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Lattice distortion in the one-dimensional double and super-exchange model

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Abstract

The effect of the interplay between magnetism and lattice distortion within an exchange model is studied in low-dimensional systems. An important magnetoelastic effect that leads to a lattice contraction is presented. The model is discussed in connection with the contraction of the rungs experimentally observed within the three-leg ladders present in the oxyborate $Fe_3O_2BO_3$.

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In 1950, Jonker and Van Santen proposed an empirical correlation between ferromagnetism and electrical conduction in certain compounds of manganese with perovskite structure [1]. This interplay between magnetism and electronic motion was interpreted by Zener as an indirect spin coupling of incomplete *d*-shells via the conducting electrons, the so-called double exchange (DE) process [2]. The origin of the DE mechanism lies in the intra-atomic Hund's spin coupling J_H of localized electrons with itinerant electrons. It is the source of a variety of magnetic behavior in transition metal and rare-earth compounds. Typically the coupling is ferromagnetic ($J_H > 0$), but it can be antiferromagnetic in more than half-filled shells [3]. This ferromagnetic tendency is expected to be thwarted by antiferromagnetic super-exchange (SE) interactions between localized spins $\vec{S}_i$. This was first discussed by de Gennes [4] who conjectured the existence of canted states. Recently, it has been shown that three-leg ladders (3LL) in the oxyborate system Fe_3BO_5 may provide evidence for the existence of spin and charge ordering resulting from such a competition [5]. The former Fe-oxyborate known as Fe-ludwigite contains subunits in the form of 3LL of Fe cations. It presents an interesting structural and charge ordering transition at $T_c \approx 283\,K$ such that long and short bonds on the rungs alternate along the ladder axis [6]. As evidenced by Mössbauer studies [7,8] and X-ray diffraction [9] each rung can be viewed as three Fe^{3+} ions (*triad*) with high-spin $S = \frac{5}{2}$ of local spins sharing an extra itinerant electron. Additional X-ray diffraction studies have shown an important contraction of the triads [10]. A DE + SE exchange model with lattice distortion in one dimension is introduced by using the following Hamiltonian:

$$H = -t\sum_i (1+\delta_i)\cos\left(\frac{\theta_i}{2}\right)(c_i^+ c_{i+1} + \text{h.c.}) + JS^2\sum_i \cos(\theta_i) + B\sum_i \delta_i^2 + V\left(\sum_i \delta_i\right)^2, \quad (1)$$

where c_i^+ (c_i) are the fermions creation (annihilation) operators of the conduction electrons at site i and t is the hopping parameter. To obtain the former model, the following strong coupling limit $J_H \to -\infty$ was used (a necessary limit) because of the half-filled shells in the Fe-ludwigite. Due to the high-spin configuration $S = \frac{5}{2}$ of local spins in the 3LL Fe-ludwigite, classical localized spins $\vec{S}_i \to \infty$ were used in this work. θ_i is the relative angle between the classical localized spins at sites i and $i+1$. J is the SE interaction energy. The effect of lattice distortion is considered by using classical springs to join the localized atoms. The spring forces are assumed to be linear

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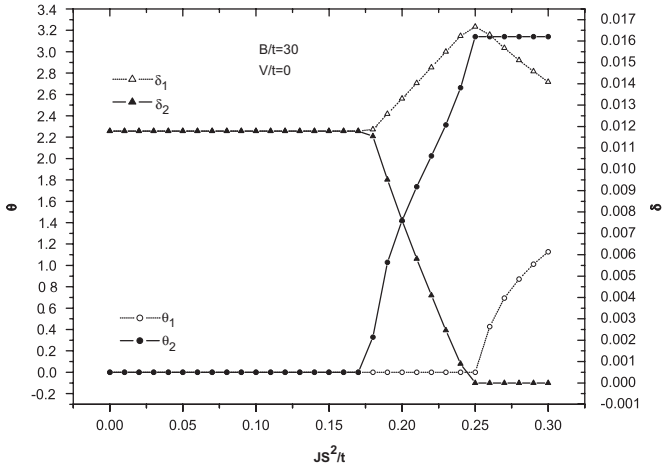

Fig. 1. Phase diagram as a function of the SE energy JS^2/t, for typical values of the elastic energy $B/t = 30$ and $V/t = 0$. The lines in this diagram represent a guide for the eyes.

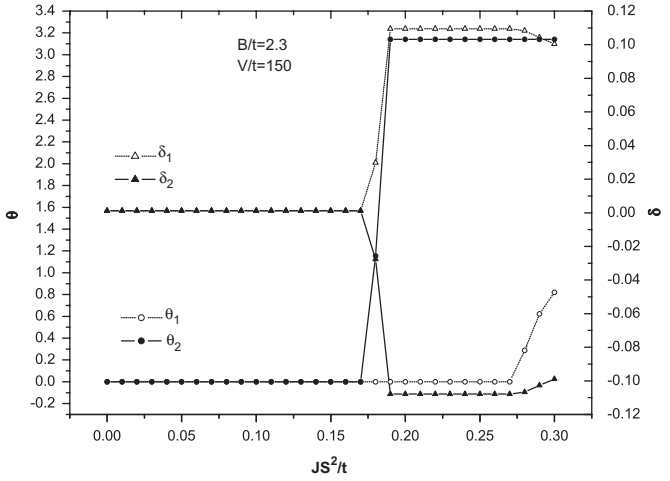

Fig. 2. The same as in Fig. 1 but in this case $B/t = 2.3$ and $V/t = 150$.

(small displacements, Hooke's law). Being δ the spring displacement because of lattice distortion. An elastic energy B is introduced and an additional spring energy V is considered to avoid a large displacement of the final atom.

Itinerant electrons in the 3LL in the Fe-ludwigite are found basically in the triads, therefore, in a first approximation a three sites one-dimensional model will be used. An analytical minimization was considered in two angles θ_1 and θ_2 and two spring displacements δ_1 and δ_2. The results of this model are summarized in Figs. 1 and 2 showing the phase diagram for two typical values of the elastic energy B and V. For low SE interaction energy $JS^2/t \lesssim 0.17$, Figs. 1 and 2 show a ferromagnetic arrangement of local spins $\theta_1 = \theta_2 = 0$. This magnetic phase has been observed experimentally in the triads at 82 K [9] and for symmetry reasons $\delta_1 \cong \delta_2$. Lattice contraction is given by $\delta_1 + \delta_2 \neq 0$ as shown in Figs. 1 and 2. This contraction is obtained because of an important magnetoelastic effect given by the interplay between magnetic interactions and lattice distortion. At low temperature (15 K), X-ray diffraction studies propose $\delta_2 \sim -\delta_1$ and $\delta_1 + \delta_2 \neq 0$ [10]. The X-ray studies are more easily obtained in this work in a $\theta_1 \neq \theta_2$ magnetic phase as shown in Fig. 2 for $JS^2/t > 0.17$. In Fig. 2 for $JS^2/t = 0.18$, two angles were found ($\theta_1 = 0$ and $\theta_2 = 1.15477$), that are in agreement with a magnetic phase observed experimentally in the triads at 10 K [9]. For the same value of JS^2/t a qualitative distortion ($\delta_2 \sim -\delta_1$ and $\delta_1 + \delta_2 \neq 0$) was found in a good agreement with X-ray diffraction studies [10].

In conclusion, an important magnetoelastic effect was found in this work due to the interplay between magnetic interactions in an exchange model and lattice distortion. Magnetic phases and lattice contraction were also obtained in a good qualitative agreement with neutron [9] and X-ray [10] studies, respectively.

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