yields a sharp anisotropy of magnetic properties of such effective spin $S = \frac{1}{2}$ models. These systems become either Ising-like or XY-like, depending on which two levels (doublet) of the real (multi-level) total moment of the site f orbital of the magnetic ion are the lowest-lying ones [4].

It is well-known that a magnetic anisotropy in spin systems can play an essential role when studying theoretically low temperature magnetic properties [5]. A magnetic anisotropy manifests itself in such a way, that a degeneracy of the energy is lifted[2]. Such a situation emerges in many-body AF spin systems, where Heisenberg AF spin-spin interaction does not prefer any direction. Hence, the states with spins directed along any vector of a lattice are energetically equivalent. Here a magnetic anisotropy leads to a situation where some crystal directions become more energetically favorable. In this case the total spin of a system is not an integral of motion. It is well known that a magnetic anisotropy appears as the manifestation of crystalline (electric) fields of ligands (*i.e.* non-magnetic neighbouring ions of magnetic ones) [4]. This field affects the spin subsystem of electrons of magnetic ions indirectly, via a spin-orbital interaction, which is usually weak. Therefore a change (appearance) of a magnetic anisotropy is caused by the change of the symmetry of non-magnetic neighbouring ions' lattice places. For only the spin subsystem the emergence of an uniaxial magnetic anisotropy reduces the symmetry of spins from $SU(2)$ for Heisenberg magnet to $U(1)$ for the uniaxial one.

A magnetic anisotropy may be of single-ion type as well as of inter-ion type [4,5]. In our paper we will study

* Dedicated to J. Zittartz on the occasion of his 60th birthday

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[1] *I.e.* at low temperatures the lowest doublets are most important there.

[2] Directions of quantization of a total spin moment are similar for only isotropic Heisenberg exchange coupling or for free spin.

essentially many-body spin systems, so we will investigate the inter-ion magnetic anisotropy influence first of all. Naturally, systems of spins $S = \frac{1}{2}$ may have only inter-ion magnetic anisotropy.

We will show that 1D AF Heisenberg spin $S = \frac{1}{2}$ chains are unstable at low temperatures under the appearance of a magnetic anisotropy of "easy-plane" type. This magnetic anisotropy appears due to a weak distortion of (3D) non-magnetic ions, and, as a consequence, the change of its crystalline electric fields. Our results have been derived in mean field approximation. Such an approximation is well based here. We deal with a model system, in which the lattice is *three-dimensional*, despite the fact that the spin-spin exchange interaction is *one-dimensional*. So the mean field method, undoubtedely, can be used here. Moreover, we study the instability of the magnetically isotropic *homogeneous* system against *homogeneous* distortions. It produces a homogeneous magnetic anisotropy along the total chain, *i.e.* we do not consider phase transitions to incommensurate phases (states). In other words, the phonon, which lifts the spin degeneracy, has a *commensurate* wave vector (quasimomentum) and the instability of the Heisenberg AF spin chain is governed by this phonon. We will consider also effects of an external magnetic field and nonzero temperature onto the instability mentioned above.

The nature of the instability studied in this paper is very similar to the phase transition of Peierls type in spin $S = \frac{1}{2}$ XY chains [6,7]. A spontaneous appearance of the biaxial magnetic anisotropy in XY chain of spins $S = \frac{1}{2}$ was predicted in reference [8]. In references [6–8] the Hamiltonians of spin XY chains were mapped exactly (using a Jordan-Wigner transformation [9]) onto *non-interacting* spinless fermion chains. In other words, in references [6–8] effectively *noninteracting* fermion systems were studied. As for the present work, we investigate here the 1D Heisenberg AF chain of spins $S = \frac{1}{2}$. Even using the Jordan-Wigner transformation one can map it onto 1D spinless fermion system *with two-particle interaction*. Hence, we study essentially *many-body* co-operative Jahn-Teller-like effects in an *interacting* 1D quantum spin system.

The Hamiltonian of a (periodic) chain of N spins $S = \frac{1}{2}$ with antiferromagnetic interaction has the form:

$$\mathcal{H}_0 = -\frac{1}{2}\sum_{l=1}^{N}(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y + \Delta\sigma_n^z\sigma_{n+1}^z), \qquad (1)$$

where σ_n^α ($\alpha = x, y, z$) are Pauli operators of α-projection of the spin in n-th site, the exchange constant is equated to unity, and Δ is the parameter of an (inter-ion) magnetic anisotropy. $|\Delta| > 1$ corresponds to the "easy-axis" type of anisotropy, while $|\Delta| < 1$ is connected with the "easy-plane" type of magnetic anisotropy. The case $\Delta = -1$ is the isotropic Heisenberg AF spin chain. The wave function of a state with M spins down can be found in the form of the so-called *Bethe ansatz*, *i.e.* the plane wave permutations:

$$\Psi = \sum_{x_1<x_2<\ldots<x_M}\sum_P A_P \exp i\sum_{j=1}^{M} p_{P_j}x_j|x_1\ldots x_M\rangle, \qquad (2)$$

where x_j are coordinates of j-th spin down, p are quasimomenta (conjugated to coordinates), and P denotes permutation of quasimomenta. The vector $|x_1\ldots x_M\rangle = \sigma_{x_1}^-\ldots\sigma_{x_M}^-|0\rangle$, where $|0\rangle$ is the spin polarized ("ferromagnetic") state with all spins up, and $\sigma_n^\pm = \sigma_n^x \pm i\sigma_n^y$. Then the energy of this AF chain with M spins down is:

$$E_{mag} = -\frac{N\Delta}{2} + 2\sum_{j=1}^{M}(\Delta - \cos p_j). \qquad (3)$$

The values of the quasimomenta that parametrize eigenfunctions and eigenvalues of the Schrödinger equation are found from the periodic boundary conditions, which have the well-known Bethe ansatz equations' form

$$Np_j = 2\pi I_j - \sum_{l=1,l\neq j}^{M}\theta(p_j, p_l), \qquad (4)$$

where

$$\theta(p_j, p_l) = 2\tanh^{-1}\left[\frac{\Delta\sin\frac{p_j-p_l}{2}}{\cos\frac{p_j+p_l}{2} - \Delta\cos\frac{p_j-p_l}{2}}\right], \qquad (5)$$

and I_j are (half)integers for M (even) odd. These numbers parametrize eigenfunctions (2) and eigenvalues (3) of our quantum problem. In the limit of $\Delta \to 0$ our system reduces to the isotropic XX spin chain, and equations (4) become the well-known periodic boundary conditions for the free 1D lattice fermion gas.

Let $\Delta = -1 + u\delta$, *i.e.* the parameter ($u\delta$) now characterizes the appearence of a magnetic anisotropy. u is the magnetoelastic constant and δ is the distortion of nonmagnetic ligands from their symmetric configuration. A magnetic anisotropy is caused by the change of the crystalline fields of ligands. Hence, it is connected with the shifts of equilibrium states of the 3D lattice of (nonmagnetic) ligands. For small δ, this process causes in the lowest order an enhancement of the energy of the totally elastic subsystem

$$E_{el} = NC\frac{\delta^2}{2}, \qquad (6)$$

where C is the elastic constant. That is why a gain in the magnetic energy (Eq. (3)) due to the magnetic anisotropy is followed by the loss in elastic energy (as it must be). In other words, the degeneracy of the Heisenberg AF spin chain is lifted due to an effect analogous to the co-operative Jahn-Teller effect [4], *i.e.* the influence of the elastic subsystem onto the electronic one. We find the energy of the spin subsystem (Eq. (3)) *exactly*, using the well known results of the classic paper [10].

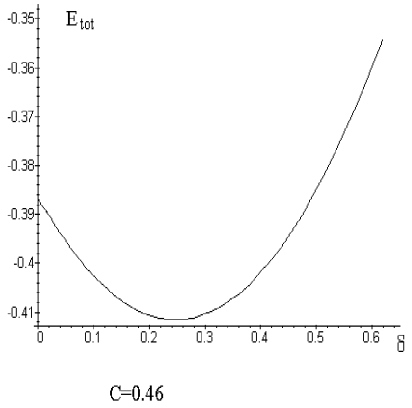

Fig. 1. The total groundstate energy of magnetic and elastic subsystems E_{tot} as function of the shift δ of lattice positions of nonmagnetic ions. The elastic constant is $C = 0.46$.

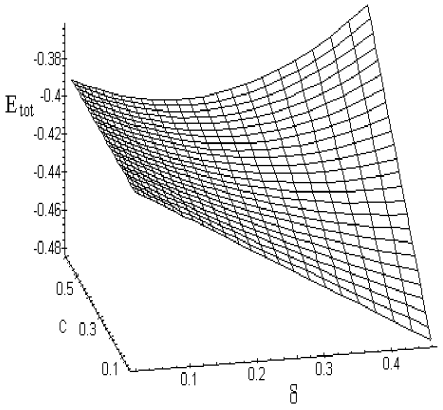

Fig. 2. The total magnetic and elastic groundstate energy E_{tot} as function of the distortion of lattice positions of nonmagnetic ligands δ and the elastic constant of the lattice C.

Let $\Delta \equiv -1 + u\delta = -\cos\mu$ ($u\delta > 0$) for the "easy-plane" type of magnetic anisotropy. Then the Bethe ansatz equations (Eqs. (4)) can be solved in the thermodynamic limit (where $N \to \infty$, $M \to \infty$ and M/N is fixed). They become

$$\frac{\sin\mu}{\cosh\alpha - \cos\mu} = 2\pi\rho(\alpha) + \int_{-Q}^{Q} d\beta\rho(\beta)\frac{\sin 2\mu}{\cosh(\alpha-\beta) - \cos 2\mu}, \tag{7}$$

where we changed the variables from the quasimomenta p_j to *rapidities* α_j

$$p_j = -i\ln\frac{\sinh(\alpha_j + i\mu)}{\sinh(\alpha_j - i\mu)}\,. \tag{8}$$

$\rho(\alpha)$ is the density of quantum rapidities α, which from now parametrize the eigenvalues and eigenvectors of our spin subsystem. The limits of integration $(-Q, Q)$ are determined by the M value ($M = N\int_{-Q}^{Q} d\alpha\rho(\alpha)$)[3]. In the absence of an external magnetic field h it was proved exactly in reference [10] that the rapidities α fill the total interval $[-\infty, \infty]$ for AF spin chain. The solution of equation (7) is found by using a Fourier transformation. This solution yields together with equation (3) in the thermodynamic limit

$$E_{mag} = -\frac{N\Delta}{2} - N\int_{-Q}^{Q} d\alpha\rho(\alpha)\frac{2\sin^2\mu}{\cosh\alpha - \cos\mu}\,. \tag{9}$$

For $h = 0$ ($Q = \infty$) we find

$$E_{mag} = -N\Delta - N\sin(\mu)\int_{-\infty}^{\infty} dx\frac{\sinh(\pi-\mu)x}{\cosh(\mu x)\sinh(\pi x)}\,. \tag{10}$$

Now we minimize $E_{tot} = E_{mag} + E_{el}$ with respect to the distortion δ of the nonmagnetic lattice. We find that the "easy-plane" AF chain minimum energy is connected with the solution of the equation

$$C\delta_{eqv} = \frac{\partial}{\partial\delta}\left[\Delta + \sin(\mu(\delta))\int dx\frac{\sinh[(\pi-\mu(\delta))]x}{\sinh(\pi x)\cosh(\mu(\delta)x)}\right]|_{\delta=\delta_{eqv}}. \tag{11}$$

Under the assumption that our lattice is in the groundstate for any scale of our problem we plot the dependence of the total groundstate energy of the elastic and magnetic subsystems as function of the shift δ of the 3D nonmagnetic lattice of ligands. In Figure 1 one can see such a dependence for the elastic constant value $C = 0.46$[4]. We see that the minimum of the total energy corresponds to a *nonzero* value of the lattice distortion. It means that in the groundstate the minimal energy is connected with a shift of the 3D nonmagnetic ions. This, in turn, produces the electric field, which causes a nonzero magnetic anisotropy for the 1D AF spin subsystem due to spin-orbit coupling.

We can ask the question whether such a behaviour emerges for any value of the elastic constant C? In Figure 2 we plot the dependence of the total groundstate energy of our system of both the elastic constant C and the shift δ. We can see that the minimum in δ, which is connected with a nonzero distorsion of the ligand lattice, appears only for large enough values of the lattice

[3] So, they are connected with the total magnetization of our system.

[4] Note that we measure everything in isotropic exchange constant units.

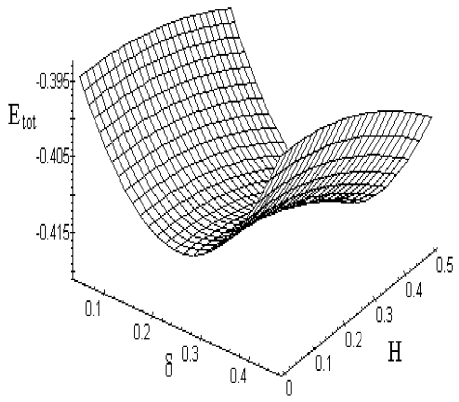

Fig. 3. The dependence of the total groundstate energy of magnetic and elastic subsystems on the distortion δ and weak external magnetic field h.

elastic constant C. This is not surprising since one needs high enough values of elastic shifts to see the magnetic anisotropy effect in the spin subsystem.

We can study the same effect for $\Delta < -1$ in a similar fashion, *i.e.*, for an "easy-axis" type of magnetic anisotropy. Working in a similar way, we solved the Bethe ansatz equations (Eq. (4)) for this case. After tedious but straightforward calculations we found that for any elastic constant C the minimal total groundstate energy of the spin and elastic subsystems corresponds to a *zero* value of the distortion δ of the 3D ligand lattice. So we conclude that for such a case there is no appearance of an additional ligand's electric field. Thus, there is no magnetic anisotropy of "easy-axis" type. This result is not surprising, because we know well that in the case of an Ising-like ("easy-axis") magnetic anisotropy, the AF spin $S = \frac{1}{2}$ chain without an external magnetic field or for low enough fields has *gapful* low-lying excitations.

Now we want to know what happens with such an instability of the 1D Heisenberg AF spin chain under the appearance of an "easy-plane" anisotropy when an external magnetic field h is applied. First, let us study the case of low magnetic fields $h \ll 1$. The Hamiltonian of the spin subsystem then has the form:

$$\mathcal{H} = \mathcal{H}_0 - h \sum_n \sigma_n^z, \tag{12}$$

where $h = g\mu_B H$, g is the gyromagnetic ratio, H is the magnetic field, and μ_B is Bohr's magneton. Using the results of reference [10], *i.e.* solving the integral equation (Eq. (7)) by the Wiener-Hopf method for small enough magnetic fields, we find

$$E_{mag} = E_{mag}|_{h=0} - Nh^2 \frac{\mu}{4\pi(\pi-\mu)\sin\mu} \cdot \tag{13}$$

Minimizing the total spin and elastic energy over the lattice shift δ we see, that for any weak magnetic field h the minimal groundstate energy corresponds to the appearance of the nonzero minimal distortion δ. The dependence of the total groudstate energy of the spin and elastic subsystems *via* the external magnetic field h and the shift δ of the ligands in 3D lattice is depicted in Figure 3. It is seen that for any value of the magnetic field h there exists a minimum (which corresponds to a nonzero shift δ) in the distortion dependence of the total energy.

For high enough magnetic field values $h > h_c$, where h_c is the critical field for the transition in the spin-saturated ("ferromagnetic") state, we can minimize the total energy E_{tot} with respect to δ. This yields:

$$\delta_{eqv} = \frac{u}{4C} \cdot \tag{14}$$

It means that for this case a high external magnetic field does not change the situation drastically: the co-operative effect of the electric crystalline in the spin subsystem and the distortion of the 3D ligand lattice in the elastic subsystem produce essentially a nonzero magnetic anisotropy of "easy-plane" type. So we can conclude that the effect of the appearence of the "easy-plane" magnetic anisotropy in a Heisenberg AF spin chain does not depend on the external magnetic field.

In the previous part we have studied the groundstate properties of the Heisenberg quantum spin chain. It is worthwile to understand what happens when switching on nonzero temperature T. It is obvious that[5] for very high temperatures the isotropic spin system will be stable. This is transparent also from symmetry arguments: usually the high temperature phase corresponds to a situation with higher symmetry. The question arises whether the critical temperature T_c of such a co-operative Jahn-Teller-like phase transition is zero[6] or a situation may exist in which for some range of temperatures the phase with nonzero "easy-plane" magnetic anisotropy emerges for the spin $S = \frac{1}{2}$ chain. To decide this question, one can use the thermal Bethe ansatz [11]. For simplicity we treat only the case of low temperatures. At low temperatures one knows well the Sommerfeld expansion, see, *e.g.*, reference [12]:

$$F_{mag} = E_{mag} - N\frac{\pi T^2}{6v_F}, \tag{15}$$

where v_F is the Fermi velocity of the lowest excitation of the AF chain (spinon). For zero magnetic field case, $h = 0$, it is given by $v_F = \pi \sin(\mu)/\mu$ [10]. We minimize the total free energy $F_{tot} = F_{mag} + E_{el}$ over the distortion of ligands δ. Once more, we consider small enough temperatures, so we suppose that the elastic subsystem is still in the groundstate. This assumption is justified because the elastic subsystem has usually a much larger energy scale than the magnetic one. In Figure 4 we plot the dependence of the total free energy as function of the shift δ and the temperature. Note that we considered only small

[5] For our case of an inter-ion magnetic anisotropy.

[6] Which is to be expected for a 1D spin system, where the only special point in T is $T = 0$.

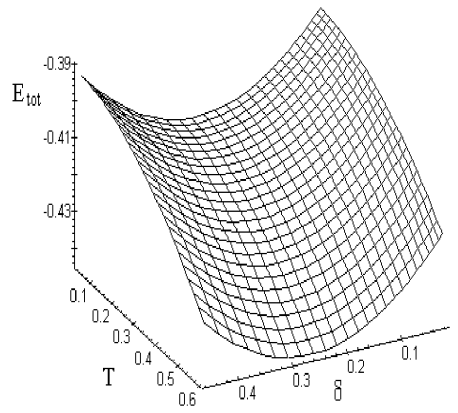

Fig. 4. The temperature (T) and lattice distortion (δ) dependences of the total free energy of the system. Temperatures are small compared to the exchange constant ($J = 1$).

enough temperatures. One can see that the minimum in the δ dependence (corresponding to a nonzero equilibrium shift, and, thus, to the nonzero magnetic anisotropy) exists in the low temperature region, while the minimum has a tendency to disappear with increasing temperature. It is worthwile to notice here that equation (15) does not describe the behavior of the spin chain for the whole temperature region. For higher temperatures a full thermal Bethe ansatz treatment is necessary. It will be reported elsewhere.

We can suppose that one may expect the appearance of the "easy-axis" type magnetic anisotropy for high enough magnetic field values, too (the field value must be larger than the gap value of the elementary spin excitation).

We want to point out that the effect does not depend on the way the interaction between the spin and elastic subsystems is introduced. The results qualitatively emerge when we study E_{mag} as a function of μ itself, and the elastic energy in a form $E_{el} = NC\mu^2/2$, see, *e.g.*, reference [7].

Unfortunately, we do not know any direct experiments on 1D quantum AF spin $S = \frac{1}{2}$ systems which revealed the spontaneous appearence of a magnetic anisotropy. However, we can speculate about results of a recent experiment [13] on quasi-two dimensional antiferromagnet $Ba_2CuGe_20_7$ with Cu^{2+} magnetic ions. There even for an almost isotropic square spin lattice, the magnetic anisotropy effect was necessary to explain the dependence of the magnetization on an external in-plane magnetic field. To our minds, such an effect is the indirect confirmation of the predicted appearence of a magnetic anisotropy, though for a 2D AF spin $\frac{1}{2}$ Heisenberg system. We strongly believe that the effect must emerge for any spin $\frac{1}{2}$ AF system with a non magnetically ordered groundstate and gapless low-lying excitations.

To conclude, in this paper we have studied a one-dimensional quantum Heisenberg spin $S = \frac{1}{2}$ antiferromagnetic chain. We have shown that under the influence of a three-dimensional lattice of nonmagnetic ions (ligands) the Heisenberg spin chain becomes unstable against the appearance of an "easy-plane" magnetic anisotropy. An external magnetic field does not affect this co-operative magneto-elastic effect of Jahn-Teller nature. We have also shown that a phase with nonzero magnetic anisotropy exists for some (nonzero) interval of low temperatures. The instability studied in this paper is analogous to the well-known spin-Peierls instability of spin $S = \frac{1}{2}$ chains [6,7]. The microscopic origin of the instability is the shift of degeneracy of the spin subsystem with isotropic exchange interaction by the appearance of magnetic anisotropy connected with the change of an electric field of lattice nonmagnetic ions (ligands).

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