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CONTRIBUTION OF ONE-SITE TWO-MAGNON BOUND STATES TO THE SPECIFIC HEAT OF S=1 HEISENBERG CHAIN WITH EASY-AXIS ANISOTROPY*

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In this work we discuss the possibility of contribution of one-site two-magnon bound states (OSTMBS's) to the thermodynamic equilibrium properties in $S = 1$ Heisenberg chain with easy-axis anisotropy. We found that for sufficiently strong anisotropy $|D/J| = 5$ a good agreement between OSTMBS's theoretical contribution to the specific heat using dilute approximation and numerical calculations for the aforementioned system was obtained for temperatures below $T = 0.12|D/k_B|$. The obtained result confirms that OSTMBS's are the lowest energy excitations in S=1 Heisenberg chains with sufficiently strong easy-axis anisotropy. Further, the compound $Ni(N_2H_5)_2(SO_4)_2$ previously identified as $S = 1$ antiferromagnetic Heisenberg chain with easy-axis anisotropy with $D/k_B = -15.6$ K, $D/J = 5$, is proposed as an appropriate system for experimental studies of OSTMBS's contribution to thermodynamic properties.

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Quantum Heisenberg chains described by Hamiltonian

$$H = \sum_i D(S_i^z)^2 - \sum_i J(S_i.S_{i+1}) \tag{1}$$

where J represents the intrachain nearest neighbour spin exchange interaction and D denotes the single-ion anisotropy were subject of both theoretical and experimental studies, owing to the presence of non-linear excitations, which play an important role in the thermodynamic properties of these systems. It has been shown that in transverse magnetic field the equation of motion of one-dimensional systems with easy-plane anisotropy, in continuum limit, can be mapped to a sine-Gordon equation [1]. Apart from linear excitations (magnons as small amplitude solutions of the linearized equation) there are also non-linear solutions known as solitons in both antiferromagnetic and ferromagnetic systems [1-4].

Magnetic excitations in classical spin chains with both non-linearity and discreteness of the lattice taken into account were theoretically investigated in [5]. These studies revealed that in the presence of a sufficiently large longitudinal magnetic field there exist intrinsic localised spin modes (ILSM) which are of a very different nature than solitons. ILSM extends over a few lattice sites and has the amplitude dependent frequencies outside the spin-wave band. The degree of

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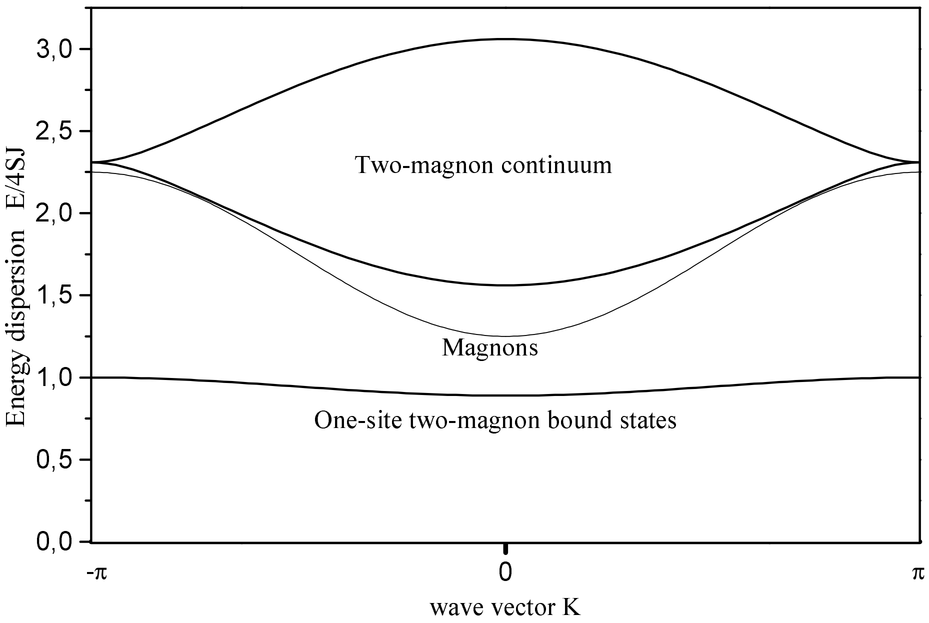

Fig.1. Energy spectrum of two-magnon states for ferromagnetic system with easy-axis type of anisotropy and $D/k_B = 15K$ and $D/J = 5$ (the dispersion branch of exchange bound states emerging from continuum at the zone boundary is not plotted for clarity).

localisation of these non-linear excitations increases with increasing maximum spin deviation and D/J ratio. Electron spin resonance and infrared spectroscopy were proposed as the most appropriate techniques for observation of ILSM due to their transverse magnetic moment rotating in the easy-plane. Nevertheless, the existence of ILSM has not been experimentally confirmed yet.

The two-magnon states in anisotropic magnetic chains of arbitrary spin have been theoretically studied in [6] by extending the original Bethe ansatz for multimagnon states [7]. These calculations furnish a simple expression for two-magnon wave function together with the energy spectrum for systems with both easy-axis (Fig.1) and easy-plane type of anisotropy. Different types of two-magnon bound states emerge when the exchange interaction is taken into account. These states can be constructed either by reducing the azimuthal spin by two units at a single site, so called OSTMBS's, or by reducing its value by one unit at two different sites, obtaining common exchange bound states. Two-magnon bound states emerge at the Brillouin zone boundary below the two-magnon continuum. We discuss the properties of OSTMBS's as a potential quantum mechanical counterpart of ILSM's. More specifically, we study the contribution

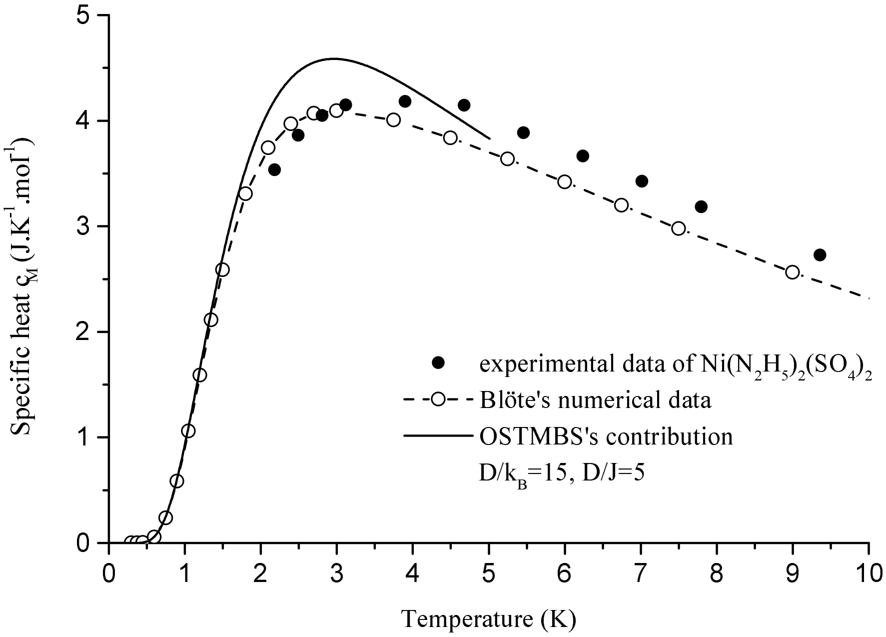

Fig.2. Comparison of magnetic contribution to the specific heat as calculated by Blöte with that of OSTMBS's contribution. The experimental data of $Ni(N_2H_5)_2(SO_4)_2$ are also plotted.

of OSTMBS's to the specific heat in $S = 1$ ferromagnetic Heisenberg chain with sufficiently strong easy-axis anisotropy where the energy dispersion of OSTMBS's is extended through the entire Brillouin zone. We calculated the specific heat of such a chain system using approximation of dilute OSTMBS's taking into account that the OSTMBS's dispersion is lying under the magnon dispersion. For sufficiently low temperatures the OSTMBS's contribution should dominate because of the absence of interaction between OSTMBS's and because of negligible thermal occupation of magnon states. Thus if we compare the numerical prediction of Blöte [8] with the contribution of OSTMBS's to the specific heat we can determine the value of critical temperature for validity of dilute OSTMBS's approximation and indirectly verify the existence of OSTMBS's in systems with sufficiently strong easy-axis anisotropy. For ratio $D/J = 5$, the good agreement between numerical data and OSTMBS's contribution to the specific heat is obtained for temperatures below $T = 0.12|D/k_B|$ (see Fig. 2). The temperature region of the applicability of the theoretical prediction for OSTMBS's is extended with increasing D/J ratio. Fig. 2 also illustrates the experimental data of the compound $Ni(N_2H_5)_2(SO_4)_2$ previously identified as $S = 1$ antiferromagnetic Heisenberg chain with easy-axis anisotropy with $D/k_B = -15.6K$, $D/J = 5$. Numerical calculations of Blöte [8] using Heisenberg linear chain model describe very well the available experimental data of Ni$(N_2H_5)_2(SO_4)_2$ obtained in temperature region 2-20K [9]. A direct comparison of experimental data with theoretical prediction for OSTMBS's cannot be accomplished because this theory is not available for antiferromagnetic system yet. Since Blöte's numerical predictions of specific heat for both ferromagnetic and antiferromagnetic systems with $D/J = 5$ differs only a little for temperatures below $(D/k_B)/8$ it can be expected that in low temperature region OSTMBS's will also dominate in Ni$(N_2H_5)_2(SO_4)_2$. The extension of the theoretical model [6] for antiferromagnetic exchange coupling is in progress [10].

The obtained result confirms that OSTMBS's are the lowest energy excitations in $S = 1$ Heisenberg chain with sufficiently strong easy-axis anisotropy and that they determine its thermodynamic properties at low temperatures. The experimental study of specific heat of aforementioned compound in temperature region from 100 mK to 2.5 K is being carried out.

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