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To cite this version:
F. Sapiña, E. Coronado, M. Drillon, Robert Georges, D. Beltrán. ALTERNATING EX-
CHANGE IN FERRIMAGNETIC ISING CHAINS. Journal de Physique Colloques, 1988, 49
(C8), pp.C8-1423-C8-1424. <10.1051/jphyscol:19888654>. <jpa-00228884>

HAL Id: jpa-00228884
https://hal.archives-ouvertes.fr/jpa-00228884
Submitted on 1 Jan 1988

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ALTERNATING EXCHANGE IN FERRIMAGNETIC ISING CHAINS

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Abstract. - We propose a general treatment for solving J-alternating ferrimagnetic Ising chains, made up of two spin sublattices (s, S). Exact expressions of the susceptibility are derived for s = 1/2 spins alternating with arbitrary S quantum spins, including a local anisotropy on the second sublattice, D_b. The magnetic properties of the ordered bimetallic chain MnCo (EDTA), 6H2O is discussed on the basis of the developed model.

Stimulated by the discovery of new quasi-one dimensional compounds MM' (EDTA), 6H2O-in short (MM'), the structure of which may be viewed as ordered bimetallic chains with alternating M – M' distances, M – M' – M – M' [1], we have focused for a time on the general behavior of ferrimagnetic chains with Heisenberg or Ising exchange couplings [2-5]. So far, all the models developed have assumed uniform chains, ignoring the alternation of the exchange parameter, J.

We present here a general treatment for solving J-alternating ferrimagnetic Ising chains, made up of two spin sublattices (s – S). Exact expressions of the thermodynamic quantities of interest can be derived for s = 1/2 spins alternating with arbitrary S quantum spins, including local anisotropies.

Theoretical treatment of the J-alternating ferrimagnetic Ising chains (1/2–S)

The full hamiltonian is written as

\[ H = -J \sum_i \hat{S}_{2i-1}^z \hat{S}_{2i}^z - J' \sum_i \hat{S}_{2i}^z \hat{S}_{2i+1}^z - \left( g_a \sum_i \hat{S}_{2i}^z + g_b \sum_i \hat{S}_{2i}^z - D_b \sum_i \left( \hat{S}_{2i}^z - \hat{S}_{2i}^z \right) \right) \mu_B H \]

where the current spin operator \( S_b \) takes the values \( S_a = 1/2 \) and \( S_b = S \) for odd and even sites, respectively, \( g_a \) and \( g_b \) are the corresponding Landé factors, and \( D_b \) is the zero field splitting on site b.

A similar procedure to that reported for other ferrimagnetic chains [5, 6] allows us to deduce the transfer matrix:

\[ T = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \]

\[ A = r^{1/2} \sum_j K(j^2 - S^2)(2 - \delta j_0) \cosh [\beta j J_{m+}] \]

\[ B = r^{1/2} \sum_j K(j^2 - S^2)(2 - \delta j_0) \cosh [\beta j J_{m-}] \]

\[ C = r^{-1/2} \sum_j K(j^2 - S^2)(2 - \delta j_0) \cosh [\beta j J_{m-}] \]

\[ D = r^{-1/2} \sum_j K(j^2 - S^2)(2 - \delta j_0) \cosh [\beta j J_{p-}] \]

where \( r = \exp (g_a \mu_B H \beta) \), \( s = \exp (g_b \mu_B H \beta) \), \( K = \exp (D_b \beta) \), \( \beta = 1 / kT \)

\[ J_p = (J + J') / 2 \]

\[ J_m = (J - J') / 2 \]

\[ J_{p \pm} = J_p \pm g_b \mu_B H \]

\[ J_{m \pm} = J_m \pm g_b \mu_B H \]

The summations are extended over \( j = 0 (1/2) \) to \( S \), for \( S \) integer (semi-integer).

Taking into account that the partition function per pair of sites corresponds to the largest eigenvalue of \( T \), we obtain the following expression for the zero-field parallel susceptibility:

\[ X_p = N / \beta \left[ S_0'' + (S_0^2 - 4P_0')^{1/2} \right] / \left[ S_0 + (S_0^2 - 4P_0)^{1/2} \right] \]

where \( S_0 \) and \( P_0 \) are the values at zero field of the trace and determinant of \( T \), respectively.

Using this expression we have calculated the magnetic behavior of the \( (1/2 - 5/2) \) Ising system for the two limiting cases, namely the regular chain \( (J = J') \) and dimer unit (solid lines of Fig. 1). In this figure, \( X_n \) represents the normalized susceptibility per spin pair defined as

\[ (10X_m) / ((N \mu_B^2 / k)(3/4g_a^2 + S(S + 1)g_b^2)) \]

These results can be compared with those obtained for J-alternating Heisenberg chains made up of \( s = 1/2 \) spins alternating with classical spins [7]. We observe that in the regular chain limit both models give a similar variation of the \( X_nT \) product with a close coincidence in the height of the minimum and in the divergence at lower temperatures. On the contrary, the
Fig. 1. - Theoretical variation of the normalized magnetic susceptibility of a (1/2-5/2) Ising chain in the limiting cases $J = J'$ (A) and $J' = 0$ (B). Dashed lines correspond to the calculated behaviors from the (1/2-classical) Heisenberg model.

Fig. 2. - Magnetic behavior of the bimetallic chain (MnCo). Solid line corresponds to the best fit from the $J$-alternating Ising model. Comparison to uniform chain (---) and dimer (-----) limits are also given.

curve of the Ising dimer is significantly above that of the Heisenberg dimer and further exhibits a narrow minimum around $kT / |J| = 1$.

This drastic difference may come from the fact that we are comparing an average susceptibility (in the Heisenberg case) with the parallel component of $X$ (in the Ising case), thus neglecting the perpendicular contribution, which decreases toward zero upon cooling down. This assumption, that is justifiable in the chain limit owing to the divergence of $X_{\perp}$, is no longer valid in the dimer limit. Thus, the value of $X_{n}T$ at absolute zero (4.2) is divided by one third when $X_{\perp}$ is taken into account and hence, the difference with the corresponding Heisenberg value (2.1) is reduced.

The above remarks allow us to emphasize that, except near the dimer limit, the magnetic susceptibility of this kind of systems is little sensitive to the symmetry of the exchange Hamiltonian.

The MnCo(EDTA).6H2O ferrimagnetic chain

Its structure consists of infinite zigzag chains involving two alternating octahedral sites selectively occupied by Mn(II) and Co(II) ions. Co(II) can be described at low temperatures by a very anisotropic Kramers doublet ($g_{\parallel} = 9, g_{\perp} = 1.3$) with an effective spin 1/2 and hence, the anisotropic Ising model is expected to describe conveniently the magnetic properties.

Accordingly, the low temperature data are reported in figure 2, along with the best fitted curves. A very close agreement with experiment has been obtained for $J = -2.7$ and $J' = -0.6$ K (solid line), which indicates a significant $J$-alternation. In order to test the validity of this result we have fit the data to a regular chain ($J = J' = -1.6$ K) and a dimer ($J = -3.4$ K; $J' = 0$) model. We observe that the uniform chain behavior gives a close agreement for temperatures around and below the minimum, but is less satisfactory at higher temperatures. Conversely, the dimeric behavior well reproduces the decrease of $X_{n}T$ upon cooling down and the position of the minimum, but does not allow to explain the sharp divergence at lower temperature.

Acknowledgments

This work was supported by the European Economic Community (grant ST2/164), and The Comision Interministerial en Ciencia y Tecnología (grant PB85-0106-CO2-02).