The magnetic properties of a ferromagnetic or ferrimagnetic mixed spin-1/2 and spin-3/2 Ising system

1993 J. Phys.: Condens. Matter 5 5331

(http://iopscience.iop.org/0953-8984/5/30/013)

J. Phys.: Condens. Matter 5 (1993) 5331–5342. Printed in the UK

The magnetic properties of a ferromagnetic or ferrimagnetic mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising system

T Kaneyoshi†, M Jaščur†§ and P Tomczak‡

† Department of Physics, Nagoya University, 464-01 Nagoya, Japan
‡ Ferromagnetic Laboratory, Institute of Molecular Physics, 60-179 Poznan, Poland

Received 9 March 1993

Abstract. The magnetic properties of a ferromagnetic or ferrimagnetic mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising system are studied by the use of the effective-field theory. The general expressions for evaluating these properties are given. In particular, the internal energy, specific heat and susceptibility of the system with the honeycomb lattice are numerically examined. Some characteristic phenomena are found in these properties.

1. Introduction

In recent years, the study of the Ising model with mixed spins of different magnitudes has attracted considerable attention. The mixed-spin Ising model has less translational symmetry than the single-spin counterparts and was originally a simple system showing a certain type of ferrimagnetism because of the complexity of the structures in real ferrimagnets. In particular, most research attention has been directed to the two-sublattice mixed-spin system consisting of spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ with a crystal-field interaction. It has been investigated by a variety of techniques, such as exact [1, 2] and approximate [3–7] methods and the high-temperature series expansion method [8]. An important point in studying the mixed-spin model including spin-1 ions is that the tricritical behaviour is predicted in the system with a coordination number Z larger than $Z = 3$ [6]. On the other hand, the mixed-spin Ising model consisting of spin-$\frac{1}{2}$ and spin-S ($S > 1$) ions has not been examined so much except for the phase diagrams of a honeycomb lattice [2]. Furthermore, as discussed in [9], the magnetic properties of the system with $S = \frac{3}{2}$ are expected to be different from those of the system with $S = 1$.

The purpose of this work is to study the magnetic properties of a mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ ferromagnetic or ferrimagnetic Ising system with a crystal-field interaction on the basis of the new formulation [10] which is superior to the standard mean-field theory. The outline of this work is as follows. In section 2, we briefly present the basic framework of the theory. In section 3, the general expressions for evaluating the magnetic properties of the system are given on the basis of the framework. The numerical results for the internal energy, specific heat and susceptibility of the system with a honeycomb lattice are obtained in section 4. We have found some characteristic phenomena in these properties.

§ Permanent address: Department of Theoretical Physics and Geophysics, Faculty of Natural Sciences, P J Safarik University, Moyzesova 16, 04154 Kosice, Slovakia.

2. Formulation

We consider a mixed-spin ferromagnetic or ferrimagnetic Ising system consisting of spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ with a crystal-field constant D. The Hamiltonian of the system is

$$H = \mp J \sum_{im} \mu_i^Z S_m^Z - D \sum_m (S_m^Z)^2 \tag{1}$$

where S_m^Z takes the values $\pm\frac{3}{2}$ and $\pm\frac{1}{2}$, μ_i^Z can be $+\frac{1}{2}$ or $-\frac{1}{2}$, and the first summation is carried out only over nearest-neighbour pairs of spins. Here, $J > 0$ and hence the minus sign and plus sign of the first term denote the ferromagnetic or ferrimagnetic interaction, respectively.

As discussed in [9, 10], for the evaluation of the mean values $\langle\mu_i^Z\rangle$ and $\langle S_m^Z\rangle$ we can use the exact Ising spin identities and the differential operator technique. Within the framework of the effective-field theory, the magnetizations per site are given by

$$\sigma = \langle\mu_i^Z\rangle = [A(J\nabla) \pm B(J\nabla)m + C(J\nabla)q \pm D(J\nabla)r]^Z f(x)|_{x=0} \tag{2}$$

and

$$m = \langle S_m^Z\rangle = [\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}J\nabla)]^Z F(x)|_{x=0} \tag{3}$$

where $\nabla = \partial/\partial x$ is a differential operator and Z is the coordination number. The functions $f(x)$ and $F(x)$ are defined by

$$f(x) = \tfrac{1}{2}\tanh(\tfrac{1}{2}\beta x)$$

and

$$F(x) = \tfrac{1}{2}[3\sinh(\tfrac{3}{2}\beta x) + \exp(-2D\beta)\sinh(\tfrac{1}{2}\beta x)]/[\cosh(\tfrac{3}{2}\beta x) + \exp(-2D\beta)\cosh(\tfrac{1}{2}\beta x)] \tag{4}$$

where $\beta = 1/k_B T$.

Here, in order to derive the sublattice magnetizations, we have used the exact Ising spin identities as well as the exact van der Waerden identities for spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$. To treat the multispin correlation functions, the decoupling approximation has then been introduced:

$$\langle\mu_j^Z S_m^Z (S_n^Z)^2 \ldots \mu_k^Z\rangle \simeq \langle\mu_j^Z\rangle\langle S_m^Z\rangle\langle(S_n^Z)^2\rangle \ldots \langle\mu_k^Z\rangle \tag{5}$$

for $j \neq m \neq n \neq \ldots \neq k$. As discussed in [10], the statistical accuracy of (5) corresponds to the Zernike [11] approximation of the spin-$\frac{1}{2}$ Ising model for the special case when $D/J = -\infty$. By the use of the exact van der Waerden identity for $S = \frac{3}{2}$, the coefficients A, B, C and D in (2) are given by

$$\begin{aligned} A(J\nabla) &= \tfrac{1}{8}[9\cosh(\tfrac{1}{2}J\nabla) - \cosh(\tfrac{3}{2}J\nabla)] \\ B(J\nabla) &= \tfrac{1}{12}[27\sinh(\tfrac{1}{2}J\nabla) - \sinh(\tfrac{3}{2}J\nabla)] \\ C(J\nabla) &= \tfrac{1}{2}[\cosh(\tfrac{3}{2}J\nabla) - \cosh(\tfrac{1}{2}J\nabla)] \\ D(J\nabla) &= \tfrac{1}{3}[\sinh(\tfrac{3}{2}J\nabla) - 3\sinh(\tfrac{1}{2}J\nabla)]. \end{aligned} \tag{6}$$

The parameters q and r in (2) are defined by

$$q = \langle (S_m^Z)^2 \rangle \tag{7}$$

$$r = \langle (S_m^Z)^3 \rangle. \tag{8}$$

By using the same procedure as that of (3), the parameters q and r are given in the following forms:

$$q = [\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}J\nabla)]^Z G(x)|_{x=0} \tag{9}$$

and

$$r = [\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}J\nabla)]^Z H(x)|_{x=0} \tag{10}$$

where the functions $G(x)$ and $H(x)$ are defined by

$$G(x) = \frac{1}{4}\frac{9\cosh(\frac{3}{2}\beta x) + \exp(-2D\beta)\cosh(\frac{1}{2}\beta x)}{\cosh(\frac{3}{2}\beta x) + \exp(-2D\beta)\cosh(\frac{1}{2}\beta x)} \tag{11}$$

and

$$H(x) = \frac{1}{8}\frac{27\sinh(\frac{3}{2}\beta x) + \exp(-2D\beta)\sinh(\frac{1}{2}\beta x)}{\cosh(\frac{3}{2}\beta x) + \exp(-2D\beta)\cosh(\frac{1}{2}\beta x)}. \tag{12}$$

Here, note that the minus sign and plus sign in (2), (3), (9) and (10) correspond to the ferromagnetic and ferrimagnetic interactions, respectively, in (1). Thus, we have a complete set of equations for studying the magnetic properties of the system. As one can see, in our treatment two new order parameters q and r naturally appear which one is able to evaluate. This is not the case of the standard mean-field theory where all correlations are neglected. It is one reason why the present framework provides better results than the standard mean-field theory.

On the other hand, the total magnetization M of the system is

$$M = \tfrac{1}{2}N(m + \sigma) \tag{13}$$

where N is the number of magnetic atoms.

3. Magnetic properties

In this section, we study the magnetic properties of the mixed-spin Ising system on the basis of the formulation in section 2.

3.1. Phase diagram

Let us first examine the phase diagram. When the temperature is higher than the transition temperature, the whole system is demagnetized. The transition temperature of the mixed-spin system can be obtained by requiring that the sublattice magnetizations m and σ and the parameter r tend to zero continuously as the temperature approaches a critical temperature, since in the present system there is no tricritical behaviour [10]. Consequently, from the coupled equations (2), (3), (9) and (10) the following linearized equations can be derived:

$$\sigma = \pm K_1 m \pm K_2 r \qquad m = \pm 2R_1\sigma \qquad r = \pm 2L_1\sigma \tag{14}$$

with

$$\begin{aligned} K_1 &= ZB(J\nabla)[A(J\nabla) + C(J\nabla)q_0]^{Z-1} f(x)|_{x=0} \\ K_2 &= ZD(J\nabla)[A(J\nabla) + C(J\nabla)q_0]^{Z-1} f(x)|_{x=0} \\ R_1 &= Z\sinh(\tfrac{1}{2}J\nabla)\cosh^{Z-1}(\tfrac{1}{2}J\nabla)\,F(x)|_{x=0} \\ L_1 &= Z\sinh(\tfrac{1}{2}J\nabla)\cosh^{Z-1}(\tfrac{1}{2}J\nabla)\,H(x)|_{x=0} \end{aligned} \tag{15}$$

where the parameter q_0 in (15) is given by

$$q_0 = \cosh^Z(\tfrac{1}{2}J\nabla)\,G(x)|_{x=0}. \tag{16}$$

These coefficients (K_1, K_2, R_1 and L_1) and q_0 for a fixed value of Z can be calculated by using a mathematical relation $\exp(a\nabla)\,\psi(x) = \psi(x+a)$. Then, the phase diagram (or transition temperature) can be determined by solving the relation

$$1 = 2K_1R_1 + 2K_2L_1. \tag{17}$$

Here, note that the transition temperature determined from (17) is independent of the $\pm$ sign in (14); the relation is valid for both (ferromagnetic and ferrimagnetic) cases. In [9], the results (or phase diagram) for $Z = 3$, 4 and 6 were obtained (see figure 1) as a function of D/J. In the figure, the exact solution for the honeycomb lattice [2] was also depicted for comparison. It indicates that our fomulation gives reasonable results.

3.2. Internal energy and specific heat

The internal energy U of the mixed-spin system is given by

$$2U/N = -\tfrac{1}{2}\langle \mu_i^Z E_i^Z\rangle - \tfrac{1}{2}\langle S_m^Z E_m^Z\rangle - \tfrac{1}{2}Dq \tag{18}$$

with

$$E_i^Z = \pm J\sum_\delta S_{i+\delta} \qquad E_m^Z = \pm J\sum_\delta \mu_{m+\delta} \tag{19}$$

where the summations in (19) are over the nearest neighbours of a site i (or a site m). Then the specific heat C of the system can be determined from the relation

$$C = \partial U/\partial T. \tag{20}$$

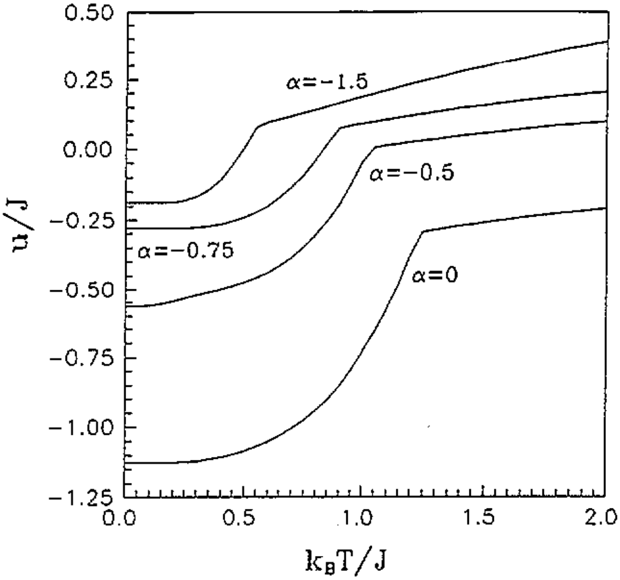

Figure 1. The internal energy U versus temperature T for the mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising system with the honeycomb lattice, when the value of α ($\alpha = D/J$) is fixed at some typical values.

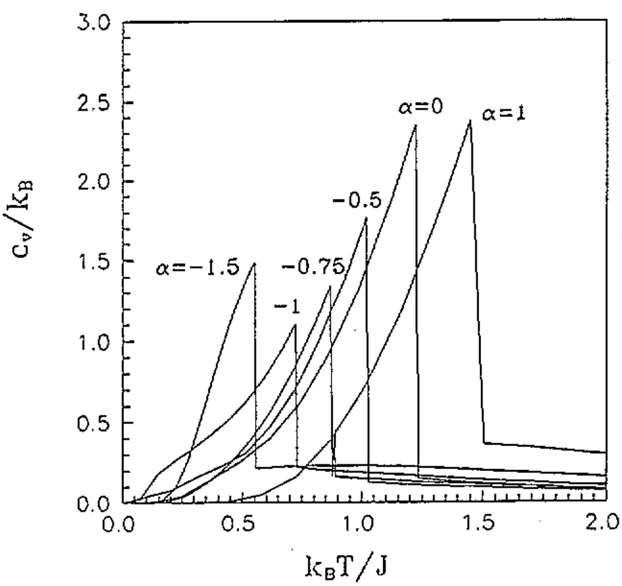

Figure 2. The specific heat C versus temperature T for the mixed-spin system with $Z = 3$, when the value of α is changed.

For the evaluation of $\langle \mu_i^Z E_i^Z \rangle$ in (18), the exact Ising spin identity can also be applied:

$$\langle \mu_i^Z E_i^Z \rangle = \langle E_i^Z \exp(E_i^Z \nabla) \rangle f(x)|_{x=0} = \{(\partial/\partial y)\langle \exp(E_i^Z y) \rangle\}_{y=\nabla} f(x)|_{x=0}. \tag{21}$$

The expectation value $\langle \exp(E_i^Z y) \rangle$ in (21) can be evaluated in the same way as that of m

by using the exact van der Waerden identity for $S = \frac{3}{2}$ and the decoupling approximation (5). It is given by

$$\langle \exp(E_i^Z y)\rangle = [A(yJ) \pm B(yJ)m + C(yJ)q \pm D(yJ)r]^Z \tag{22}$$

from which the expectation value $\langle \mu_i^Z E_i^Z \rangle$ is obtained as

$$\begin{aligned}\langle \mu_i^Z E_i^Z \rangle = \tfrac{1}{2} JZ[-\tfrac{9}{8}D(J\nabla) \pm 2A(J\nabla)m + E(J\nabla)q \pm 2C(J\nabla)r]\\ \times [A(J\nabla) \pm B(J\nabla)m + C(J\nabla)q \pm D(J\nabla)r]^{Z-1} f(x)|_{x=0}\end{aligned} \tag{23}$$

with

$$E(J\nabla) = \tfrac{1}{2}[3\sinh(\tfrac{3}{2}J\nabla) - \sinh(\tfrac{1}{2}J\nabla)]. \tag{24}$$

On the other hand, the contribution from $\langle S_m^Z E_m^Z \rangle$ in (18) can be easily calculated in the same way as that of $\langle \mu_i^Z E_i^Z \rangle$:

$$\langle S_m^Z E_m^Z \rangle = \tfrac{1}{2} JZ[\sinh(\tfrac{1}{2}J\nabla) \pm 2\sigma \cosh(\tfrac{1}{2}J\nabla)][\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}J\nabla)]^{Z-1} F(x)|_{x=0}. \tag{25}$$

Thus, the internal energy and the specific heat can be determined from (18) and (20).

3.3. Susceptibility

The initial susceptibility of the mixed-spin system is also an important physical property which can be measured experimentally. In order to obtain the expression, we must include the applied field term in the Hamiltonian (1):

$$H = \mp J \sum_{im} \mu_i^Z S_m^Z - D\sum_m (S_m^Z)^2 - H\left(\sum_i \mu_i^Z + \sum_m S_m^Z\right) \tag{26}$$

where H is the applied magnetic field.

For $H \neq 0.0$, equations for σ, m, q and r have the same forms as those for $H = 0.0$, except that the functions $f(x)$, $F(x)$, $G(x)$ and $H(x)$ in (2), (3), (9) and (10) must be replaced by $f(x+H)$, $F(x+H)$, $G(x+H)$ and $H(x+H)$, respectively. The initial susceptibility χ is defined by

$$\chi = \lim_{H\to 0}(\partial M/\partial H) = (\partial M/\partial H)_0 = \tfrac{1}{2}N[(\partial m/\partial H)_0 + (\partial \sigma/\partial H)_0]. \tag{27}$$

By differentiating σ, m, q and r with respect to H, one obtains

$$\begin{aligned}(\partial\sigma/\partial H)_0 &= \beta\Delta_1 \pm \Gamma_1(\partial m/\partial H)_0 + \Gamma_2(\partial q/\partial H)_0 \pm \Gamma_3(\partial r/\partial H)_0\\ (\partial m/\partial H)_0 &= \beta\Delta_2 \pm 2\Gamma_4(\partial\sigma/\partial H)_0\\ (\partial q/\partial H)_0 &= \beta\Delta_3 \pm 2\Gamma_5(\partial\sigma/\partial H)_0\\ (\partial r/\partial H)_0 &= \beta\Delta_4 \pm 2\Gamma_6(\partial\sigma/\partial H)_0\end{aligned} \tag{28}$$

where the coefficients Δ_i ($i = 1$–4) and Γ_i ($i = 1$–6) are defined in appendix 1. From these relations, the initial susceptibility χ is given by

$$\chi = \tfrac{1}{2}N\beta\Delta/\Gamma \tag{29}$$

with

$$\Delta = \Delta_2[1 - 2(\Gamma_1\Gamma_4 + \Gamma_2\Gamma_5 + \Gamma_3\Gamma_6)] + (1 \pm 2\Gamma_4)(\Delta_1 \pm \Gamma_1\Delta_2 + \Gamma_2\Delta_3 \pm \Gamma_3\Delta_4) \tag{30}$$

and

$$\Gamma = 1 - 2(\Gamma_1\Gamma_4 + \Gamma_2\Gamma_5 + \Gamma_3\Gamma_6). \tag{31}$$

In particular, in the temperature region above the transition temperature determined from (17), the coefficients Γ_i (i = 1–6) are given; putting $m = \sigma = 0$ and $q = q_0$ into these gives

$$\Gamma_2 = \Gamma_5 = 0 \qquad \Gamma_1 = K_1 \qquad \Gamma_2 = K_2 \qquad \Gamma_4 = R_1 \qquad \Gamma_6 = L_1. \tag{32}$$

The inverse paramagnetic susceptibility χ_{para}^{-1} is then given by

$$\chi_{\text{para}}^{-1} = (2k_BT/N)\{[1 - (K_1R_1 + K_2L_1)]/\Delta_0\} \tag{33}$$

with

$$\Delta_0 = \Delta_2^0[1 - 2(K_1R_1 + K_2L_1)] + (1 \pm 2R_1)(\Delta_1^0 \pm K_1\Delta_2^0 \pm K_2\Delta_4^0) \tag{34}$$

where Δ_1^0, Δ_2^0 and Δ_4^0 are defined by

$$\begin{aligned} \Delta_1^0 &= [A(J\nabla) + C(J\nabla)q_0]^Z I(x)|_{x=0} \\ \Delta_2^0 &= \cosh^Z(\tfrac{1}{2}J\nabla)O(x)|_{x=0} \\ \Delta_4^0 &= \cosh^Z(\tfrac{1}{2}J\nabla)R(x)|_{x=0}. \end{aligned} \tag{35}$$

Thus, the initial susceptibility and the paramagnetic susceptibility can be determined from (29) and (33).

4. Numerical results

In sections 2 and 3, we have derived the general expressions for evaluating the magnetic properties of the spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ mixed (ferromagnetic or ferrimagnetic) Ising system. In particular, in the previous work [9] we have demonstrated the temperature dependences of m, σ and M for the honeycomb lattice ($Z = 3$) by solving the coupled equations (2), (3), (9) and (10) numerically. As depicted in figure 2 of [9], they may exhibit some characteristics different from the corresponding mixed spin-$\frac{1}{2}$ and spin-1 system [12]. In this section, let us show some typical results of the internal energy, specific heat and initial susceptibility in the present system by solving the expressions in section 3 numerically for the case when $Z = 3$. Then, we have also used the numerical results for m and σ obtained in previous work [9].

4.1. Internal energy and specific heat

Figure 1 shows the thermal variations in the internal energy U when the parameter α defined by

$$\alpha = D/J \tag{36}$$

is changed. As discussed in [9], the parameter α has an important physical meaning for distinguishing the magnetization curve of m (or M). For the system with $\alpha < -0.75$ the saturation magnetization of m at $T = 0$ K is given by $m = \frac{1}{2}$, and for the system with $\alpha > -0.75$ it is given by $m = \frac{3}{2}$. On the other hand, the saturation magnetization of the system with $\alpha = -0.75$ is $m = 1.0$, which indicates that in the ground state the spin configuration of S_m^Z in the system consists of the mixed phase; the S_m^Z are randomly in the $S_m^Z = \pm\frac{3}{2}$ or $S_m^Z = \pm\frac{1}{2}$ state with equal probabilities. As is seen from figure 1, however, the internal energy does not express any characteristic feature depending on the value of α, although in detail a small change in curvature is seen in the curve for $\alpha = -0.5$ especially in the very-low-temperature region near $k_B T/J = 0.3$. Here, one should note that the internal energy obtained is independent of the $\pm$ sign in the Hamiltonian (1). The results are valid for both (ferromagnetic and ferrimagnetic) cases.

In figure 2, the thermal variations in specific heat in the system are plotted by changing the value of α. As is seen from the figure, for the system with a value of α near $\alpha = -0.75$ (the curves for $\alpha = -1.0$ and -0.5) the specific heat may show a characteristic behaviour in the very-low-temperature region in comparision with the results for other values of α which express a monotonic decrease to $C = 0.0$ at $T = 0$ K. The phenomenon is closely related to the anomalous behaviour of the magnetization curve m, as depicted in figure 2 of [9]. Here, our formulation is the effective-field theory, so that the specific heat exhibits a discontinuity at the transition temperature T_c. However, one should note that for $T > T_c$ the specific heat takes finite values. It also indicates that our formulation is superior to the standard mean-field theory.

4.2. Susceptibility

Let us now find the inverse susceptibility of the ferromagnetic or ferrimagnetic mixed-spin system by changing the value of α. Figures 3 and 4 correspond to the ferromagnetic and ferrimagnetic cases, respectively.

Figure 3 expresses the typical variations in χ^{-1} for the ferromagnetic system with $Z = 3$. As is seen from the figure, the inverse paramagnetic susceptibility satisfies the Curie–Weiss law except for the region near $T = T_c$ for the curve with $\alpha = -1.5$ in which a weak upward curvature is observed. On the other hand, the behaviour of χ^{-1} becomes dramatic in the region below T_c. When the value of α approaches the critical value $\alpha = -0.75$ where the ground state of S_m^Z may change from the $S_m^Z = \pm\frac{3}{2}$ (or $S_m^Z = \pm\frac{1}{2}$) state to the $S_m^Z = \pm\frac{1}{2}$ (or $S_m^Z = \pm\frac{3}{2}$) state, the outstanding features of χ^{-1} are obtained, as depicted for $\alpha = -0.6$ and -0.5. In particular, χ^{-1} for the system with $\alpha = -0.75$ may exhibit a broad maximum in the region $0 < T < T_c$ and then reduces to zero at $T = 0$ K. It is completely different from others which express the divergence of χ^{-1} at $T = 0$ K (or the normal behaviour in a ferromagnet). The anomalous result of $\alpha = -0.75$ which reduces to zero at $T = 0$ K arises only from the nature of the ground state where the spin configuration of S_m^Z is in the mixed phase, namely the $S_m^Z = \pm\frac{3}{2}$ or $S_m^Z = \pm\frac{1}{2}$ state with equal probabilities. Thus, the outstanding behaviour of χ^{-1} for the system with a value of α at or near $\alpha = -0.75$ results from the characteristic features of the magnetization curve m, as shown in figure 2 of [9].

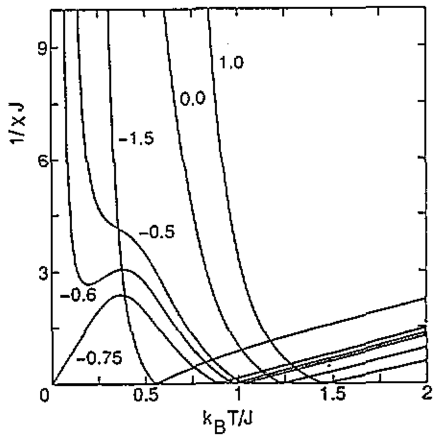

Figure 3. The inverse susceptibility χ^{-1} versus temperature for the ferromagnetic mixed-spin system with $Z = 3$, when the value of α is fixed at some typical values.

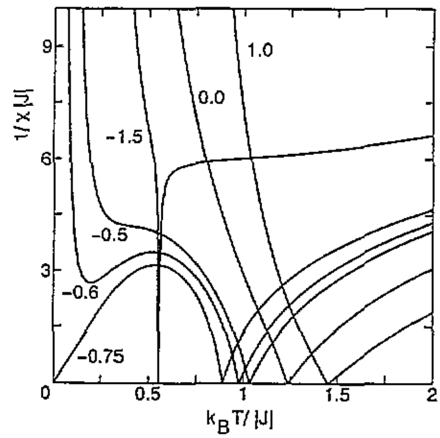

Figure 4. The inverse susceptibility χ^{-1} versus temperature for the ferrimagnetic mixed-spin system with $Z = 3$, when α is fixed at the same values as in figure 3.

In figure 4, the χ^{-1} values for the ferrimagnetic system are depicted by selecting the same values of α as those in figure 3. On comparison of figure 4 with figure 3, the behaviour of χ^{-1} for $T < T_c$ is very similar on the whole, although some differences in detail are observed. On the other hand, the inverse paramagnetic susceptibility in figure 4 clearly exhibits some features depending on whether the interaction is ferrimagnetic (or antiferromagnetic) and the value of α is larger (or smaller) than $\alpha = -0.75$. That is to say, firstly, when $\alpha > -0.75$, the spin state of S_m^Z at $T = 0$ K is in the $S_m^Z = \pm\frac{3}{2}$ state and hence χ_{para}^{-1} may show an upward curvature near $T = T_c$ which is characteristic for the ferrimagnetic systems. Secondly, for $\alpha < -0.75$, the spin state of S_m^Z at $T = 0$ K is in the $S_m^Z = \pm\frac{1}{2}$ state, so that the ground state of the mixed-spin system must be antiferromagnetic. As depicted for the system with $\alpha = -1.5$, χ_{para}^{-1} may express the characteristic of antiferromagnetism, although χ^{-1} may still reduce to zero at the transition temperature. However, as is discussed in appendix 2, for $\alpha \to -\infty$, χ_{para}^{-1} has a finite value at the transition temperature (or the Néel temperature), since only the $S_m^Z = \pm\frac{1}{2}$ state is then allowed energetically in the whole temperature region. Thus, the results in figure 4 express the outstanding features due to the crossing from the ferrimagnetic case to the antiferromagnetic case on decrease in α.

5. Conclusions

In this work, we have developed general expressions for evaluating the magnetic properties of the mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ ferromagnetic or ferrimagnetic Ising system on the basis of the new effective-field theory which includes the two order parameters q and r in addition to the magnetization. In fact, the parameters have to be taken into account when the theory is constructed beyond the standard mean-field theory. However, the expressions depend only on the coordination number Z and hence the critical properties at the transition temperature are essentially of the mean-field type, as shown in figure 2.

In section 4 as well as in the previous work [9], we have found the magnetic properties of the system with the honeycomb lattice ($Z = 3$) by solving the general expressions numerically. As depicted in previous work, our formulation gives reasonable results for the transition temperature in comparison with the exact results. Furthermore, the magnetization curves have exhibited some characteristics different from the corresponding mixed spin-$\frac{1}{2}$ and spin-1 system. As shown in figures 1–4, on the other hand, the specific heat and susceptibility of the present system have also exhibited a number of interesting behaviours. In particular, the susceptibility may express many anomalous behaviours for both (ferromagnetic and ferrimagnetic) cases, when the value of α is selected at or near the critical value $\alpha = -0.75$ where the ground state of S_m^Z changes from the $S_m^Z = \pm\frac{3}{2}$ (or $S_m^Z = \pm\frac{1}{2}$) state to the $S_m^Z = \pm\frac{1}{2}$ (or $S_m^Z = \pm\frac{3}{2}$) state. Moreover, the paramagnetic susceptibility of the ferrimagnetic system with the plus sign in (1) clearly exhibited a crossing from ferrimagnetic behaviour to antiferromagnetic behaviour on decrease in α. As far as we know, these findings have not been previously reported. These results may be helpful when the experimental data of a ferromagnetic or ferrimagnetic material are analysed.

Appendix 1

The coefficients Δ_i $(i = 1–4)$ and Γ_i $(i = 1–6)$ in (28) are given by

$$\begin{aligned}
\Delta_1 &= [A(a) \pm B(a)m + C(a)q \pm D(a)r]^Z I(x)|_{x=0} \\
\Delta_2 &= [\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}J\nabla)]^Z O(x)|_{x=0} \\
\Delta_3 &= [\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}J\nabla)]^Z Q(x)|_{x=0} \\
\Delta_4 &= [\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}J\nabla)]^Z R(x)|_{x=0}
\end{aligned} \tag{A1.1}$$

and

$$\begin{aligned}
\Gamma_1 &= ZB(a)[A(a) \pm B(a)m + C(a)q \pm D(a)r]^Z f(x)|_{x=0} \\
\Gamma_2 &= ZC(a)[A(a) \pm B(a)m + C(a)q \pm D(a)r]^Z f(x)|_{x=0} \\
\Gamma_3 &= ZD(a)[A(a) \pm B(a)m + C(a)q \pm D(a)r]^Z f(x)|_{x=0} \\
\Gamma_4 &= Z \sinh(\tfrac{1}{2}J\nabla)\,[\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}J\nabla)]^{Z-1} F(x)|_{x=0} \\
\Gamma_5 &= Z \sinh(\tfrac{1}{2}J\nabla)\,[\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}\nabla)]^{Z-1} G(x)|_{x=0} \\
\Gamma_6 &= Z \sinh(\tfrac{1}{2}J\nabla)\,[\cosh(\tfrac{1}{2}J\nabla) \pm 2\sigma \sinh(\tfrac{1}{2}J\nabla)]^{Z-1} H(x)|_{x=0}
\end{aligned} \tag{A1.2}$$

where $a = J\nabla$ and the functions $I(x)$, $O(x)$, $Q(x)$ and $R(x)$ are defined by

$$\begin{aligned}
\beta I(x) &= [(\partial/\partial H)f(x+H)]_{H=0} \\
\beta O(x) &= [(\partial/\partial H)F(x+H)]_{H=0} \\
\beta Q(x) &= [(\partial/\partial H)G(x+H)]_{H=0} \\
\beta R(x) &= [(\partial/\partial H)H(x+H)]_{H=0}.
\end{aligned} \tag{A1.3}$$

Appendix 2

We examine here the paramagnetic susceptibility analytically for the special case when $\alpha = -\infty$. For this case, the spin S_m^Z in the mixed-spin system is only allowable in the $S_m^Z = \pm\frac{1}{2}$ state energetically and hence the system looks like a standard ferromagnetic or antiferromagnetic spin-$\frac{1}{2}$ Ising model.

To prove this fact, let us at first note that for $\alpha = -\infty$ the functions $F(x)$, $G(x)$ and $H(x)$ are given by

$$\begin{aligned} F(x) &= \tfrac{1}{2}\tanh(\tfrac{1}{2}\beta x) = f(x) \\ G(x) &= \tfrac{1}{4} \\ H(x) &= \tfrac{1}{4}F(x) \end{aligned} \tag{A2.1}$$

from which

$$\begin{aligned} &q = q_0 = \tfrac{1}{4} \qquad r = \tfrac{1}{4}m \\ &A(J\nabla) + C(J\nabla)q_0 = \cosh(\tfrac{1}{2}J\nabla). \end{aligned} \tag{A2.2}$$

From these results, one can easily obtain the relations

$$L_1 = \tfrac{1}{4}R_1 \qquad K_1 + \tfrac{1}{4}K_2 = 2R_1 \tag{A2.3}$$

so that equation (17) reduces to

$$1 = (2R_1)^2 \tag{A2.4}$$

or

$$Z\sinh(\tfrac{1}{2}J\nabla)\cosh^{Z-1}(\tfrac{1}{2}J\nabla)\tanh(\tfrac{1}{2}\beta_c x)|_{x=0} = 1$$

with

$$\beta_c = 1/k_B T_c.$$

Here, equation (A2.4) is simply that of the spin-$\frac{1}{2}$ Ising model in the Zernike approximation [13]. In fact, for $Z = 6$ it reproduces the well known Zernike [11] equation for the spin-$\frac{1}{2}$ simple cubic lattice. The solution is given by

$$4k_B T_c/J = 5.073 \qquad \text{for } Z = 6 \tag{A2.5}$$

which is superior to the standard mean-field theory result ($4k_B T_c/J = 6$).

From (A2.1) and (A2.3), for $\alpha = -\infty$ we obtain

$$\begin{aligned} I(x) &= O(x) = \tfrac{1}{4}\,\mathrm{sech}^2(\tfrac{1}{2}\beta x) \\ R(x) &= \tfrac{1}{4}I(x) \end{aligned} \tag{A2.6}$$

from which (35) reduces to

$$\Delta_1^0 = \Delta_2^0 \qquad \Delta_4^0 = \tfrac{1}{4}\Delta_1^0. \tag{A2.7}$$

Therefore, the paramagnetic susceptibility (33) is given, for $\alpha = -\infty$, by

$$\chi_{\text{para}} = \tfrac{1}{2}N\beta\Delta_0/[1-(2R_1)^2] \tag{A2.8}$$

with

$$\Delta_0 = \Delta_1^0[1-(2R_1)^2] + \Delta_1^0(1 \pm 2R_1)^2. \tag{A2.9}$$

Then, the paramagnetic susceptibility $\chi_{\text{para}}^{(+)}$ for the ferromagnetic interaction (or the plus sign in (A2.9)) is given by

$$\chi_{\text{para}}^{(+)} = (N/k_B T)[\Delta_1^0/(1-2R_1)]. \tag{A2.10}$$

Thus, the paramagnetic susceptibility (A2.10) for the ferromagnet with $\alpha = -\infty$ diverges at the transition temperature T_c determined from (A2.4). On the other hand, the paramagnetic susceptibility $\chi_{\text{para}}^{(-)}$ for the antiferromagnetic interaction (or the minus sign in (A2.9)) is given by

$$\chi_{\text{para}}^{(-)} = (N/k_B T)[\Delta_1^0/(1+2R_1)]. \tag{A2.11}$$

Thus, the paramagnetic susceptibility (A2.11) for the antiferromagnet with $\alpha = -\infty$ takes a finite value at the transition temperature (or the Néel temperature T_N) determined from (A2.4), namely

$$\chi_{\text{para}}^{(-)} = (N/2k_B T_N)\Delta_1^0(T_N) \tag{A2.12}$$

with

$$\Delta_1^0 = \tfrac{1}{4}\cosh^z(\tfrac{1}{2}J\nabla)\,\text{sech}^2(x/2k_B T_N)|_{x=0}. \tag{A2.13}$$

References

[1] Domb C 1960 *Adv. Phys.* **9** 149
[2] Goncalves L L 1985 *Phys. Scr.* **32** 248
[3] Iwashita T and Uryu N 1979 *Phys. Lett.* **96A** 311; 1984 *J. Phys. Soc. Japan* **53** 721
[4] Schafield S L and Bowers R G 1980 *J. Phys. A: Math. Gen.* **13** 3697
[5] Siqueira A F and Fittipaldi I P 1986 *J. Magn. Magn. Mater.* **54–7** 678
[6] Kaneyoshi T 1987 *J. Phys. Soc. Japan* **56** 2675
[7] Kaneyoshi T 1988 *Z. Phys.* B **71** 109
[8] Bowers R G and Yousif B Y 1983 *Phys. Lett.* **96A** 49
Hunter G J A, Jenkins R C L and Tinsley C J 1990 *J. Phys. A: Math. Gen.* **23** 4547
[9] Kaneyoshi T, Jaščur M and Tomczak P 1992 *J. Phys.: Condens. Matter* **4** L653
[10] Kaneyoshi T, Tucker J W and Jaščur M 1992 *Physica* A **186** 495
[11] Zernike F 1940 *Physica* **7** 565
[12] Kaneyoshi T and Chen J C 1991 *J. Magn. Magn. Mater.* **98** 201
[13] Honmura R and Kaneyoshi T 1979 *J. Phys. C: Solid State Phys.* **12** 3979