

### Mean-field solution for random mixtures $A_x B_{1-x}$ of an Ising site model

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An exact solution for random mixtures  $A_x B_{1-x}$  of an Ising model is presented. The solution is obtained in the mean-field version of the model and exhibits a spin-glass phase transition. The explicit dependence of the critical temperature  $T_c$  on the exchange integrals  $J_{AA} > 0, J_{BB} > 0, J_{AB} < 0$ , and concentration  $x$ , are found. The results are in good agreement with the previous Monte Carlo simulation.

Various theoretical models and approaches<sup>1</sup> have been proposed to explain the qualitative features of spin-glass transitions observed in experiments,<sup>2,3</sup> especially a sharp cusplike peak in the low-field susceptibility. Of these efforts, exactly solvable models<sup>1</sup> with either bond randomness<sup>4,5</sup> or site randomness<sup>6,7</sup> play an important role. In this note we will show that a random mixture of an Ising model is exactly soluble in the mean-field theory and exhibits spin-glass transition. Extensive researches have been carried out on the model.<sup>8-11</sup> In 1977, Tatsumi found its spin-glass phase with Monte Carlo method. As we will see later, our mean-field solution is in good agreement with the Monte Carlo simulation.

Random mixtures of an Ising site model can be considered as a quenched magnetic alloy of the form  $A_x B_{1-x}$ , both kinds of atoms being magnetic, with exchange integrals  $J_{AA}, J_{BB}, J_{AB}$ . The Hamiltonian of this model is of the form,<sup>1,8</sup>

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} s_i s_j - \mu_0 H \sum_i s_i \tag{1}$$

where  $\mu_0$  is the magnetic moment of each spin (we consider both kinds of atoms with the same magnetic moment for simplicity) and  $J_{ij}$  are given by

$$\begin{aligned} J_{ij} &= J_1 + J_2 \epsilon_i \epsilon_j + J_3 (\epsilon_i + \epsilon_j), \\ J_1 &= (J_{AA} + 2J_{AB} + J_{BB})/4, \\ J_2 &= (J_{AA} - 2J_{AB} + J_{BB})/4, \\ J_3 &= (J_{AA} - J_{BB})/4, \end{aligned} \tag{2}$$

where  $\epsilon_i = 1$  if the site  $i$  is taken by an  $A$  atom,  $\epsilon_i = -1$  otherwise. If we take the mean-field version of the model, then  $J_{ij}$  is given by

$$J_{ij} = [J_1 + J_2 \epsilon_i \epsilon_j + J_3 (\epsilon_i + \epsilon_j)]/N, \tag{3}$$

where  $N$  is the number of spins,  $J_1, J_2, J_3$  are still given by Eq. (2), and the interaction is chosen for any pair of spins irrespective of distance.

$A$  and  $B$  atoms are randomly distributed under a certain concentration of  $A_x B_{1-x}$ . Thus the quenched free energy with concentration  $x$  is given by

$$F = \langle F[J] \rangle = \left[ \frac{N!}{n_+! n_-!} \right]^{-1} \sum_{\{\epsilon_i\}} F[J] \tag{4}$$

where the summation is over different distributions of  $A$  and  $B$  atoms under a given concentration  $x$ .  $n_+$  is the number of  $A$  atoms with  $\epsilon_i = 1$  and  $n_-$  the number of  $B$  atoms with  $\epsilon_j = -1$ . We can follow the procedure similar to Ref. 7.

By using (3), the partition function becomes

$$Z = \sum_{m_1 m_2} W_N(m_1, m_2) \exp N \left[ \frac{1}{2} (k_1 m_1^2 + k_2 m_2^2 + 2k_3 m_1 m_2) + h m_1 \right] \tag{5}$$

where  $k_l = \beta J_l (l=1,2,3)$ ,  $h = \beta \mu_0 H$ ,  $m_1 = \sum_i s_i / N$ ,  $m_2 = \sum_i s_i \epsilon_i / N$ , and the summation is over all possible values of  $m_1$  and  $m_2$  under a given concentration of  $x$ .  $W_N(m_1, m_2)$  is the number of spin states for a set of given  $m_1, m_2$ .

The number of spin states for given  $m_1, m_2$  is given by

$$W_N(m_1, m_2) = \frac{n_+!}{(N_+^+)(N_+^-)!} \frac{n_-!}{(N_-^+)(N_-^-)!}, \tag{6}$$

where  $N_+^+$  is the number of sites with  $s_i = +1$  and  $\epsilon_i = +1$ ,  $N_+^-$  is the number of sites with  $s_i = +1$  and  $\epsilon_i = -1$ ,  $N_-^+$  is the number of sites with  $s_i = -1$  and  $\epsilon_i = +1$ , and  $N_-^-$  is the number of sites with  $s_i = -1$  and  $\epsilon_i = -1$ . Using these definitions, one finds after a simple calculation

$$\begin{aligned} N_+^+ &= N(1 + m_1 + m_2 + \lambda)/4, \\ N_+^- &= N(1 - m_1 - m_2 + \lambda)/4, \\ N_-^+ &= N(1 + m_1 - m_2 - \lambda)/4, \\ N_-^- &= N(1 - m_1 + m_2 - \lambda)/4, \\ n_+ &= N(1 + \lambda)/2, \quad n_- = N(1 - \lambda)/2, \end{aligned} \tag{7}$$

in which  $\lambda = \sum_i \epsilon_i / N$ . It is straightforward to relate  $\lambda$  with concentration  $x$ , yielding

$$\lambda = 2x - 1. \tag{8}$$

For large  $N$ , Eq. (6) becomes

$$W_N(m_1, m_2) = 2^N \exp N \left\{ -\frac{1}{4} [(1+m_1+m_2+\lambda) \ln(1+m_1+m_2+\lambda) + (1-m_1-m_2+\lambda) \ln(1-m_1-m_2+\lambda) \right. \\ \left. + (1+m_1-m_2-\lambda) \ln(1+m_1-m_2-\lambda) + (1-m_1+m_2-\lambda) \ln(1-m_1+m_2-\lambda)] \right. \\ \left. + \frac{1}{2} [(1+\lambda) \ln(1+\lambda) + (1-\lambda) \ln(1-\lambda)] \right\}. \quad (9)$$

Combining Eqs. (5) and (9), we obtain the following form of  $Z$ :

$$Z = \sum_{m_1, m_2} \exp [Ng(m_1, m_2, \lambda)] \quad (10)$$

where  $g$ , independent of the size of system  $N$ , is a function of  $m_1, m_2, \lambda$ . In order to find  $\ln Z$ , we need only take the maximum term in the summation.<sup>7</sup> That is,

$$\ln Z = N \max_{m_1, m_2} [g(m_1, m_2, \lambda)]. \quad (11)$$

The free quenched energy can be written as

$$F = \left[ \frac{N!}{n_+! n_-!} \right]^{-1} \left[ -\frac{N}{\beta} \right] \max_{m_1, m_2} [g(m_1, m_2, \lambda)] P_N(\lambda), \quad (12)$$

$$f(a_1, a_2) = \frac{1}{4} \{ \beta^{-1} [(1+a_1+\lambda) \ln(1+a_1+\lambda) + (1-a_1+\lambda) \ln(1-a_1+\lambda) + (1+a_2-\lambda) \ln(1+a_2-\lambda) \\ + (1-a_2-\lambda) \ln(1-a_2-\lambda) - 4 \ln 2] - (J_{11} a_1^2 + J_{22} a_2^2 + 2J_{12} a_1 a_2) - 2\mu_0 H(a_1 + a_2) \} \quad (16)$$

and

$$\begin{aligned} J_{11} &= \frac{1}{2}(J_1 + J_2) + J_3, \\ J_{22} &= \frac{1}{2}(J_1 + J_2) - J_3, \\ J_{12} &= \frac{1}{2}(J_1 - J_2). \end{aligned} \quad (17)$$

The minimum of  $f(a_1, a_2)$  yields

$$(2\beta)^{-1} \ln[(1+\lambda+a_1)/(1+\lambda-a_1)] \\ = J_{11} a_1 + J_{12} a_2 + \mu_0 H, \quad (18)$$

$$(2\beta)^{-1} \ln[(1-\lambda+a_2)/(1-\lambda-a_2)] \\ = J_{12} a_1 + J_{22} a_2 + \mu_0 H. \quad (19)$$

Equations (18) and (19) are similar to, but physically different from the Luttinger's. Of the various solutions of (18) and (19) (if there are several), the one which makes  $f(a_1, a_2)$  smallest must be taken. This solution is denoted by  $a_1^0, a_2^0$ , corresponding to  $m_1^0, m_2^0$ . Obviously,  $m_1^0$ , which is proportional to the mean magnetic moment of the system, is the conventional order parameter for magnetic problem.  $m_2^0$  is the order parameter of spin-glass transition.<sup>7,11</sup>

If the concentration of  $A$  atoms  $x=0.5$ , i.e.,  $\lambda=0$ , Eqs. (18) and (19) turn out to be the Luttinger's equations. Thus it is straightforward to show the typical feature of spin-glass transition, i.e., the cusplike peak in low-field susceptibility. A complete discussion of the equations is complicated and will be given elsewhere. We

where  $P_N(\lambda)$  is the distribution number of spins under a given concentration  $x$  and obviously given by

$$P_N(\lambda) = \frac{N!}{n_+! n_-!}. \quad (13)$$

Therefore the quenched free energy is simply taken to be

$$F = -\frac{N}{\beta} \max_{m_1, m_2} [g(m_1, m_2, \lambda)]. \quad (14)$$

Introducing  $m_1=(a_1+a_2)/2$  and  $m_2=(a_1-a_2)/2$ , we can write the free energy per spin  $f$  as follows:

$$f = F/N = \min_{a_1, a_2} [f(a_1, a_2, \lambda)] \quad (15)$$

where

shall limit ourselves to the case of no magnetic field. In order to compare with the Monte Carlo results,<sup>11</sup> we are further specialized in the case of  $J_{AA}, J_{BB} > 0$ , and  $J_{AB} < 0$ , which means  $J_2 > J_1$  and  $J_1 + J_2 > 0$ . There is always exactly one second-order phase transition at  $T = T_c$ , which means that both order parameters  $m_1^0$  and  $m_2^0$  vanish at the same temperature and is in agreement with the Monte Carlo results.<sup>11</sup> The critical temperature  $T_c(x) = T_s(x)$  ( $T_s$  is the spin-glass transition temperature), dependent on the concentration  $x$  or  $\lambda$ , is given by

$$\begin{aligned} k_B T_c(x) &= \frac{1}{2}(J_1 + J_2) + J_3 \lambda \\ &+ \frac{1}{2} [(J_1 - J_2)^2 + 4J_3^2 \\ &+ 4(J_1 + J_2)J_3 \lambda + 4J_1 J_2 \lambda^2]^{1/2}, \end{aligned} \quad (20)$$

where  $\lambda = 2x - 1$ . For  $T > T_c$  the only solution is  $a_1 = a_2 = 0$ . For  $T$  just below  $T_c$ , there is nonzero solution  $a_1 = a_1^0$ , and  $a_2 = a_2^0$ ,

$$a_2^0 = \frac{J_{12}(1-\lambda)}{(k_B T_c) - J_{22}(1-\lambda)} a_1^0, \quad (21)$$

$$a_1 = \left[ \left[ 3(1+\lambda)^3 J_{11} \right. \right. \\ \left. \left. + \frac{3(1+\lambda)^3(1-\lambda)J_{12}^2}{k_B T_c - J_{22}(1-\lambda)} \right] (T_c - T) \right]^{1/2}, \quad (22)$$

$$m_1^0 = \frac{1}{2} \left[ 1 + \frac{J_{12}(1-\lambda)}{k_B T_c - J_{22}(1-\lambda)} \right] a_1^0, \quad (23)$$

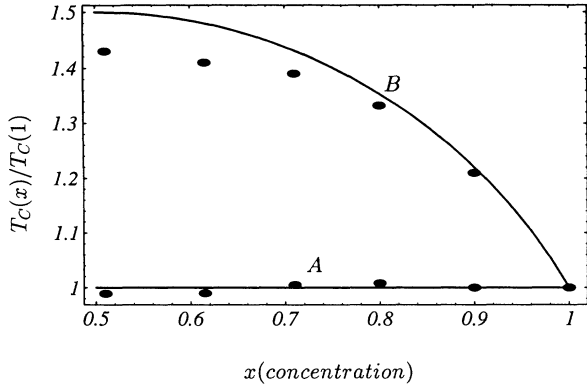


FIG. 1. Phase diagram. A: case 1 ( $J_{AA}=J_{BB}=-J_{AB}=J$ ); B: case 2 ( $J_{AA}=J_{BB}=J, J_{AB}=-2J$ ). Solid lines represent our results and black points the Monte Carlo simulation (Ref. 11).

$$m_2^0 = \frac{1}{2} \left[ 1 - \frac{J_{12}(1-\lambda)}{k_B T_c - J_{22}(1-\lambda)} \right] a_1^0. \quad (24)$$

In general, there is nonvanishing magnetic order  $m_1^0$  and nonvanishing spin-glass order  $m_2^0$  below  $T_c$ . We notice that in the particular case of  $J_{AA}=J_{BB}$  (i.e.,  $J_3=0$ ) and concentration  $x=0.5$ , the only spin-glass order exists, i.e.,  $M_2 \neq 0$  and  $m_1=0$  for  $T < T_c$ . This is the so-called pure spin-glass state. The derivative of the free energy (14) with respect to  $T$  is discontinuous at  $T=T_c$ , since that of the order parameters is discontinuous at  $T=T_c$ . It means that the derivative of magnetic susceptibility  $\chi (= \partial^2 F / \partial H^2)$  with respect to  $T$ , is also discontinuous at  $T=T_c$ , which gives rise to cusplike behavior of  $\chi$  as in Ref. 7.

Now we can compare our results with the Monte Carlo simulation.<sup>11</sup> Some caution must be taken in comparison, since the meanings of exchange integrals  $J$  for Monte Carlo simulation (nearest-neighbor interaction) and for ours (infinite-range interaction) are different. Therefore, we compare the scaled transition temperature as Tatsumi did, i.e.,  $T_c(x)/T_c(1)$ , which is independent of exchange integral  $J$ . Actually it is expectable in our result, since the temperature is always proportional to the exchange integral  $J$  for any concentration  $x$ . First one notes from Eq. (20),  $T_c(x) = T_c(1-x)(\lambda=2x-1)$  for  $J_{AA}=J_{BB}$ , i.e.,  $J_3=0$ , which is in excellent agreement with the simulation.<sup>11</sup>

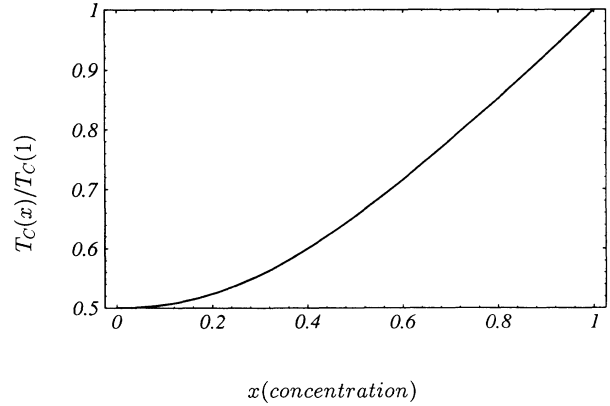


FIG. 2. Phase diagram. Case 3 ( $J_{AA}=2J, J_{BB}=-J_{AB}=J$ ). Solid lines represent our results.

Case 1 ( $J_{AA}=J_{BB}=-J_{AB}=J$ ): we simply have  $k_B T_c(x) = J$ , independent of concentration  $x$ . We can trivially rewrite it as  $T_c(x)/T_c(1) = 1$ , compared with the numerical simulation<sup>11</sup> which is  $0.989 \mp 0.011$ . The result is shown in Fig. 1.

Case 2 ( $J_{AA}=J_{BB}=J, J_{AB}=-2J$ ): we have

$$k_B T_c = J \{ 1 + [4 - 3(2x-1)^2]^{1/2} \} / 2,$$

which has a maximum of  $x=0.5$ . It is easy to show that  $T_c(0.5)/T_c(1) = 1.5$ , compared with the numerical simulation<sup>11</sup> which is  $1.411 \mp 0.011$ . The result is shown in Fig. 1.

Case 3 ( $J_{AA}=2J, J_{BB}=-J_{AB}=J$ ): we have

$$k_B T_c(x)/J = \frac{3}{4} + \frac{2x-1}{4} + \frac{1}{2} \left[ \frac{5}{4} + \frac{3(2x-1)}{2} + \frac{5(2x-1)^2}{4} \right]^{1/2}$$

and  $k_B T_c(1) = 2J$ . The result is shown in Fig. 2. No Monte Carlo result is available for this case.

In summary, the mean-field model can give us the results such as the spin-glass transition temperatures and phase diagram, which are in good agreement with the Monte Carlo simulation.

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<sup>1</sup>K. Binder and A. P. Young, Rev. Mod. Phys. **58**, 801 (1986).

<sup>2</sup>J. A. Mydosh, in *Magnetism and Magnetic Materials-1974*, edited by C. D. Graham, Jr., J. J. Rhyne, and G. H. Lander, AIP Conf. Proc. No. 24 (AIP, New York, 1975), p. 131.

<sup>3</sup>L. E. Wenger and P. H. Keesom, Phys. Rev. B **13**, 4053 (1976).

<sup>4</sup>S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).

<sup>5</sup>D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1792 (1975).

<sup>6</sup>D. C. Mattis, Phys. Lett. **56A**, 421 (1976).

<sup>7</sup>J. M. Luttinger, Phys. Rev. Lett. **37**, 772 (1976).

<sup>8</sup>A. Aharony, Phys. Rev. Lett. **34**, 590 (1975); A. Aharony and Y. Imry, Solid State Commun. **20**, 899 (1976).

<sup>9</sup>F. Wegner, Solid State Commun. **12**, 785 (1973); A. D. Bruce and S. Aharony, Phys. Rev. B **11**, 478 (1975); E. Eggarter and T. P. Eggarter, *ibid.* **15**, 2804 (1977).

<sup>10</sup>D. P. Landau, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1986).

<sup>11</sup>T. Tatsumi, Prog. Theor. Phys. **57**, 1799 (1977); **59**, 1428 (1978); **59**, 1437 (1978).