

# The effects of transverse field on the magnetic properties in a diluted mixed spin-2 and spin-5/2 Ising system

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## Abstract

The magnetic properties of a diluted mixed spin-2 and spin-5/2 ferrimagnetic Ising system are investigated on the basis of the effective-field theory with correlation. The influences of transverse fields and concentrations of magnetic atoms on the magnetic properties are examined numerically. © 2000 Elsevier Science B.V. All rights reserved.

*Keywords:* Ferrimagnetism; Ising model; Molecular magnetism

A number of experimental studies have accumulated recently in the area of molecular-based magnetic materials, and the magnetic properties, namely molecular magnetism, have become an important focus of scientific interest [1]. Theoretically, the systems can be rather well described by a mixed spin (Ising or Heisenberg) model. In recent work [2], we have proposed that the mixed spin-2 and spin-5/2 ferrimagnetic Ising system on honeycomb lattice can explain the characteristic temperature dependence of magnetization observed at low temperatures in the molecular-based magnetic material,  $N(n-C_4H_9)_4Fe^{II}Fe^{III}(C_2O_4)_3$  [3].

The aim of this work is to report some characteristic effects of a transverse field and concentrations of magnetic atoms on the magnetic properties in the diluted mixed spin-2 and spin-5/2 ferrimagnetic Ising system on honeycomb lattice, using the effective-field theory with correlations (EFT) [2,4]. As far as we know, only a few studies have dealt with the effects of a transverse field on molecular magnetism [2,5].

The Hamiltonian of the system is given by

$$H = J \sum_{\langle ij \rangle} S_{iA}^x S_{jB}^x \zeta_{iA} \zeta_{jB} - \Omega_A \sum_i S_{iA}^x \zeta_{iA} - \Omega_B \sum_j S_{jB}^x \zeta_{jB}, \quad (1)$$

where  $J (> 0)$  is the exchange interaction,  $S_{iA}^\alpha$  ( $\alpha = x$  or  $z$ ) is the spin-5/2 operator and  $S_{jB}^z$  is the spin-2 operator. The first summation is over all nearest-neighbor pairs of atoms.  $\zeta_{iA}$  (or  $\zeta_{jB}$ ) is a random variable which takes the value 1 with a probability  $p_A$  (or  $p_B$ ) or 0 with a probability  $1 - p_A$  (or  $1 - p_B$ ), depending on whether the site  $i$  (or  $j$ ) is occupied by a magnetic atom or not.  $\Omega_A$  and  $\Omega_B$  are the transverse fields on the  $A$  and  $B$  sublattices.

We are here interested in studying the phase diagram and the thermal variation of the total longitudinal magnetization in the system, since there is an order with a finite total transverse magnetization at all temperatures. The total longitudinal magnetization  $M_z$  of the system is

$$M_z = \frac{1}{2}(p_A m_A^z + p_B m_B^z) \quad (2)$$

with

$$m_A^z = \frac{\langle \langle \zeta_{iA} S_{iA}^z \rangle \rangle_r}{\langle \zeta_{iA} \rangle_r} \quad \text{and} \quad m_B^z = \frac{\langle \langle \zeta_{jB} S_{jB}^z \rangle \rangle_r}{\langle \zeta_{jB} \rangle_r}, \quad (3)$$

where  $\langle \dots \rangle$  and  $\langle \dots \rangle_r$  denote the thermal and random averages. Within the EFT, the magnetizations and the transition temperature  $T_C$  can be easily obtained by the use of the formulation in Refs. [2,4]. The compensation temperature  $T_\kappa$ , if it exists in the system, can be determined from the relation  $M_z = 0$ .

Fig. 1(A) shows a typical phase diagram of the system with  $\Omega_A = \Omega_B = \Omega = 0.0$  in the  $(k_B T/J, p_A)$  plane, when the concentration  $p_B$  is changed from  $p_B = 1.0$  to 0.3. The  $T_C$  curves exhibit the characteristic behavior expected for

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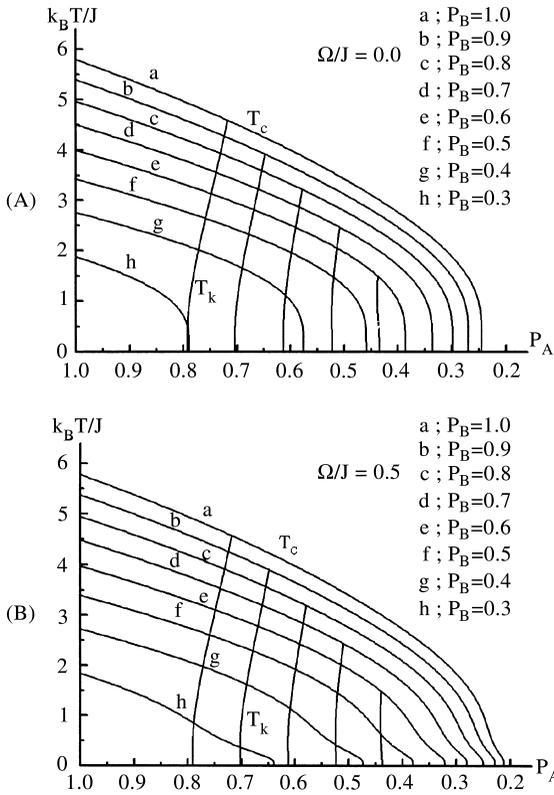


Fig. 1. Phase diagram in the  $(k_B T/J, p_A)$  plane with transverse field  $\Omega/J = 0.0$  (A) and  $\Omega/J = 0.5$ . (B)

diluted magnetic systems. But  $T_k$  could not be obtained when  $p_B$  is lower than  $p_B = 0.6$ . Fig. 1(B) shows how the phase diagram is modified, when a finite transverse field ( $\Omega/J = 0.5$ ) is applied.

Fig. 2 shows the temperature dependencies of  $M_z$  in the system with  $p_A = 0.6$  and  $p_B = 0.8$ , when the

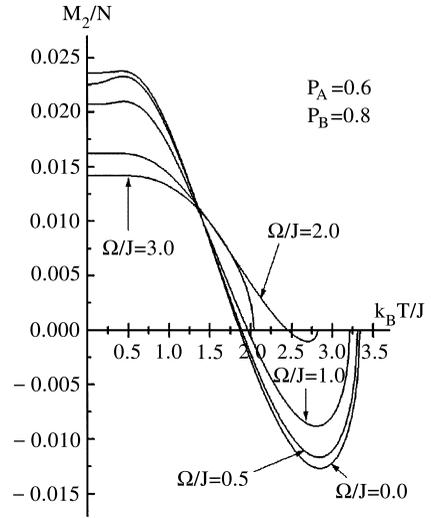


Fig. 2. The temperature dependencies of  $M_z$  in the system with  $p_A = 0.6$  and  $p_B = 0.8$ .

transverse field is changed from  $\Omega/J = 0.0$  to 3.0. The compensation point can be observed for relatively small transverse fields.

**References**

- [1] O. Kahn, in: E. Coronado, et al., (Eds.), *Molecular Magnetism: From Molecular Assemblies to the Devices*, Kluwer Academic Publishers, Dordrecht, 1996.
- [2] T. Kaneyoshi, Y. Nakamura, S. Shin, *J. Phys.: Condens. Matter* 10 (1998) 7025.
- [3] C. Mathoniere, C.J. Nuttall, S.G. Carling, P. Day, *Inorg. Chem.* 35 (1996) 1201.
- [4] T. Kaneyoshi, M. Jascur, I.P. Fittipaldi, *Phys. Rev. B* 48 (1993) 250.
- [5] M. Jascur, A. Bobak, *J. Magn. Magn. Mater.* 161 (1996) 148.