

## Spin glasses in the Bethe-Peierls-Weiss and other mean-field approximations

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We obtain the thermodynamic properties of a system of Ising spins interacting with various random potentials in the Bethe-Peierls-Weiss (BPW) approximation. When the effective number of neighbors  $z$  approaches infinity, we show that all the magnetic properties arising from the BPW approximation, the mean random field (MRF) and the Sherrington-Kirkpatrick (SK) replica treatment are identical. Also, the internal energy in the BPW method is identical to that obtained by SK, while the MRF neglects correlations and thus gives a different internal energy. Introducing a plausible phenomenological constant of integration we obtain the microscopic free energy derived by Thouless, Anderson, and Palmer (TAP). Using this free energy, we show that the BPW method with a random distribution of fields reproduces *all* the results of SK including a negative entropy of  $-k/(2\pi)$  at  $T = 0$ , and that all probability distributions which do not go to zero at zero field give a negative entropy at  $T = 0$ . For finite  $z$ , we obtain the phase diagram for the MRF method as a function of  $z$  and find that for  $z > 8$  the phase diagram is already very close to that of the  $z \rightarrow \infty$  case. We also derive the thermodynamic properties for the Ruderman-Kittel-Kasuya-Yosida system near the spin-glass transition temperature in the BPW method. We find that the method gives a discontinuous slope in the magnetic susceptibility  $\chi$  and the specific heat  $C_M$  at the spin-glass transition temperature  $T_g$ , however the maxima in  $\chi$  and  $C_M$  occur well below  $T_g$ .

### I. INTRODUCTION

Several different approaches have been used to discuss the thermodynamic properties of random magnetic systems. One of these is the well-known replica trick proposed by Edwards and Anderson<sup>1</sup> and used by Sherrington and Kirkpatrick (SK)<sup>2</sup> to treat a system of spins interacting via a normally distributed potential of infinite range. However, since the replica method gives a negative entropy at  $T=0$ , it clearly is an approximation, valid over some limited temperature range.<sup>3</sup> Some mean-field methods which avoid the replica trick are the Bethe-Peierls-Weiss (BPW) method,<sup>4</sup> the self-consistent mean-random-field approximation (MRF)<sup>5,6</sup> and the method presented by Thouless *et al.*<sup>7</sup> (TAP) for the Gaussian random potential using the properties of random matrices.

The MRF method<sup>6</sup> has been used previously to treat (i) the spin-glass transition for the Ruderman-Kittel-Kasuya-Yosida (RKKY)-system as well as for the Gaussian random potential, (ii) the random dipole system,<sup>8</sup> (iii) the random strain system,<sup>9</sup> (iv) the NMR linewidth of the ortho-para-hydrogen system,<sup>10</sup> and (v) the phase diagram of palladium-based alloys.<sup>11</sup> In every one of these cases some interesting properties are explored which cannot be obtained by the usual molecular field approximation. Whereas the MRF procedure greatly simplifies the treatment of a complicated system by reducing the problem to the evaluation of the Fourier transform of a single potential, its validity has not been estab-

lished beyond the fact that it is self-consistent.

The purpose of this paper is to use a modified BPW method coupled with the probability distribution of internal fields to compare the predictions of various mean-field approximations with each other. In particular we show that as the range of interaction goes to infinity, the BPW, the MRF, and the SK methods give identical magnetic properties. However, the internal energy arising from the MRF method differs from that of BPW and SK because MRF does not take into account correlations correctly. Furthermore, by integrating the BPW internal energy and adding a plausible phenomenological constant of integration, we obtain the TAP free energy. Using this free energy we find that any probability distribution of fields  $H$  which does not go to zero near  $H \approx 0$  faster than  $H^{1/2+6}$  with  $\delta > 0$  is unphysical in that it gives a negative entropy. Indeed, computer calculations<sup>7,12</sup> give a hole at the center of the distribution. However, the BPW method does not, and in fact, reproduces all the results of SK including the unphysical negative entropy of  $-k/2\pi$  at  $T=0$ .

To obtain the thermodynamic quantities in the BPW approximation, we write the Hamiltonian for  $z$  particles in the molecular field approximation and then treat the interaction of the  $(z+1)$ th spin  $S_0$ , placed at the origin, with all the other spins exactly. In this procedure the interaction potentials  $J_{0j}$  and the  $z$  internal fields  $H_i$  are independent random variables. We then obtain the single spin magnetization  $\langle S_i \rangle$  and the pair-correlation function  $\langle S_0 S_i \rangle$  using the Hamiltonian for

$z+1$  spins in terms of the variables  $J_{0i}$  and  $H_i$ . Any correlations between the  $H_i$ 's and  $\langle S_0 \rangle$  are neglected. The probability distributions of the  $J_{0i}$  are assumed *a priori* to be given, from which one derives self-consistently the expression for the probability distribution  $P_1(H_i)$ . The procedure is then to expand the  $\langle S_i \rangle$  and  $\langle S_0 S_i \rangle$  in terms of the  $J_{0i}$  and  $H_i$  and average over the independent random distributions. This procedure is used instead of the Gaussian random matrix method of TAP.<sup>7</sup>

We also use the BPW method to derive the expression for the thermodynamic properties of the RKKY system, where the random matrix method used by TAP is not applicable. We then compare the results with those derived for the RKKY system in the MRF approximation. Although it is difficult to solve the problem in the BPW method in general, we are able to describe the probability distribution of the internal fields  $H_0$  for large  $H_0$  and small  $H_0$ . Again, we find that at  $T=0$  the BPW method as well as the MRF method give  $P(H=0) \neq 0$ , in contrast to the computer results.<sup>7,12</sup> We then obtain the probability distribution of the fields, the phase diagram, the magnetic susceptibility, the internal energy, and the specific heat of the RKKY system near the spin-glass transition temperature  $T_g$ . We find that whereas the magnetic susceptibility  $\chi$  as well as the specific heat  $C_M$  have a discontinuous derivative at  $T=T_g$ , for low concentrations both continue to increase below  $T_g$  and have a maximum at  $T$  well below  $T_g$ . The susceptibility result is in qualitative agreement with previous MRF calculations.<sup>6</sup>

In order to examine the variation of the magnetic properties with the number of neighbors  $z$ , we calculate the phase diagram for a Gaussian potential with various values of  $z$  from  $z=2$  to  $z=20$  in the MRF method. We find that whereas for small  $z$  the phase diagram changes quite strongly with  $z$ , once we have reached the value of  $z$  around 8 there is very little further change in the phase diagram with increasing  $z$ . Thus for  $z>8$  the MRF calculation already gives a phase diagram very close to that obtained by SK.

## II. BETHE-PEIERLS-WEISS APPROXIMATION

In the BPW approximation, one writes a Hamiltonian for a cluster of  $z$  spins in the molecular field approximation and then treats the interaction of the  $(z+1)$ th spin  $S_0$  with the cluster exactly. The BPW Hamiltonian is

$$\mathcal{H}_{\text{BPW}} = - \sum_{i=1}^z H_i S_i - \sum_{i=1}^z J_{0i} S_0 S_i, \quad (2.1)$$

where  $H_i$  is the internal field at site  $i$  and  $J_{0i}$  is the interaction potential between the spins  $S_0$  and  $S_i$ , where the  $S$  are Ising spins. Using Eq. (2.1) one obtains the following exact expressions in the BPW approximation:

$$\langle S_0 S_i \rangle = (1 - t_i^2 g_{0i}^2)^{-1} [g_{0i}(1 - t_i^2) + t_i(1 - g_{0i}^2) \langle S_0 \rangle], \quad (2.2)$$

$$\langle S_0 \rangle = \tanh \left( \sum_{i=1}^z \tanh^{-1}(t_i g_{0i}) \right), \quad (2.3)$$

$$\langle S_i \rangle = (1 - t_i^2 g_{0i}^2)^{-1} [t_i(1 - g_{0i}^2) + g_{0i}(1 - t_i^2) \langle S_0 \rangle], \quad (2.4)$$

where the averaging  $\langle \rangle$  is done in the  $(z+1)$ -particle BPW system. In the above equations,

$$t_i = \tanh \beta H_i, \quad (2.5)$$

$$g_{0j} = \tanh \beta J_{0j}. \quad (2.6)$$

The internal energy  $U$  in the BPW approximation is

$$U = - \frac{1}{2} \sum_{ij} J_{ij} \langle S_i S_j \rangle. \quad (2.7)$$

In the expression for  $U$  there are two random variables, the quantities  $J_{0i}$  and  $t_i$ . We find that the problem can be formulated self-consistently such that each of these two quantities are independent random variables. The probability distribution  $P_2(J_{ij})$  is assumed to be given and we then find the probability distribution of the fields  $P_1(H_i)$ . From  $P_1(H_i)$  and  $P_2(J_{ij})$  we will obtain the thermodynamic variables using the BPW approximation.

Letting  $\langle S_0 \rangle = \tanh \beta H_0$  in Eq. (2.3) gives for the field  $H_0$  at spin  $S_0$  (for BPW method)

$$H_0 = \beta^{-1} \sum_{i=1}^z \tanh^{-1}(t_i g_{0i}). \quad (2.8)$$

For comparison we also write the expression for the internal field  $H_0$  in the MRF approximation which is<sup>5,6</sup>

$$H_0 = \sum J_{0j} t_j. \quad (2.9)$$

The  $z$  variables  $H_i$  are assumed to be independent of each other in the spirit of the BPW approximation. The interactions  $J_{0i}$  are *a priori* independent variables of the model. The  $H_i$ 's are assumed to be independent of the  $J_{0i}$  (and  $\langle S_0 \rangle$ ) because the fields  $H_i$  arise from the spins and interactions outside the cluster of  $z+1$  spins. This assumption, typical of BPW, neglects the fact that the spins outside the cluster are not totally independent of the spins in the cluster. With these assumptions the distribution  $H_0, P_0(H_0)$ , is<sup>6</sup>

$$P_0(H_0) = \prod_{i=1}^z \int_{-\infty}^{\infty} P_1(H_i) dH_i \prod_{i=1}^z \int_{-\infty}^{\infty} P_2(J_{0i}) dJ_{0i} \delta\left(H_0 - \beta^{-1} \sum_{i=1}^z \tanh^{-1}(t_i g_{0i})\right). \quad (2.10)$$

At the end of our calculations we will require that the distributions  $P_0(H)$  and  $P_1(H)$  be identical. For the BPW case this introduces an error of order  $z^{-1/2}$  which goes to zero as  $z \rightarrow \infty$ .

For the MRF case no additional error is intro-

duced by this requirement (since the  $H_i$ 's are the total fields),<sup>5</sup> however, there is already an error of order  $z^{-1/2}$  due to neglect of correlations included in the BPW.

Rewriting Eq. (2.10) gives

$$P_1(H_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\rho H_0} d\rho \prod_{i=1}^z \left( \int P_1(H_i) dH_i \int P_2(J_{0i}) dJ_{0i} \exp[-i\rho\beta^{-1} \tanh^{-1}(t_i g_{0i})] \right). \quad (2.11)$$

It is convenient to write Eq. (2.11) in the form,

$$P_1(H_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\rho H_0} d\rho \{1 - V'(\rho)\}^z, \quad (2.12)$$

where

$$V'_{\text{BPW}} = \int_{-\infty}^{\infty} P_1(H_i) dH_i \int P_2(J_{0i}) dJ_{0i} \{1 - \exp[-i\rho\beta^{-1} \tanh^{-1}(t_i g_{0i})]\}. \quad (2.13)$$

For a symmetric probability distribution  $P_2(J_{ij})$ , Eq. (2.13) becomes

$$V'_{\text{BPW}} = \int_{-\infty}^{\infty} P_1(H_i) dH_i \int_{-\infty}^{\infty} P_2(J_{0i}) dJ_{0i} \{1 - \cos[\rho\beta^{-1} \tanh^{-1}(t_i \tanh\beta J_{0i})]\}. \quad (2.14)$$

To obtain the expression for  $P_1(H_0)$  in the MRF approximation we replace<sup>5</sup>

$$[\tanh^{-1}(t_i \tanh\beta J_{0i})]_{\text{BPW}} \rightarrow [\beta t_i J_{0i}]_{\text{MRF}} \quad (2.15)$$

as can be seen by comparing Eqs. (2.9) and (2.8). Thus in MRF we get

$$V'_{\text{MRF}} = \int_{-\infty}^{\infty} P_1(H_i) dH_i \int P_2(J_{0i}) dJ_{0i} (1 - e^{-i\rho t_i J_{0i}}). \quad (2.16)$$

### III. GAUSSIAN DISTRIBUTION OF INTERACTION STRENGTHS

#### A. Infinite-range potential

Here we show that when the range of the interaction becomes infinite, the probability distribution of fields obtained in the BPW approximation is identical to that obtained in the MRF approximation.

Let the number of neighbors  $z \rightarrow \infty$  and let  $\langle J_{0i} \rangle_c \propto z^{-1}$  and  $\langle J_{0i}^2 \rangle_c \propto z^{-1}$ , where  $\langle \rangle_c$  denotes a configurational average. In this limit  $\tanh^{-1}(t_i g_{0i}) = t_i J_{0i} + O(1/z)$ . The field  $H_0$  is given by Eq. (2.8) becomes identical to Eq. (2.9) which is the MRF expression.<sup>5</sup> The probability distribution of the random internal fields was studied for this case in the MRF approximation by Klein<sup>6</sup> and in the BPW approximation by Plefka,<sup>13</sup> the resultant expression for  $P_1(H_0)$  being identical for the two. For orientational purposes we briefly rederive these results using the method of Plefka.<sup>13</sup> Let

$$P_2(J_{0i}) = (2\pi J^2)^{-1/2} \exp\left[-\frac{1}{2} \left(\frac{J_{0i} - J_0}{J}\right)^2\right]. \quad (3.1)$$

Expanding the exponential in Eq. (2.16) and keeping only terms of lowest power in  $1/z$  (note that  $\langle J_{0i}^{2k} \rangle \propto z^{-k}$  and  $\langle J_{0i}^{2k+1} \rangle \propto z^{-k-1}$ ) gives

$$V' = -i\rho m J_0 + \frac{1}{2} \rho^2 J^2 q + O(\rho^3 \langle t_i^3 \rangle z^{-2}) \quad (3.2)$$

with  $m$  being the magnetization defined by

$$m = \langle t_i \rangle = \int_{-\infty}^{\infty} P_1(H_i) \tanh(\beta H_i) dH_i \quad (3.3)$$

and  $q$  being the spin-glass order parameter given by

$$q = \langle t_i^2 \rangle = \int_{-\infty}^{\infty} P_1(H_i) \tanh^2(\beta H_i) dH_i. \quad (3.4)$$

In the limit  $z \rightarrow \infty$  we have (letting  $\bar{J}_0 = J_0/z$  and  $\bar{J}^2 = J^2/z$ )

$$\{1 - V'\}^z = \exp(i\rho m \bar{J}_0 - \frac{1}{2} \rho^2 \bar{J}^2 q). \quad (3.5)$$

Substituting Eq. (3.5) into Eq. (2.12) gives

$$P_1(H_0) = (2\pi\sigma^2)^{-1/2} \exp\left[-\frac{1}{2} \left(\frac{H_0 - \bar{J}_0 m}{\sigma}\right)^2\right], \quad (3.6)$$

where for this case

$$\sigma_{\text{BPW}} = \sigma_{\text{MRF}} = (\bar{J}^2 q)^{1/2}. \quad (3.7)$$

Thus the temperature dependence of the spin-glass order parameter, the phase diagram and the magnetic properties are *identical* for the case  $z \rightarrow \infty$  in the MRF, BPW, and SK treatments.

The internal energy in the BPW approximation is obtained following the method of Plefka,<sup>13</sup> where  $U$  is given by Eq. (2.7). The evaluation of  $U$  has to be done carefully as is discussed in Sec. V, since the internal fields and the  $J_{0i}$  are independent random variables. Thus  $\langle S_0 S_i \rangle$  and  $\langle S_0 \rangle$  must be expanded in variables involving the  $t_i$ 's and the  $J_{0i}$ 's neglecting higher powers in  $1/z$ . We have

$$\langle S_0 S_i \rangle = \beta J_{0i} (1 - t_i^2) + t_i \langle S_0 \rangle + O(J_{0i}^2), \quad (3.8)$$

$$\langle S_0 \rangle = t_0 + \beta J_{0i} (1 - t_0^2) t_i + O(J_{0i}^2). \quad (3.9)$$

We must keep all terms of order  $J_{0i}$  in Eqs. (3.8) and (3.9), whereas terms of order  $J_{0i}^2$  can be neglected.

Substituting Eqs. (3.8) and (3.9) into Eq. (2.7) gives

$$U_{\text{BPW}}/N = -\bar{J}_0 m^2/2 - \beta \bar{J}^2 (1 - q^2)/2. \quad (3.10)$$

Equation (3.10) is identical to the SK internal energy.

The internal energy using the MRF approximation is

$$U_{\text{MRF}}/N = \frac{1}{2} \int_{-\infty}^{\infty} P(H) H \tanh(\beta H) dH \\ = -\frac{1}{2} \bar{J}_0 m^2 - \frac{1}{2} \bar{J}^2 q (1 - q). \quad (3.11)$$

This result has also been derived by Kaneyoshi<sup>14</sup> using a different method.<sup>15</sup> The difference in the internal energy  $U_{\text{MRF}}$  given by Eq. (3.11) and  $U_{\text{BPW}}$  given by Eq. (3.10) is the correlation energy considered in the BPW model and not considered in the MRF method. The fact that  $U_{\text{BPW}}$  for the infinite-range potential agrees with the SK calculation suggests that even for the case when one obtains  $P_1(H_0)$  from the MRF method one should use BPW to calculate the internal energy and the specific heat. However, the magnetic properties are identical in the BPW and MRF methods in the limit as  $z \rightarrow \infty$ .

#### B. Finite-range potential

Here we consider the magnetic properties of a system with a Gaussian distribution of finite-range interactions. First, the MRF approximation is used to calculate the distribution of internal fields  $P_1(H_0)$  and to find the phase diagram of this system as a function of  $z$ . We expect this to be a more realistic approximation of some physical amorphous ferromagnets and spin-glasses than the  $z \rightarrow \infty$  case. However, we find that for  $z \geq 8$ , the phase diagram of the system differs little from the  $z \rightarrow \infty$  results for which we have already shown that the magnetic properties from the MRF are identical to BPW and SK. Finally, BPW is used to calculate  $P_1(H_0)$  near  $T_c$  when  $J_0 = 0$ . We find that the resultant transition temperature is reduced from the MRF result by a correction term proportional to  $1/z$ .

Substituting Eq. (3.1) into Eq. (2.16) gives

$$1 - V'_{\text{MRF}} = \int_{-\infty}^{\infty} dH_i P_1(H_i) \\ \times \exp\left[-\frac{1}{2} (J\rho t_i)^2 + i\rho J_{0i} t_i\right]. \quad (3.12)$$

Using Eq. (2.12), the distribution of internal fields is given by

$$P_1(H_0) = \prod_{i=1}^z \int_{-\infty}^{\infty} P_1(H_i) dH_i [2\pi J^2 Q]^{-1/2} \\ \times \exp\left[-\frac{1}{2Q} \left(\frac{H_0 - J_0 M}{J}\right)^2\right], \quad (3.13)$$

where  $M = \sum_{i=1}^z \tanh \beta H_i$  and  $Q = \sum_{i=1}^z \tanh^2 \beta H_i$ .

At high temperatures the system is in the paramagnetic phase and only the trivial solution  $P_1(H_0) = \delta(H_0)$  is possible. For temperatures just below  $T_c$ ,  $P_1(H_0)$  will be a narrow distribution centered very close to  $H_0 = 0$  so that  $\tanh \beta H_i$  can be expanded about  $H_i = 0$  in Eqs. (3.3) and (3.4). In this way, the critical temperature is determined to be the greater of

$$T_c = \bar{J} \quad (3.14)$$

or

$$T_g = (\bar{J}_0^2/z + \bar{J}^2)^{1/2}. \quad (3.15)$$

The system orders as a ferromagnet if  $\bar{J}_0/\bar{J} > (1 - 1/z)^{-1/2}$  and as a spin-glass if the converse is true. Note that  $T_c$  is identical to the  $z \rightarrow \infty$  results, however,  $T_g$  is greater than the  $z \rightarrow \infty$  result due to the addition of the  $\bar{J}_0^2/z$  term within Eq. (3.15).

At  $T=0$ , Eq. (3.13) reduces to

$$P_1(H_0) = 2^{-z} (2\pi\bar{J}^2)^{-1/2} \times \sum_{n=0}^z \binom{z}{n} (1+m)^{z-n} (1-m)^n \times \exp\{- (2\bar{J}^2)^{-1} [H_0 - \bar{J}_0(z-2n)/z]^2\}, \quad (3.16)$$

where the binomial coefficient  $\binom{z}{n} = z!/[n!(z-n)!]$ . Thus,  $P_1(H_0)$  near  $T=0$  is the sum of  $z+1$  Gaussians. Each Gaussian is centered about  $S_1 J_0$  where  $S_1$  can range through the  $z+1$  eigenvalues of the total spin of the  $z$  nearest neighbors. For

$$D = \frac{(2/\pi)^{1/4}}{zR_c} \sum_{n=0}^{z/2} \left[ \binom{z}{n} (z-2n)^2 \exp\left(-\frac{\frac{1}{2}(z-2n)^2}{(zR_c)^2}\right) \right] \left\{ \sum_{n=0}^{z/2} \binom{z}{n} \left[ n(z-2n) - \binom{z-2n}{3} \right] \Phi\left(\frac{z-2n}{zR_c\sqrt{2}}\right) \right\}^{-1}. \quad (3.20)$$

Note that a ferromagnetic state is not possible for nonzero  $\bar{J}$  if  $z \leq 2$ . In the  $z \rightarrow \infty$  limit,  $R_c = (2/\pi)^{1/2}$  and  $D = (72/\pi)^{1/4}$  in agreement with SK. [Note, however, that there is a misprint in Eq. (2.22) of Kirkpatrick and Sherrington.<sup>12</sup>] We have evaluated  $R_c$  and  $D$  numerically for values of  $z$  ranging from  $z=3$  to 20 and find that for  $z > 8$ ,  $R_c$  and  $D$  change very slowly. Table I tabulates  $R_c$  and  $D$  for several values of  $z$ .

The phase diagrams for several values of  $z$  are shown in Fig. 1. Once a value of  $z$  around 8 is reached there is very little further change in the phase diagrams (less than 10%) as a function of  $z$ . This suggests that the  $z \rightarrow \infty$  results adequately

TABLE I. Numerical values of  $R_c$  and  $D$ , which are defined in Eqs. (2.19) and (2.20), are listed for various values of  $z$ . If  $\bar{J}/\bar{J}_0 < R_c$  then the system is ferromagnetic at  $T=0$ , otherwise the system is in the spin-glass phase.

$z$	$R_c$	$D$	$z$	$R_c$	$D$
2	0	...	10	0.736	2.44
3	0.594	3.12	12	0.746	2.43
4	0.645	2.87	16	0.758	2.37
6	0.695	2.61	20	0.765	2.34
8	0.721	2.50	$\infty$	0.798	2.19

small fluctuations,  $(\bar{J}/\bar{J}_0 \ll 1)$ ,

$$m \approx 1 - (2/\pi)^{1/2} (\bar{J}/\bar{J}_0) \exp[-\frac{1}{2} (\bar{J}_0/\bar{J})^2] \quad (3.17)$$

which is identical to the  $z \rightarrow \infty$  result of SK. Near the spin-glass boundary, the magnetization is given by

$$m \approx D(R_c - \bar{J}/\bar{J}_0)^{1/2}. \quad (3.18)$$

$R_c$  is determined by the condition,

$$\sum_{n=0}^{z/2} \binom{z}{n} (z-2n) \Phi[(z-2n)/zR_c] = 2^{z-1}, \quad (3.19)$$

where  $\Phi(x) = (2/\pi)^{1/2} \int_0^x e^{-t^2} dt$  is the error function and  $[z/2]$  is the largest integer  $\leq z/2$ . The coefficient  $D$  is given by,

describe typical materials as  $z$  is generally greater than 8.

As observed by Kirkpatrick and Sherrington,<sup>12</sup> the magnetization increases with temperature near  $T=0$ . Actually, it is possible to show that within the MRF approximation at very low temperatures,

$$m(T) = m(T=0) + BT + \dots, \quad (3.21)$$

for any distribution of potentials  $P_2(J_{0i})$ , where  $B \propto P_1(0)$ .

We now consider the derivation of  $P_1(H_0)$  in the BPW approximation. In order to simplify the calculations, we only treat the case when  $J_0 = 0$ .

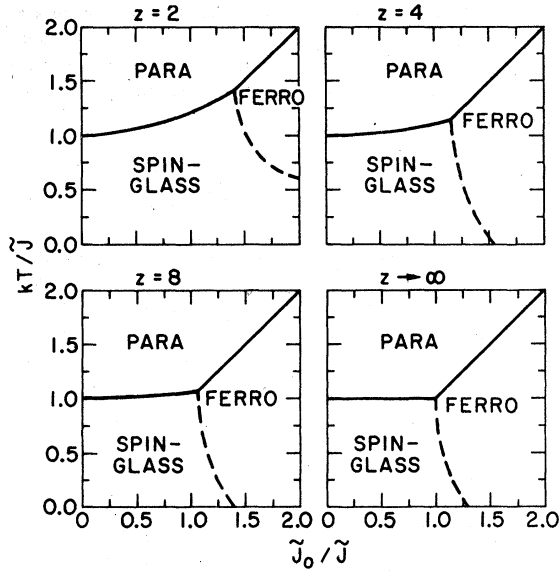


FIG. 1. Phase diagrams of a spin system in which each spin interacts with  $z$  nearest neighbors, as calculated within the MRF, are shown for several values of  $z$ . The end points of the dotted line are calculated exactly (see the text), however, the exact shape of this line is not known. Note that the phase diagram for  $z=8$  is already very close to that  $z \rightarrow \infty$  case.

Even with this simplification, the calculations become complicated as  $T \rightarrow 0$  (it is simpler for the RKKY interaction as will be shown later). However, at  $T$  near  $T_c$  the correction to the  $z \rightarrow \infty$  is rather straightforward, within the assumptions mentioned immediately following Eq. (2.10).

From Eq. (2.14) we have

$$1 - V'_{BPW} = \int_{-\infty}^{\infty} P_1(H_i) dH_i \int_{-\infty}^{\infty} P_2(J_{0i}) dJ_{0i} \times \cos[\rho\beta^{-1} \tanh^{-1}(t_i g_{0i})]. \quad (3.22)$$

For  $T$  near  $T_c$ , the quantity  $\mu_k$ , defined by

$$\mu_k = \langle t_i^k \rangle = \int P(H_i) \tanh^k \beta H_i dH_i, \quad (3.23)$$

is small for all integer  $k$ . Furthermore,  $\mu_{k+2} \ll \mu_k$ . We thus expand Eq. (3.22) in a power series of  $t_i$  to give

$$1 - V'_{BPW} = 1 - \frac{\rho^2}{2\beta^2} \langle x^2 \rangle + \frac{\rho^4}{4! \beta^4} \langle x^4 \rangle + \dots \quad (3.24)$$

In the above equation  $\langle x^2 \rangle \approx \mu_2 g_2 + \frac{2}{3} \mu_4 g_4$  and  $\langle x^4 \rangle \approx \mu_4 g_4$  with

$$g_k = \int_{-\infty}^{\infty} P_2(J_{0i}) dJ_{0i} (\tanh \beta J_{0i})^k. \quad (3.25)$$

Substituting the above in Eq. (2.12) gives

$$P_1(H_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\rho H_0} d\rho \exp\left(-\frac{z}{2} \frac{\rho^2}{\beta^2} \langle x^2 \rangle - \frac{z\rho^4}{12\beta^4}\right) \times [3\mu_2^2 g_2^2 - \mu_4 g_4]. \quad (3.26)$$

Evaluating Eq. (3.26) for large but finite  $z$ , we have

$$P_1(H_0) = (2\pi\sigma^2)^{-1/2} \exp\left[-\frac{1}{2}(H/\sigma)^2\right] \times \left\{1 + \frac{1}{4z} [3 - 6(H/\sigma)^2 + (H/\sigma)^4]\right\}, \quad (3.27)$$

where

$$\sigma = [z\langle x^2 \rangle]^{1/2} / \beta.$$

In the limit as  $z \rightarrow \infty$ ,  $g_2 = \beta^2 J^2$ , and Eq. (3.27) reduces to Eq. (3.6).

Using Eq. (3.27) to calculate the spin-glass temperature, we find

$$T_c = (\tilde{J}/k)(1 - 1/z) + O(1/z^2). \quad (3.28)$$

Note that for  $z \geq 8$  the correction to the  $z \rightarrow \infty$  transition temperature is less than 12%.

#### IV. RKKY INTERACTION

##### A. Probability distribution of the internal fields

We next consider the probability distribution for the RKKY interaction. We assume that  $J_{ij}$  is of the form<sup>5</sup>

$$J_{0i} = \pm a/r_{0i}^3, \quad (4.1)$$

with a probability for the + and - sign each equal to  $\frac{1}{2}$ . We also let the spins be randomly and uniformly distributed throughout the volume  $V$  of the solid. Then

$$P_2(|J_{0i}|) d|J_{0i}| \rightarrow 4\pi r_{0i}^2 dr_{0i} / V. \quad (4.2)$$

Let  $N_0$  be the number of sites in the solid and  $c$  be the fractional impurity concentration ( $c = N/N_0$ ). Replacing  $z$  in Eq. (2.12) with  $N_0 c$ , we obtain in the thermodynamic limit

$$P_1(H_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\rho H_0} e^{-V'(\rho)cN_0}, \quad (4.3)$$

where  $V'$  is given by Eq. (2.14) for the BPW case and by Eq. (2.16) for the MRF case.

Using the potential in Eq. (4.1), integrating from a near-neighbor distance  $r_0$  to infinity, and changing the variable of integration to  $y = \beta a/r^3$ , gives

$$V'_{\text{BPW}} = \frac{4\pi}{3V} a\beta \int_{-\infty}^{\infty} P_1(H_i) dH_i \int_0^{\beta a/r_0^3} \frac{1 - \cos[\rho\beta^{-1} \tanh^{-1}(t_i \tanh y)]}{y^2} dy. \quad (4.4)$$

We now treat several different cases of interest.

$P(H_0)$  for the RKKY potential at  $T=0$ . For  $T=0$  the expression for  $\tanh^{-1}(t_i g_{0i})$  is, for both  $J_{0i}$  and  $H_i$  positive,

$$\tanh^{-1}(t_i \tanh \beta J_{0i}) = \begin{cases} \beta J_{0i}, & J_{0i} < H_i \\ \beta H_i, & J_{0i} > H_i \end{cases}. \quad (4.5)$$

Substituting Eq. (4.5) into Eq. (4.4) and integrating by parts gives

$$V'_{\text{BPW}} = \frac{8\pi}{3V} \rho a \left\{ \int_0^{a/r_0^3} P_1(H_i) dH_i \left( \int_0^{\rho H_i} \frac{\sin x}{x} dx + \frac{r_0^3}{\rho a} (\cos \rho H_i - 1) \right) + \int_{a/r_0^3}^{\infty} P_1(H_i) dH_i \left[ \int_0^{\rho a/r_0^3} \frac{\sin x}{x} dx + \frac{r_0^3}{\rho a} \left( \cos \frac{\rho a}{r_0^3} - 1 \right) \right] \right\}. \quad (4.6)$$

Equation (4.6) is to be compared with the corresponding expression for the MRF case which is

$$V'_{\text{MRF}} = \frac{4\pi}{3} \frac{\rho a}{V} \int_{-\infty}^{\infty} P(H_i) t_i dH_i \left\{ \int_0^{\rho a t_i / r_0^3} \frac{\sin x}{x} dx + \frac{r_0^3}{\rho a t_i} \left[ \cos \left( \frac{\rho a t_i}{r_0^3} \right) - 1 \right] \right\}. \quad (4.7)$$

Whereas Eq. (4.6) is only valid for  $T=0$ , Eq. (4.7) is valid for all temperatures. At  $T=0$ ,  $t_i$  in Eq. (4.7) becomes unity and if we replace  $\rho H_i$  in Eq. (4.6) by  $\rho a/r_0^3$ ; Eqs. (4.6) and (4.7) become identical.

Even though the integrals Eq. (4.6) and Eq. (4.7) are not simple to evaluate in general, it is easy to discuss the behavior of the probability distribution for very large and very small fields. To determine the wings of  $P_1(H_0)$  ( $H_0 \rightarrow \infty$ ) we are only interested in small values of  $\rho$ . Expanding Eq. (4.7) in a power series of  $\rho$  and letting  $\lim_{\beta \rightarrow \infty} |t_i| = 1$  gives

$$V'_{\text{MRF}} = \frac{2}{3} \pi (\rho a)^2 / V r_0^3, \quad \rho \rightarrow 0. \quad (4.8)$$

Substituting Eq. (4.8) into Eq. (4.3) and letting  $V = N_0 v_c = N_0 k r_0^3$ , where  $v_c$  is the volume per site and  $k$  is a geometrical factor of order unity, we obtain

$$P_1(H_0) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-\frac{1}{2}(H/\sigma)^2], \quad H_0 \rightarrow \infty, T=0, \quad (4.9)$$

where

$$\sigma_{\text{MRF}}^2 = (4\pi/3k)(a/r_0^3)^2 c. \quad (4.10)$$

Expanding Eq. (4.6) for  $\rho \rightarrow 0$  we obtain the probability distribution in the BPW method for the RKKY interaction. Again we obtain a Gaussian with a width

$$\sigma_{\text{BPW}} = \frac{8\pi}{3} \frac{ac}{k r_0^3} \left( h_1 - \frac{r_0^3}{2a} h_2 \right) + O[\exp(-c^{-\alpha})], \quad (4.11)$$

where

$$h_k = 2 \int_0^{\infty} P_1(H_i) H_i^k dH_i, \quad \text{and } 2 \geq \alpha \geq 1.$$

Since  $a/r_0^3$  is the near-neighbor interaction,  $h_k$  is always less than  $(a/r_0^3)^k$ . Thus the width of the distribution which describes the wings of  $P(H_0)$  at  $T=0$  is always smaller in the BPW case than in the MRF case.

We next examine the behavior of  $P_1(H_0)$  for very low  $c$  in the limit as  $H_0 \rightarrow 0$ . For this case all values of  $\rho$  in Eq. (4.3) contribute. The contribution to  $V'$  for both MRF and BPW is proportional to  $\rho$  for large  $\rho$  and to  $\rho^2$  for small  $\rho$ . In the limit as  $c \rightarrow 0$ , the integral, Eq. (4.3), used to evaluate  $P_1(H_0 \approx 0)$  is dominated by the part of the contribution to  $V'$  which is proportional to  $\rho$  (large  $\rho$  limit). Therefore the center portion of  $P_1(H_0)$  at  $T=0$  is Lorentzian-like for both the BPW and MRF cases. The probability distribution has a maximum at  $H_0=0$ . We thus obtain

$$P_1(H_0) \approx \frac{1}{\pi} \frac{\Delta}{\Delta^2 + H_0^2}, \quad (4.12)$$

with

$$\Delta_{\text{MRF}} = \Delta_{\text{BPW}} \approx \frac{2\pi^2}{3} \frac{ac}{k r_0^3}. \quad (4.13)$$

The case of the MRF distribution has been explored in detail in Ref. 6, where it was found that for  $T$  near zero the wings of the distribution are approximately Gaussian with width proportional to  $c^{1/2}$ , whereas the center of the distribution is

approximately Lorentzian for  $c < 5\%$  and approximately Gaussian for  $c > 5\%$ . Near and above  $T_c$  the distribution becomes a  $\delta$  function at  $H_0 = 0$ .

#### B. RKKY potential near $T = T_g$ , BPW method

Near  $T = T_g$ ,  $t_i$  in Eq. (3.3) is small and therefore for  $\rho$  not too large we can expand Eq. (4.4) in a power series in  $t_i$  keeping only terms up to  $t_i^2$ . We obtain for the wings of the distribution function ( $H_0 \rightarrow \infty$ ) a Gaussian with width

$$\sigma_{\text{BPW}}^2 = \frac{8\pi}{3k} \frac{ac}{r_0^3} \frac{q}{\beta_g} \left( \frac{7}{\pi^2} \zeta(3) - \frac{r_0^3}{2a\beta_g} \right) + O[e^{-2c} c^{-\alpha/2}], \quad (4.14)$$

where the Riemann zeta function  $\zeta(3) = 1.2021$ ,  $(H/\sigma) \gg 1$ , and  $\beta_g = T_g^{-1}$ . This is to be compared with the width of the Gaussian describing the wings in the MRF case.

$$\sigma_{\text{MRF}}^2 = (4\pi/3k)qc(a/r_0^3)^2, \quad (4.15)$$

where  $q$  is defined in Eq. (3.4). Again, the width of the BPW distribution is less than that for the MRF distribution.

The width of the distribution near  $T_g$  with  $H_0$  near zero is next obtained. Again, all values of  $\rho$  contribute to the integral Eq. (4.3). Examining the integrand we find that for  $c \rightarrow 0$  the part of  $V'$  proportional to  $\rho$  (large  $\rho$ ) predominates the integrand in Eq. (4.3). Thus  $P_1(H_0)$  near  $H_0 \approx 0$  is approximately a Lorentzian with width

$$\sigma_{\text{BPW}} = \sigma_{\text{MRF}} \approx \frac{2}{3} \pi^2 (a/k r_0^3) |t| c, \quad (4.16)$$

where

$$|t| = \int_{-\infty}^{\infty} P_1(H) |\tanh \beta H| dH. \quad (4.17)$$

The fact that the form of  $P_1(H)$  near  $H \approx 0$  is a Lorentzian will have important consequences on the concentration dependence of the spin-glass transition temperature.

We conclude this section by emphasizing that the qualitative behavior of the probability distribution does not change in going from the MRF approximation to the BPW approximation, however, the quantitative values of the width may differ somewhat. Again, the difficulty with the BPW approximation is that it is very cumbersome, albeit in principle possible, to obtain the probability distribution for all temperatures and all impurity concentrations, whereas the MRF distribution is in general easier to calculate.

#### C. Spin-glass transition temperature and the magnetic susceptibility

We next evaluate the spin-glass transition temperature and the magnetic susceptibility for the

RKKY system. For  $T \approx T_c$ ,  $q \rightarrow 0$  and the width of the distribution also approaches zero. For  $T$  near  $T_g$  we have to solve self-consistently for the width of the distribution near the wings given by Eqs. (4.14) and (4.15) and for the width of the distribution near the center which is given by Eqs. (4.16) and (4.17). The transition temperature will occur when the width of the distribution becomes nonzero. This solution can only be obtained using computer calculations. However, near  $T_g$  the BPW distribution is close to the MRF distribution and therefore we present the MRF results.<sup>6</sup> Let

$$n_k(0) = 2 \int_0^{\infty} P_1(H) H^k dH, \quad (4.18)$$

where  $\eta_k(0)$  is the  $k$ th moment of the distribution evaluated at  $T = 0$ . Then as found in Ref. 6

$$T_g = \eta_1(0) = (a/k r_0^3) c^\alpha, \quad (4.19)$$

with  $\alpha \approx 0.66$  for  $0.01 < c < 0.04$  and  $\alpha \approx 0.5$  for  $c > 0.06$  (6%).

Note that  $T_g$  is not proportional to  $c$  and thus our result differs from that derived by Smith<sup>16</sup> for the BPW case using a different method. The expression for  $T_g$  does not obey the usual scaling laws discussed for the RKKY potential by Souletie and Tournier<sup>17</sup> and derived independently by Klein<sup>5</sup> (according to these  $T_g \propto c$ ). The reason the scaling laws<sup>5,17</sup> are not obeyed is because of the cutoff of the interaction potential at a near-neighbor distance. The experimental results are not inconsistent with a value of  $\alpha$  around 0.67.<sup>18</sup> The spin-glass order parameter is near  $T_g$

$$q \approx [3T^2/\eta_3(0)](T_g - T), \quad (4.20)$$

where<sup>6</sup>  $\eta_3(0) \propto c^{1.2}$  for  $0.01 < c < 0.04$  and  $\eta_3(0) \propto c^{1.5}$  for  $c > 6\%$ .

The average magnetization  $M_1$  per impurity is

$$M_1 = \int_{-\infty}^{\infty} P(H) \tanh \beta H dH, \quad (4.21)$$

and the magnetic susceptibility is obtained from Eq. (4.21) using the result that  $P_1(H)$  depends only on the square of the external field, we have

$$\chi = \beta \int P_1(H) \text{sech}^2(\beta H) dH = \beta(1 - q). \quad (4.22)$$

The slope of the magnetic susceptibility is

$$\frac{d\chi}{dT} = -\frac{1}{k_B T^2}; \quad T \geq T_g. \quad (4.23)$$

For  $T = T_g^-$ , where  $T_g^-$  is the temperature just be-



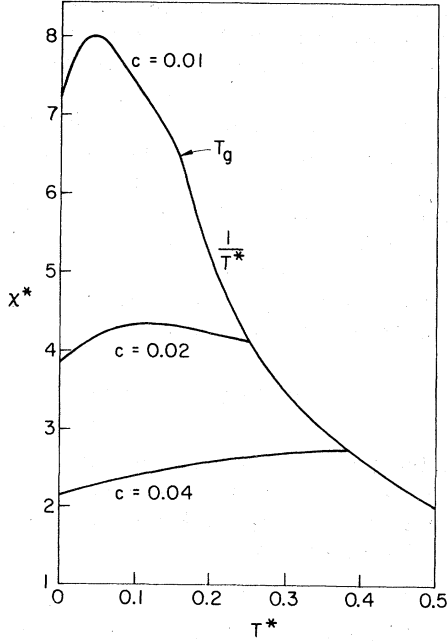


FIG. 2. Magnetic susceptibility per impurity  $\chi^*$  in arbitrary units as a function of the impurity concentration  $c$ , where  $T^* = T/(a/kr_0^3)^{-1}$  and  $a/r_0^3$  is the strength of the nearest-neighbor interaction. For the 1% concentration the calculated slope is discontinuous at  $T = T_c$ .

low  $T_g$ , we have

$$\left(\frac{d\chi}{dT}\right)_{T=T_g^-} = -\frac{1}{k_B T_g^2} \left(1 - \frac{3\eta_2(0)\eta_1(0)}{\eta_3(0)}\right), \quad (4.24)$$

where it is discussed in Ref. 6 that the slope of  $\chi$  below  $T_c$  is still negative for  $c$  of the order of 1% or less.

The computer-calculated results of the magnetic susceptibility for several impurity concentrations are shown in Fig. 2. Note that for the higher concentrations the susceptibility is very much like the one of SK whereas for low  $c$  the maximum in  $\chi$  occurs well below the discontinuous slope at  $T = T_g$ . Note that the results in Fig. 2 are for a static field, whereas the experiments were done in an alternating field.<sup>18</sup>

We next evaluate the internal energy  $U$  and the specific heat for the RKKY system using the BPW method. The expression for  $U$  is given by Eq. (2.7). To evaluate  $\langle S_0 S_i \rangle$  we expand  $\langle S_0 \rangle$  in a power series of  $g_{0i} t_i$ , since near  $T = T_g$ ,  $\langle t_i^n \rangle$  is small and  $\langle t_i^{2n} \rangle \ll \langle t_i^{2n+2} \rangle$  for all positive  $n$ . We then have

$$\langle S_0 S_j \rangle = g_{0j} [1 - q^2(1 - g_{0j}^2)] + O(q^3). \quad (4.25)$$

Substituting Eq. (4.25) into Eq. (2.7) gives

$$U = -\frac{1}{2} \sum_{i,j} J_{ij} \tanh \beta J_{ij} [1 - q^2(1 - \tanh^2 \beta J_{ij})], \quad (4.26)$$

with  $J_{ij}$  given in Eq. (4.1). This result agrees with that obtained by Smith<sup>16</sup> using a somewhat different approach.

The magnetic specific heat  $C_M$  is given by

$$C_M = \frac{2\pi N_0 c^2 \beta a}{3V} \int_0^{Ba/r_0^3} \left[ \text{sech}^2 z - q^2 (\text{sech}^2 z - 3 \tanh^2 z \text{sech}^2 z) - 2q\beta \frac{dq}{d\beta} \left(\frac{\tanh z}{z}\right) \text{sech}^2 z \right] dz. \quad (4.27)$$

Letting  $b = a/(r_0^3 k)$ , gives

$$C_M = \frac{2\pi N_0 c^2 k_B \beta b}{3} \left(1 - 2\beta A q \frac{dq}{d\beta}\right), \quad (4.28)$$

where

$$A = \int_0^{Ba/r_0^3} (\tanh z/z) \text{sech}^2 z dz = \frac{8}{\pi^2} \sum_{n=0}^{\infty} (2n+1)^{-3} = 0.8525.$$

The upper limit  $a/r_0^3$  in Eq. (4.27) was allowed to be infinity, since the error introduced by this approximation is only of the order of  $\exp(-1/c)$  which becomes very small for small  $c$ .

Using the expression for  $q$  from Eq. (4.20) we obtain

$$\frac{dC_M}{dT} = -\frac{2\pi N_0 c^2 b}{3T^2}, \quad T \geq T_g. \quad (4.29)$$

For  $T = T_g^-$ , i.e., just below the transition temperature we obtain

$$\frac{dC_M}{dT} = -\frac{2\pi N_0 c^2 b}{3T^2} \left(1 - \frac{18AT_g^6}{\eta_3^2}\right), \quad T \approx T_g^-. \quad (4.30)$$

For low concentrations,  $c \lesssim 1\%$ , it is found that the slope of  $C_M$  is discontinuous at  $T = T_g$  and continues to be negative for  $T$  just below  $T_g$ .

## V. FREE ENERGY

We next discuss the expression for the internal energy and the free energy for the random system and show that in order to obtain consistent results for the  $z \rightarrow \infty$  case one must expand the expression for the spin  $\langle S_0 \rangle$  and  $\langle S_i \rangle$  in terms of the  $J_{ij}$  and  $\langle S_i \rangle = \tanh \beta H_i$  as is done in Eq. (3.9).

Solving Eq. (2.3) for  $\langle S_0 \rangle$  and substituting into Eq. (2.2) gives for  $z \rightarrow \infty$

$$U = -\frac{1}{2} \sum_{i,j} J_{ij} \langle S_i S_j \rangle = -\frac{1}{2} \sum_{i,j} J_{ij} [\langle S_i \rangle \langle S_j \rangle + \beta J_{ij} (1 - \langle S_i \rangle^2)(1 - \langle S_j \rangle^2)]. \quad (5.1)$$

Equation (5.1) is identical with the value of  $U$  obtained by TAP.<sup>7</sup> At first it would seem that Eq. (5.1) is in disagreement with the SK result which gives for a symmetric potential  $U = -\frac{1}{2}NJ^2\beta(1-q^2)$ , whereas if one sets the average of  $\langle S_0 \rangle = 0$  because of the even symmetry of the potential one obtains  $U = -\frac{1}{2}NJ^2\beta(1-q^2)$ . The resolution of this difficulty is immediate when it is realized that  $\langle S_0 \rangle$  is a function of both the  $J_{ij}$  and the  $t_i$  given in Eq. (2.3) and therefore the averaging can only be done after we have expressed  $\langle S_0 \rangle$  in the form given by Eq. (3.9). Keeping terms to order  $1/z$  only, gives

$$U = -\frac{1}{2} \left( \sum_{i,j} J_{ij} t_i t_j + \beta J_{ij}^2 [(1-t_j^2)(1-t_i^2) + t_j^2 + t_i^2 - 2t_i^2 t_j + O(J_{ij}^3)] \right). \quad (5.2)$$

Now Eq. (5.2) can be averaged over  $J_{ij}$  and  $t_i$  independently and we obtain for the case when  $\langle t_i \rangle = 0$ ,

$$U = -\frac{1}{2} \beta NJ^2 (1-q^2), \quad (5.3)$$

which is the SK result.

The BPW method does not give any prescription for obtaining the free energy. However, we can write an expression for the microscopic free energy (for a given configuration of  $J_{ij}$ 's) in terms of the internal energy  $U(\beta)$  and a constant of integration  $S^0$  as follows:

$$F = \frac{1}{\beta} \left( \int_0^\beta U(\beta') d\beta' - S^0 \right). \quad (5.4)$$

In Eq. (5.4) only the explicit dependence of  $U(\beta')$  upon  $\beta'$  is taken into account. Substituting for  $U(\beta')$  from Eq. (5.1), which is exact in the BPW, and the phenomenological expression

$$S_0 = \sum_i \left[ \left( \frac{1+\langle S_i \rangle}{2} \right) \ln \left( \frac{1+\langle S_i \rangle}{2} \right) + \left( \frac{1-\langle S_i \rangle}{2} \right) \ln \left( \frac{1-\langle S_i \rangle}{2} \right) \right], \quad (5.5)$$

which is the entropy of a set of independent spins constrained to have a value  $\langle S_i \rangle$ , we obtain

$$F = - \sum_{i,j} J_{ij} \langle S_i \rangle \langle S_j \rangle - \frac{\beta}{2} \sum_{i,j} J_{ij}^2 (1-\langle S_i \rangle^2)(1-\langle S_j \rangle^2) + \frac{1}{\beta} S^0. \quad (5.6)$$

This expression for  $F$  is identical to the one obtained by TAP by diagrammatic methods. It therefore offers an intuitive approach for understanding the diagrammatic derivation.

The free energy in Eq. (5.6) is the free energy for a given configuration of the random interactions  $J_{ij}$ . This is a variational free energy with respect to the variable  $\langle S_i \rangle$  and  $\beta$ . Thermodynamic quantities appropriate for the quenched system can be obtained by first obtaining the appropriate quantity from Eq. (5.6) for a given configuration *and then* averaging it over all configurations. The internal energy obtained in this manner is obviously the same as in Eq. (5.1).

Differentiating Eq. (5.6) with respect to  $\langle S_i \rangle$  we obtain the microscopic equation

$$\sum J_{0j} \langle S_j \rangle - \langle S_0 \rangle \beta \sum J_{0j}^2 (1-\langle S_j \rangle^2) = T \tanh^{-1} \langle S_0 \rangle. \quad (5.7)$$

Multiplying Eq. (5.7) by  $\langle S_0 \rangle$  and expanding in a power series of  $J_{ij}$ , keeping terms to order  $z^{-1}$ , and then averaging over the distribution of the  $J_{ij}$ 's and the  $H_i$ 's gives, for  $T$  near  $T_g$ ,

$$q(\beta \bar{J}^2 - T) - q^2(\beta \bar{J}^2 + \beta^3 \bar{J}^4) + O(q^3) = 0. \quad (5.8)$$

Equation (5.8) gives  $T_g = \bar{J}$  and

$$q \propto (T_g - T), \quad T \lesssim T_g. \quad (5.9)$$

The entropy  $S$  for a given configuration is

$$S = \beta^2 \frac{\partial F}{\partial \beta} = -\frac{1}{2} \beta^2 \sum_{i,j} J_{ij}^2 (1-\langle S_i \rangle^2)(1-\langle S_j \rangle^2) - \left( \frac{1+\langle S_i \rangle}{2} \right) \ln \left( \frac{1+\langle S_i \rangle}{2} \right) - \left( \frac{1-\langle S_i \rangle}{2} \right) \ln \left( \frac{1-\langle S_i \rangle}{2} \right). \quad (5.10)$$

Averaging  $S$  over a probability distribution for  $H_i$  and  $J_{0i}$  gives the quenched entropy  $\bar{S}$  per particle,

$$\bar{S} = -\frac{\beta^2 \bar{J}^2}{4} (1-q)^2 + \frac{1}{\beta} \int_0^\infty P_1 \left( \frac{x}{\beta} \right) \left( \ln(1+e^{-2x}) + \frac{x e^{-x}}{\cosh x} \right) dx, \quad (5.11)$$

where  $q$  is given by Eq. (3.4). If  $P_1(H)$  given by Eq. (3.6) is used to evaluate Eq. (5.11) at  $T=0$  one obtains  $S = -1/2\pi$  which is the same as obtained by SK. It is important to note that unless the quantity  $(1-q)^2$  falls off faster than  $T^3$  the first term in Eq. (5.11) dominates and gives a negative entropy as  $T \rightarrow 0$ . This clearly indicates that any probability distribution for the fields which is such that  $P_1(0) \neq 0$  would produce a negative entropy near zero temperature and is therefore unphysical. The distributions arising in the SK theory (which is also a Gaussian<sup>6</sup>) as well as the MRF and the BPW treated here are all equally unphysical. Specifically, inspection of

Eq. (5.11) reveals that  $P_1(H)$  for  $H \rightarrow 0$  must decrease faster than  $H^{1/2}$  in order to realize a non-negative entropy using TAP's free energy. No such probability distribution arises from the simple molecular field treatments discussed so far (SK, MRF, BPW). Computer calculations by TAP and SK which take into account correlations more completely show that the probability distribution of  $\bar{h}_i = \sum J_{ij} \langle S_j \rangle$  has a hole at  $\bar{h}_i = 0$ . We reiterate that, within the BPW,  $H_0$  is defined by Eq. (2.8), and is a different quantity than  $\bar{h}_i$ . If we calculate  $p(\bar{h}_i)$  in the BPW we obtain  $p(\bar{h}_i) = 0$  for  $\bar{h}_i = 0$ . However, the quantitative behavior of our  $p(\bar{h})$  for finite  $\bar{h}$  differs from the computer results.

## VI. SUMMARY

A generalization of the Bethe-Peierls-Weiss (BPW) method employing a self-consistent distribution of internal fields has been devised to study random spin systems. This method gives directly all the thermodynamic observables except the entropy which is obtained by the addition of a plausible phenomenological constant of integration. Our method also gives a convenient framework to examine the interrelationship between various molecular field theories for spin-glasses.

In the limit as  $z \rightarrow \infty$  we have shown that the mean-random-field (MRF) method gives identical magnetic properties to that obtained in the BPW and Sherrington-Kirkpatrick (SK) calculations. However, the MRF internal energy differs from the corresponding result of BPW and SK due to neglect of correlations in MRF. For finite  $z$  we

use MRF to obtain the phase diagram of a system with Gaussian distribution of interactions. For  $z > 8$  we find that the quantitative differences between the finite  $z$  and infinite  $z$  phase diagram is less than 10%.

We use the BPW method to study the properties of a system with a RKKY interaction. We find a discontinuous slope in the magnetic susceptibility and the specific heat  $C_M$  at the spin-glass transition temperature  $T_g$ . However, the maxima in  $\chi$  and  $C_M$  occur well below  $T_g$ . The result for  $\chi$  is in qualitative agreement with the MRF method. However, to our knowledge the discontinuous slope in the specific heat has so far not been observed experimentally.

Returning to the  $z \rightarrow \infty$  case, we would like to emphasize that our BPW results duplicate every observable thermodynamic quantity calculated by SK. In particular this includes the negative entropy  $-k/2\pi$  at  $T=0$ . This suggests that our method of using the distribution of internal fields is entirely equivalent to the SK approach. The negative entropy is shown to arise from the Thouless-Anderson-Palmer (TAP) free energy whenever the probability distribution of the internal fields  $P_1(H)$  is finite at  $H=0$ . In fact, from our free energy any  $P_1(H)$  which does not go to zero as  $H^{1/2+\delta}$  ( $\delta > 0$ ) is unphysical and gives a negative entropy.

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