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Random mixture of Ising systems of different values of spins: II. Possibility of spin glasses

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Abstract. A mixture of the site Ising models, each constituent of which has a different value of spin, is investigated. The phase boundaries between paramagnetic and ferromagnetic phases, paramagnetic and antiferromagnetic phases, and paramagnetic and spin glass phases are calculated. The condition under which the spin glass phase is realised is obtained.

1. Introduction

A random mixture of site Ising models of A and B, when both spins are $\frac{1}{2}$, has been considered by many authors (for example, Katsura and Matsubara 1974, Aharony 1975, 1978, Eggarter and Eggarter 1977). The possibility of a spin glass (glass-like phase) in the site model was discussed by Oguchi and Ueno (1979) and Katsura *et al* (1979, referred to as KFI hereafter) for the case $S_A = S_B = \frac{1}{2}$. However, in compounds like $K_2Cu_xFe_{1-x}F_4$ (Oguchi and Ueno 1979) and $K_2Cu_xMn_{1-x}F_4$ (Ikeda and Okamura 1979), which are regarded as mixtures of the site models, each constituent has a different value of spin. K_2CuF_4 is ferromagnetic, in which the spin of Cu is $\frac{1}{2}$, K_2FeF_4 is antiferromagnetic, in which the spin of Fe is 2, and K_2MnF_4 is antiferromagnetic, in which the spin of Mn is $\frac{5}{2}$.

From the above it is shown to be interesting to study the mixtures of different values of spins in the site Ising model. Such mixtures were investigated by Kudō *et al* (1978) and Katsura (1979, referred to as K, hereafter). The former discussed the one-dimensional case and obtained the magnetisation process. The latter obtained expressions for the phase boundaries between paramagnetic (P) and ferromagnetic (F) phases and paramagnetic and antiferromagnetic (AF) phases in the Bethe approximation without presenting numerical results. In this paper we show the possibility of finding a spin glass in the Ising site mixture of different values of spins and give the phase boundary between the paramagnetic phase and the spin glass (G) phase. Numerical calculations of the phase boundaries between P–F and P–AF are also given in § 2. In § 3 we give the condition under which the spin glass phase is realised.

2. Phase boundaries

We consider a mixture of spin A ($S_A = 1$) and spin B ($S_B = \frac{1}{2}$) in the Bethe approximation. The Hamiltonian $\mathscr{H}$ of a cluster consisting of a central atom in the external magnetic field H and its z nearest-neighbour atoms under the effective field H_i^* is given in (K, 2.1). (In the following the meanings of the symbols are the same as in K.) In the low-field limit the thermal averages of spins in the cluster for a given configuration, which consists of a central spin A and k nearest-neighbour A, and $z-k$ nearest-neighbour B, are given in (K, 5.13) and (K, 5.14).

Now we carry out the average over all possible configurations of the clusters using the distribution functions g_A and g_B, which satisfy the integral equations (with a finite field) (K, 3.1) and (K, 3.2). The averages of $\langle S_A\rangle$, $\langle S_B\rangle$, $\langle S_A\rangle^2$ and $\langle S_B\rangle^2$ can be calculated in the same way as in K to give

$$\overline{\langle S_A\rangle}=\left[1+\frac{e^{-D}}{2}\left(\frac{u+2}{u+2\cosh K_{AA}}\right)^{zp}\left(\frac{1}{\cosh K_{AB}}\right)^{z(1-p)}\right]^{-1} \times[C_A+zpt_{AA}\bar{L}_A+z(1-p)t_{AB}\bar{L}_B] \tag{2.1}$$

$$\overline{\langle S_B\rangle}=C_B+zpt_{BA}\bar{L}_A+z(1-p)t_{BB}\bar{L}_B \tag{2.2}$$

$$\overline{\langle S_A\rangle^2}=\left[1+\frac{e^{-D}}{2}\left(\frac{u+2}{u+2\cosh K_{AA}}\right)^{zp}\left(\frac{1}{\cosh K_{AB}}\right)^{z(1-p)}\right]^{-2} \times[C_A^2+2C_Ap_Azt_{AA}\bar{L}_A+2C_Ap_Bzt_{AB}\bar{L}_B+p_Azt_{AA}^2\overline{L_A^2} +p_A^2z(z-1)t_{AA}^2\bar{L}_A^2+p_Bzt_{AB}^2\overline{L_B^2}+p_B^2z(z-1)t_{AB}^2\bar{L}_B^2 +2p_Ap_Bz(z-1)t_{AA}t_{AB}\bar{L}_A\bar{L}_B] \tag{2.3}$$

and

$$\overline{\langle S_B\rangle^2}=C_B^2+2C_Bp_Azt_{BA}\bar{L}_A+2C_Bp_Bzt_{BB}\bar{L}_B +p_Azt_{BA}^2\overline{L_A^2}+p_A^2z(z-1)t_{BA}^2\bar{L}_A^2+p_Bzt_{BB}^2\overline{L_B^2} +p_B^2z(z-1)t_{BB}^2\bar{L}_B^2+2p_Ap_Bz(z-1)t_{BA}t_{BB}\bar{L}_A\bar{L}_B \tag{2.4}$$

where

$$t_{AA}=B_1(K_{AA},u) \qquad t_{BA}=B_1(K_{BA},u)$$

$$t_{AB}=B_{\frac{1}{2}}(K_{AB}) \qquad t_{BB}=B_{\frac{1}{2}}(K_{BB})$$

$$B_{\frac{1}{2}}(x)=\tanh x \qquad B_1(x,u)=\frac{2\sinh x}{u+2\cosh x}.$$

In (2.1)–(2.4) we approximated $\overline{B_1(K,u_i)}=B_1(K,u)$ $(u\equiv\overline{u_i})$ and

$$\overline{B_1(K_{AA},u_i)B_1(K_{AA},u_j)L_{Ai}L_{Aj}}=\begin{cases}t_{AA}^2\bar{L}_A^2 & (i\neq j)\\ t_{AA}^2\overline{L_A^2} & (i=j)\end{cases}$$

The uniform magnetisation M_u, staggered magnetisation M_s and spin glass magnetisation M_g are defined as (KFI, 13)

$$\left.\begin{matrix}M_u\\ M_s\\ M_g\end{matrix}\right\}\equiv[\mu_A^np_A\ \mu_B^np_B]\begin{bmatrix}\overline{\langle S_{A\alpha}\rangle^n}\pm\overline{\langle S_{A\beta}\rangle^n}\\ \overline{\langle S_{B\alpha}\rangle^n}\pm\overline{\langle S_{B\beta}\rangle^n}\end{bmatrix}, \tag{2.5}$$

where μ_A and μ_B are magnetic moments and the upper and lower signs for $n=1$ correspond to M_u and M_s, and the upper sign for $n=2$ corresponds to M_g. From (2.5) the phase boundaries are obtained in a similar way to (K, 5.23) and (KFI, 16) to be

$$[1\mp(z-1)t_{AA}^np_A][1\mp(z-1)t_{BB}^np_B]-(z-1)^2t_{BA}^nt_{AB}^np_Ap_B=0 \qquad (2.6)\text{–}(2.8)$$

where the upper sign for $n=1$ (referred to as (2.6)) corresponds to P–F, the lower sign for $n=1$ (referred to as (2.7)) to P–AF and the upper sign for $n=2$ (referred to as (2.8)) to P–G boundaries. Here u is determined by

$$u=\mathrm{e}^{-D}\left(\frac{u+2}{u+2\cosh K_{\mathrm{AA}}}\right)^{p(z-1)}\left(\frac{1}{\cosh K_{\mathrm{AB}}}\right)^{(1-p)(z-1)}. \tag{2.9}$$

This equation can be solved for q ($\equiv p_{\mathrm{A}}-\frac{1}{2}$) after taking logarithms of both sides:

$$q=\frac{\ln u+D+\frac{1}{2}(z-1)\ln[(u+2\cosh K_{\mathrm{AA}})\cosh K_{\mathrm{AB}}(u+2)^{-1}]}{(z-1)\ln[(u+2)\cosh K_{\mathrm{AB}}(u+2\cosh K_{\mathrm{AA}})^{-1}]}. \tag{2.10}$$

The phase boundaries are obtained from the intersection in the $q-u$ plane of both solutions of the quadratic equations (2.6–2.8) for q, i.e. $q=q_1(T,u)$, and $q=q_2(T,u)$ given by (2.10) for each fixed T.

Results for $z=4$ are shown in figures 1 and 2 for the two cases in which the spin glass phase is realised. The result for $z=3$ is shown in figure 3.

3. The possible region of the appearance of the spin glass

Next we determine the condition for the appearance of the glass-like phase. By using (2.6) and (2.7), (2.8) is rewritten as

$$t_{\mathrm{BA}}t_{\mathrm{AB}}=1+(z-2)t_{\mathrm{AA}}t_{\mathrm{BB}} \tag{3.1}$$

which is of the same form as that in KFI. Eliminating $t_{\mathrm{BA}}t_{\mathrm{AB}}$ from (2.6) by using (3.1) we

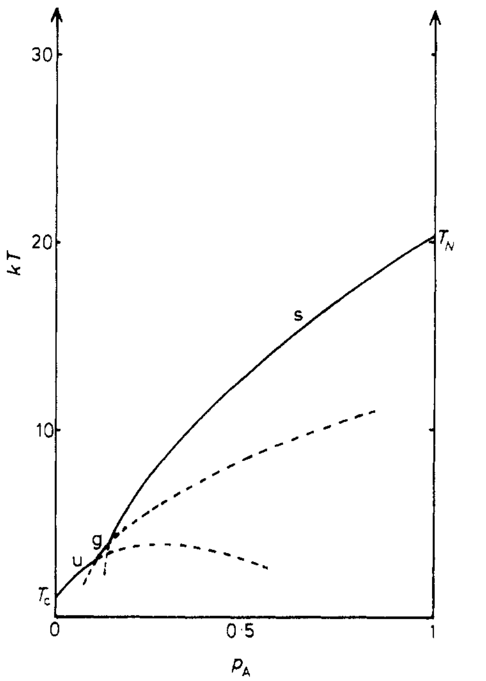

Figure 1. Phase boundaries for $z=4$, $|J_{\mathrm{AA}}|>J_{\mathrm{BB}}|$, $J_{\mathrm{AA}}=-5$, $J_{\mathrm{AB}}=5$, $J_{\mathrm{BB}}=1$, $\lambda_{\mathrm{A}}=0$.

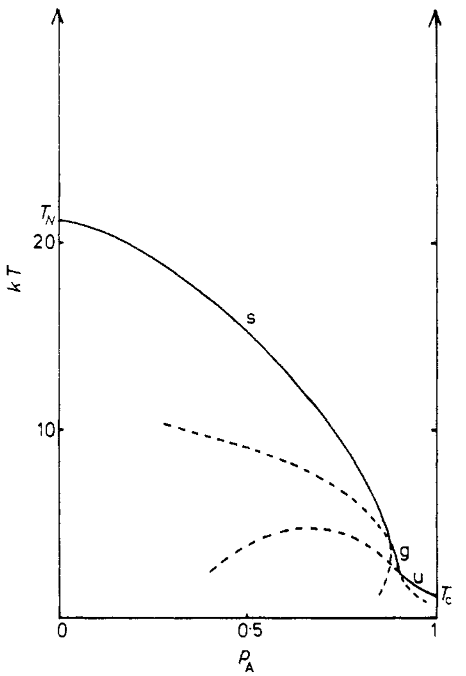

Figure 2. Phase boundaries for $z=4$, $|J_{\mathrm{AA}}|<|J_{\mathrm{BB}}|$, $J_{\mathrm{AA}}=0{\cdot}25$, $J_{\mathrm{AB}}=7{\cdot}5$, $J_{\mathrm{BB}}=-15$, $\lambda_{\mathrm{A}}=0$.

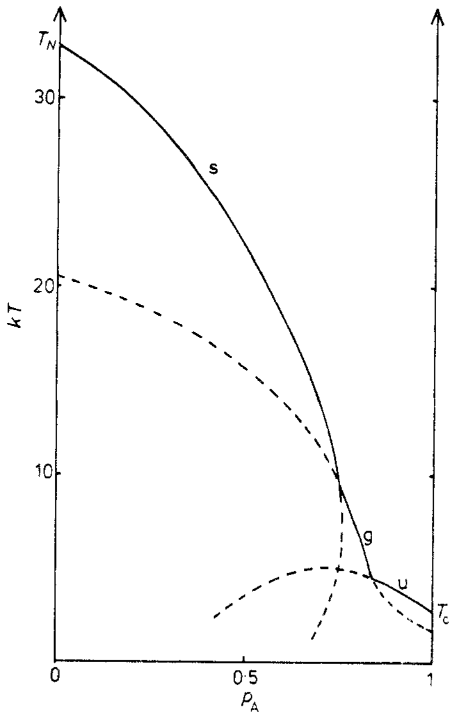

Figure 3. Phase boundaries for $z=3$, $|J_{AA}|<|J_{BB}|$, $J_{AA}=1$, $J_{AB}=18$, $J_{BB}=-36$, $\lambda_A=0$.

obtain the relation between t_{AA} and t_{BB}:

$$[1+(z-1)^2(z-3)t_{AA}^2]t_{BB}^2+[(z-1)^2-2]t_{AA}t_{BB}+t_{AA}^2=0 \tag{3.2}$$

which is the same as in KFI. From the definition of t_{AA},

$$t_{AA}=\frac{2\sinh K_{AA}}{u+2\cosh K_{AA}} \tag{3.3}$$

we have the relation

$$\cosh K_{AA}=\frac{ut_{AA}^2+(u^2t_{AA}^2-4t_{AA}^2+4)^{1/2}}{2(1-t_{AA}^2)}. \tag{3.4}$$

From equation (3.1) we have

$$\cosh K_{AB}=\frac{uA+[(uA)^2-16A+16]^{1/2}}{4(1-A)} \tag{3.5}$$

where

$$A\equiv 1+(z-2)t_{AA}t_{BB}. \tag{3.6}$$

From (3.5) and (3.4) we obtain

$$\frac{J_{AB}}{J_{BB}}=\frac{1}{2\tanh^{-1}t_{BB}}\cosh^{-1}\left(\frac{uA+[(uA)^2-16A+16]^{1/2}}{4(1-A)}\right) \tag{3.7}$$

and

$$\frac{J_{AA}}{J_{BB}} = \frac{1}{4\tanh^{-1} t_{BB}} \cosh^{-1}\left(\frac{ut_{AA}^2 + (u^2 t_{AA}^2 - 4t_{AA}^2 + 4)^{1/2}}{2(1-t_{AA}^2)}\right) \tag{3.8}$$

respectively. The condition that curves (2.6–2.8) intersect at a point in the T–p_A plane is given by equations (3.7) and (3.8) with two independent parameters u and t_{AA} satisfying (2.9) and (3.2). If the anisotropy $\lambda_A = 0$, then the condition can be given by a curve in the J_{AB}/J_{BB}–J_{AA}/J_{BB} plane, i.e. the condition can be given only by the ratios J_{AB}/J_{BB} and J_{AA}/J_{BB}, because $D \equiv \lambda_A/kT = 0$ in (2.9) so that T does not appear in (2.9) explicitly. The numerical calculation is achieved for given z, changing u and t_{AA} (or t_{BB}) as two independent variables. Results for $z = 4$ are given by two non-equivalent curves in figures 4 and 5. For values of J_{AA}, J_{AB} and J_{BB} which correspond to points lying in the upper left region bounded by the curve in figure 3 or 4 the spin glass phase is realised.

The condition does not depend on the sign of J_{AB} provided that $J_{AA}J_{BB} < 0$. The symmetry between the two cases $|J_{AA}/J_{BB}| > 1$ and $|J_{AA}/J_{BB}| < 1$ which exists in KFI is lost in our case. Other qualitative properties are similar to KFI. For $z = 6$ the region corresponding to the realisation of the spin glass phase is given by curves far from the origin in figures 4 and 5. For $z = 3$ the region is given by the whole quarter planes in figures 4 and 5†.

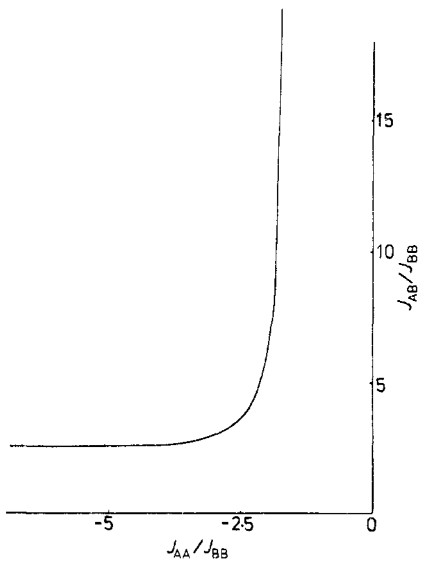

Figure 4. The condition for the realisation of the spin glass phase for $z = 4$, $J_{AB}/J_{BB} > 0$, $\lambda_A = 0$.

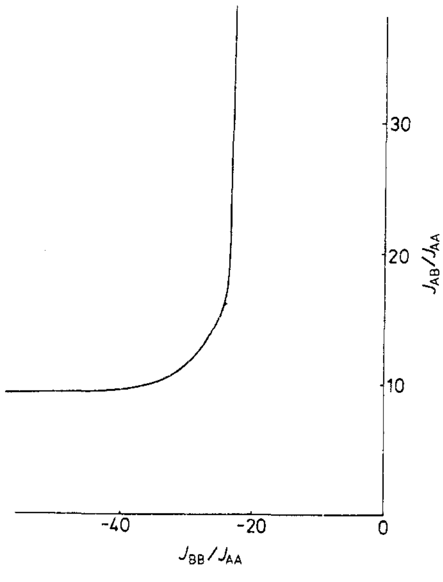

Figure 5. The condition for the realisation of the spin glass phase for $z = 4$, $J_{AB}/J_{AA} > 0$, $\lambda_A = 0$.

4. Conclusion

We investigated a mixture of the site Ising models, each constituent of which has a different value of spin. The phase boundaries between P–F, P–AF and P–G phases were calculated. For certain values of the parameters z, λ_A, J_{AA}, J_{AB} and J_{BB} the

† Precisely speaking, a curve corresponding to a line in the case of $S_A = S_B = \frac{1}{2}$ is excluded.

possibility of a realisation of the spin glass phase was shown. Experiments corresponding to the results in the present paper are expected to be carried out on such substances as $K_2Cu_xFe_{1-x}F_4$ or $K_2Cu_xMn_{1-x}F_4$. Similar results to ours (figures 1–3) have been obtained by other methods (Oguchi and Ueno 1979, Nambu 1979). Whether the existence of the spin glass phase depends on these theoretical methods or not is still open to question (Bray *et al* 1978, Southern *et al* 1979, Fisch and Harris 1977) and will be discussed in a forthcoming paper.

In § 3 we obtained the condition under which the spin glass phase is realised. Conditions are expressed in a similar form to the result of KFI when $t_{AA} = B_1(K_{AA}, u)$, etc, are replaced. The condition for $z = 4$ in the case $\lambda_A = 0$ is shown by curves in the J_{AB}/J_{BB}–J_{AA}/J_{BB} and J_{AB}/J_{AA}–J_{BB}/J_{AA} planes.

The determination of the phase boundaries between the F–G, AF–G and F–AF phases, and the discussion of the mixed phase (Eggarter and Eggarter 1977), requires information on the higher-order terms and will be discussed in future work.

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