

Disordered magnetic lattice gas: Formulation by the method of the distribution function

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A spin-1 model of a disordered magnetic lattice gas with magnetic and nonmagnetic interactions is presented as an extension of the magnetic gas introduced in the previous paper. A formulation using the method of the distribution functions is given. The concept of an effective potential is introduced along with the usual effective field in order to describe this system. Integral equations for the distribution functions are derived as a natural extension of the Bethe-Peierls-Weiss approximation to the disordered magnetic system. The form of the thermodynamic potential is given and shown to be stationary for the distribution function which satisfies the integral equation. The relationship of this work to those of previous studies utilizing the distribution-function method is presented and clarified.

I. INTRODUCTION

One of the most exciting and fascinating problems in modern statistical mechanics is the study of disordered systems, in particular the magnetic-disordered system. A magnetic system with randomly distributed exchange interactions was studied by Edwards and Anderson¹ (EA) giving the so-called spin-glass state. To calculate the free energy of the disordered system, EA introduced the “*n*-replica” method which has been further employed by numerous workers in the field. In particular, Sherrington and Kirkpatrick² obtained a solution for the random Ising model with infinitely-long-ranged interactions.

On the other hand, another approach to the problem which does not use the “*n*-replica” method has been developed and applied to the disordered magnetic system, rendering the same results as those of Sherrington and Kirkpatrick² in the limit of infinitely-long-ranged interactions.³⁻⁶

In 1975, two of us⁷ [Frankel and Thompson (FT)] introduced a completely different approach for portraying the amorphous ferromagnet. In that model, the spatial and spin configurations of the particles were treated on an equal footing. This work has been generalized and discussed further by others.⁸⁻¹⁰ This model of FT has since been mapped into an appropriate spin-1 lattice-gas model with magnetic and nonmagnetic interactions and analyzed in the limit of infinitely-long-ranged interactions.¹¹ Another model for the magnetic lattice gas was used by Ausloos *et al.*¹² and the detailed comparison with ours has been given in Ref. 11.

We now present the generalization of our magnetic lattice-gas model to the case of random distribution

of interactions. In this paper, we give a general formulation of the problem using the method of distribution functions.

We will first give the motivation for this work and discuss the physical systems where this model may be most applicable and then give a comprehensive history of the technique of distribution functions in studies of disordered systems.

Lee and Yang¹³ in a classic paper many years ago introduced the lattice-gas model where each lattice point is either vacant or occupied by an atom and no two atoms can be on the same site. The model has served as an excellent model of binary alloys¹³ and has provided valuable insights into the gas-liquid condensation problem.¹³ When dealing with amorphous systems such as glasses and amorphous ferromagnets (e.g., Ref. 14), however, their structure is irregular with no underlying structural long-range order corresponding to a precise, regularly ordered crystalline lattice. In these substances, there can be varying distances between nearest-neighbor (NN) atoms as well as more distant neighbors and also varying coordination numbers. These systems resemble more closely a network of atoms interlaced with a network of vacancies. If the diffusion coefficient for these systems is small enough (relaxation time large enough) we can think of applying equilibrium statistical mechanics to studies of these systems even though these networks are continuously changing their irregular topology in time. In many respects these systems resemble a real liquid wherein the molecules array themselves in something like irregular networks (which vary in time) as most vividly shown for fluids by computer simulation using molecular dynamics.¹⁵

It would, therefore, be most interesting and valu-

able to attempt to incorporate these kinds of irregularities in the original lattice-gas model. Within the framework of the lattice-gas model, this can be done in various ways, e.g., (i) by assigning random interactions between the lattice sites, (ii) by assigning random coordination numbers to the lattice sites, and (iii) by assigning random cell volumes about the lattice sites.

The disordered magnetic lattice gas will be referred to as the DMLG, hereafter, and will be thought of as representing disordered systems such as amorphous ferromagnets and in an appropriate limit (which we discuss later) spin-glasses. The DMLG without magnetic interaction will reduce to the disordered lattice gas and will be referred to as the DLG, hereafter. As discussed above, the DLG may be thought of as a first attempt to introduce irregularities into the original lattice gas and in so doing becomes a refined version of a lattice-gas model for describing the liquid state. In this sense the DLG is perhaps closer to the situation in real fluids and certainly closer to the philosophy of the cellular theory of liquids enunciated in the so-called lattice theories (not Lee-Yang lattice gas) of the liquid state as discussed, for example, in Barker's book.¹⁶

To our knowledge, there have been two main streams followed in the development of the method using the distribution function. One stream was initiated by Marshall¹⁷ in connection with the problem of dilute magnetic alloys, and has been developed by Klein and others.^{3,4,18-20} The other was started by Matsubara,²¹ independently from the above, in his treatment of disordered spin systems and then applied to the study of the spin-glass state in a binary-bond mixture.²² This approach has been further developed by others,^{5,6,23-26} as we now describe in some detail.

In treating a disordered magnetic system, Matsubara introduced the concept of a fictitious thermal average of the spin²¹ which was calculated by assuming that one interaction bond was removed from the z (coordination number) interaction bonds surrounding the spin. He further introduced the distribution function for the fictitious thermal average of the spin, and derived a nonlinear integral equation for it. Matsubara and Sakata applied the method of the distribution function to a binary-bond mixture, i.e., an Ising spin system with a random distribution of ferromagnetic and antiferromagnetic interaction bonds, and successfully obtained a spin-glass state named GLP (glasslike phase).²² A distribution function for an effective field was used to calculate the internal field of amorphous ferromagnets.⁵ Katsura and Fujiki²³ also used another effective field, under which a thermal average of a spin gave the fictitious thermal average of Matsubara,²¹ and derived an integral equation, using the δ function in a compact form for an arbitrary distribution of the interaction bonds,

which of course reduced to the integral equation of Matsubara in the case of the binary-bond mixture. Morita²⁶ introduced a concept of a single-bond effective field acting upon a spin through a single interaction bond, and gave a free energy for the disordered system and an integral equation for the distribution function of the single-bond effective field (which will be referred to as the single-bond distribution function). He also showed that the stationarity condition for the free energy led to an appropriate integral equation. Katsura, Fujiki, and Inawashiro²⁴ showed that the two integral equations derived by Katsura and Fujiki²³ and by Morita²⁶ were equivalent to each other. They²⁴ used a relation which expressed the effective field of Katsura and Fujiki as a synthesis of $(z-1)$ single-bond effective fields which they called the $(z-1)$ -bond field, thereafter.²⁵ In the case of the binary-bond mixture, the stationary character of the free energy was examined in detail for $z=3$ and 4 at absolute zero.²⁵

The notations and descriptions used in the above works seem to us to be complicated and often confusing and thus it is most worthwhile to give a self-contained and compact formulation of the method of the distribution function including the proof of the stationarity of the free energy. This program is carried out in detail in this paper. In the course of our generalization of the method of the distribution function to describe the DMLG we will find it necessary to introduce the new concept of an effective potential besides that of an effective field.

In Sec. II, the spin-1 lattice-gas model is presented and a pair approximation for the random distribution of magnetic and nonmagnetic interactions is described. It is emphasized here that the concept of an effective potential is necessary along with that of the effective field for portraying the disordered spin-1 system. In Sec. III, two distribution functions are introduced for both the single-bond and the $(z-1)$ -bond field and potential. Appropriate integral equations are then derived. The thermodynamic potential for the magnetic lattice gas is given in Sec. IV. It is also shown that the stationarity condition for the thermodynamic potential is satisfied by the integral equation derived in Sec. III. In Sec. V, the standard disordered spin system, wherein each lattice site is occupied by a single spin, is discussed as a limiting case of our model. This enables us to then discuss and clarify the relationship between the integral equations derived by previous authors. Section VI is devoted to a summary and discussion.

II. MODEL AND A PAIR APPROXIMATION

We consider the DMLG where particles with spins interact with each other through magnetic and non-

magnetic interactions which are randomly distributed over the lattice with a certain specified probability. Spin-1 operators are used to represent a particle with up or down spin at a lattice site by $S = 1$ or -1 , respectively, and a vacant site by $S = 0$. Then the disordered magnetic system is described by

$$\mathfrak{H} = - \sum_{(i,j)} J_{ij} S_i S_j - \sum_{(i,j)} U_{ij} S_i^2 S_j^2 - B \sum_i S_i - \mu \sum_i S_i^2 \quad (S_i = 1, 0, -1) , \quad (2.1)$$

where J_{ij} denotes the magnetic interaction between lattice sites i and j , U_{ij} is the potential interaction between lattice sites i and j , B is an external magnetic field, and μ is the chemical potential. It is assumed that J_{ij} and U_{ij} are distributed randomly over the lattice bonds with a probability distribution $\mathcal{P}(J, U)$.

The method of the distribution function for the effective field has been successfully applied to disordered magnetic systems, e.g., spin-glasses and amorphous ferromagnets. In order to apply the method to the DMLG, a specific generalization is necessary. In addition to the effective field, we must introduce an effective potential at each lattice site and represent the distribution function as a function of both the effective field and effective potential.

We formulate the problem utilizing the pair approximation which is a natural generalization of the Bethe-Peierls-Weiss approximation to a disordered system, as shown in detail in Sec. III. Within the pair approximation we consider a single-site Hamiltonian and a pair-site Hamiltonian simultaneously, and require a self-consistency between the single-site density matrix and the pair-site density matrix.

The single-site Hamiltonian is introduced by

$$\mathfrak{H}_1 = -(h_1^{(z)} + B) S_1 - (l_1^{(z)} + \mu) S_1^2 , \quad (2.2)$$

where $h_1^{(z)}$ ($l_1^{(z)}$) represents an effective field (potential) at the site 1 coming from z neighbors through each interaction bond, and is hereafter referred to as the z -bond field (potential) for simplicity (see Fig. 1). The pair-site Hamiltonian for a neighboring pair of

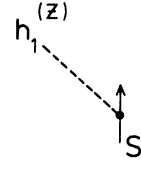


FIG. 1. Spin S_1 and the z -bond field which is denoted by a single dashed line. The external field and the z -bond potential are not shown.

lattice sites is given by

$$\begin{aligned} \mathfrak{H}_{12} = & -JS_1 S_2 - US_1^2 S_2^2 - (B + h_1^{(z-1)}) S_1 \\ & - (B + h_2^{(z-1)}) S_2 - (\mu + l_1^{(z-1)}) S_1^2 \\ & - (\mu + l_2^{(z-1)}) S_2^2 , \end{aligned} \quad (2.3)$$

where $h_i^{(z-1)}$ and $l_i^{(z-1)}$ ($i = 1, 2$), respectively, denote an effective field and an effective potential at the i th site coming from the $(z-1)$ neighbors outside the pair sites. The quantities $h_i^{(z-1)}$ and $l_i^{(z-1)}$ are referred to as the $(z-1)$ -bond field and $(z-1)$ -bond potential hereafter (see Fig. 2).

A single-site density matrix is given by

$$\rho_1 = \exp(-\beta \mathfrak{H}_1) , \quad (2.4)$$

and the trace of it is expressed as

$$\text{Tr} \rho_1 = Z_1(h_1^{(z)}, l_1^{(z)}) , \quad (2.5)$$

where

$$Z_1(x, y) \equiv 1 + 2e^{\beta(\mu+y)} \cosh \beta(B+x) . \quad (2.6)$$

A pair-site density matrix is given by

$$\rho_{12} = \exp(-\beta \mathfrak{H}_{12}) , \quad (2.7)$$

and the trace of it is expressed as

$$\begin{aligned} \text{Tr} \rho_{12} = & 1 + 2 \exp \beta(\mu + l_1^{(z-1)}) \cosh \beta(B + h_1^{(z-1)}) + 2 \exp \beta(\mu + l_2^{(z-1)}) \cosh \beta(B + h_2^{(z-1)}) \\ & + 4 \exp \beta(2\mu + l_1^{(z-1)} + l_2^{(z-1)} + U) [\cosh \beta J \cosh \beta(B + h_1^{(z-1)}) \cosh \beta(B + h_2^{(z-1)}) \\ & + \sinh \beta J \sinh \beta(B + h_1^{(z-1)}) \sinh \beta(B + h_2^{(z-1)})] . \end{aligned} \quad (2.8)$$

As a self-consistent condition, we require that

$$\text{Tr}_2 \rho_{12} \propto \rho_1 , \quad (2.9)$$

where the index 2 on Tr means that the trace is to be taken with respect to the lattice site 2. The condition (2.9) leads to a certain relationship between the z -bond field and potential and the $(z-1)$ -bond field and potential.

Performing the partial trace over the site 2, we have

$$\text{Tr}_2 \rho_{12} = \exp[\beta(B + h_1^{(z-1)})S_1 + \beta(\mu + l_1^{(z-1)})S_1^2] [1 + 2 \exp\beta(\mu + l_2^{(z-1)} + US_1^2) \cosh\beta(B + h_2^{(z-1)} + JS_1)] . \quad (2.10)$$

Making use of the formulas

$$\sinh XS = S \sinh X, \quad \cosh XS = 1 + S^2(\cosh X - 1), \quad \exp(XS^2) = 1 + S^2(e^X - 1) \quad (S = 0, \pm 1) , \quad (2.11)$$

we find that (2.10) can be rewritten as

$$\begin{aligned} \text{Tr}_2 \rho_{12} = & \exp[\beta(B + h_1^{(z-1)})S_1 + \beta(\mu + l_1^{(z-1)})S_1^2] Z_1(h_2^{(z-1)}, l_2^{(z-1)}) \\ & \times \left[1 + \frac{2 \exp\beta(\mu + l_2^{(z-1)} + U) \sinh\beta(B + h_2^{(z-1)}) \sinh\beta J}{Z_1(h_2^{(z-1)}, l_2^{(z-1)})} S_1 \right. \\ & \left. + \frac{2 \exp\beta(\mu + l_2^{(z-1)}) \cosh\beta(B + h_2^{(z-1)}) (e^{\beta U} \cosh\beta J - 1)}{Z_1(h_2^{(z-1)}, l_2^{(z-1)})} S_1^2 \right] . \quad (2.12) \end{aligned}$$

The expression within the large parentheses on the right-hand side of (2.12) can be written as

$$1 + e^{\beta L}(\sinh\beta H)S_1 + (e^{\beta L} \cosh\beta H - 1)S_1^2 , \quad (2.13)$$

where

$$e^{\beta L} \sinh\beta H = [Z_1(h_2^{(z-1)}, l_2^{(z-1)})]^{-1} 2 \exp\beta(\mu + l_2^{(z-1)} + U) \sinh\beta(B + h_2^{(z-1)}) \sinh\beta J \quad (2.14)$$

and

$$e^{\beta L} \cosh\beta H - 1 = [Z_1(h_2^{(z-1)}, l_2^{(z-1)})]^{-1} 2 \exp\beta(\mu + l_2^{(z-1)}) \cosh\beta(B + h_2^{(z-1)}) (e^{\beta U} \cosh\beta J - 1) . \quad (2.15)$$

From (2.14) and (2.15), we obtain

$$H \equiv H(h_2^{(z-1)}, l_2^{(z-1)}, J, U) = \beta^{-1} \tanh^{-1} \left[\frac{Z_1(h_2^{(z-1)} + J, l_2^{(z-1)} + U) - Z_1(h_2^{(z-1)} - J, l_2^{(z-1)} + U)}{Z_1(h_2^{(z-1)} + J, l_2^{(z-1)} + U) + Z_1(h_2^{(z-1)} - J, l_2^{(z-1)} + U)} \right] \quad (2.16)$$

and

$$L \equiv L(h_2^{(z-1)}, l_2^{(z-1)}, J, U) = \frac{1}{2\beta} \ln \left[\frac{Z_1(h_2^{(z-1)} + J, l_2^{(z-1)} + U) Z_1(h_2^{(z-1)} - J, l_2^{(z-1)} + U)}{[Z_1(h_2^{(z-1)}, l_2^{(z-1)})]^2} \right] . \quad (2.17)$$

Using the formula

$$\exp\beta(XS + YS^2) = 1 + Se^{\beta Y} \sinh\beta X + S^2(e^{\beta Y} \cosh\beta X - 1) , \quad (2.18)$$

we have

$$\text{Tr}_2 \rho_{12} = Z_1(h_2^{(z-1)}, l_2^{(z-1)}) \exp\beta[(B + h_1^{(z-1)} + H)S_1 + (\mu + l_1^{(z-1)} + L)S_1^2] . \quad (2.19)$$

Then it easily follows that

$$\text{Tr} \rho_{12} = Z_1(h_2^{(z-1)}, l_2^{(z-1)}) Z_1(h_1^{(z-1)} + H, l_1^{(z-1)} + L) . \quad (2.20)$$

The z -bond field and potential at the site 1 now consists of the $(z-1)$ -bond field and a single-bond field h_1 coming from the site 2,

$$h_1^{(z)} = h_1^{(z-1)} + h_1 , \quad (2.21)$$

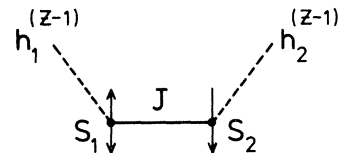


FIG. 2. Pair of spins S_1 and S_2 and two sets of the $(z-1)$ -bond fields. The $(z-1)$ -bond potentials are not shown.

as shown in Fig. 3. Likewise we have

$$l_1^{(z)} = l_1^{(z-1)} + l_1, \quad (2.22)$$

where l_1 denotes a single-bond potential coming from the site 2. The single-site density matrix can now be written as

$$\rho_1 = \beta [(B + h_1^{(z-1)} + h_1) S_1 + (\mu + l_1^{(z-1)} + l_1) S_1^2] . \quad (2.23)$$

From (2.9), (2.19), and (2.23), we obtain finally

$$h_1 = H(h_2^{(z-1)}, l_2^{(z-1)}, J, U) \quad (2.24)$$

and

$$l_1 = L(h_2^{(z-1)}, l_2^{(z-1)}, J, U) , \quad (2.25)$$

which are the two important results expressing relationships between the single-bond field and potential at the site 1 and the $(z-1)$ -bond field and potential at the site 2; pictorially this now means that Fig. 2 can be replaced by Fig. 3.

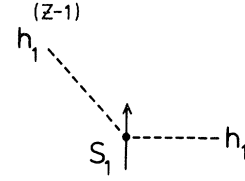


FIG. 3. Spin S_1 , the single-bond field h_1 , and the $(z-1)$ -bond field.

III. DISTRIBUTION FUNCTION FOR THE EFFECTIVE FIELD AND POTENTIAL

The single-bond field and potential vary from bond to bond and also from site to site. We assume that the distribution function for both of them over the entire lattice is denoted by a single-bond distribution function $g(h, l)$. Further, the distribution function for the $(z-1)$ -bond field and potential is denoted by $g^{(z-1)}(h, l)$. The single-bond field and potential at the site 1 is connected to the $(z-1)$ -bond fields and potentials at the site 2 through (2.24) and (2.25); the relation between the single bond and the $(z-1)$ -bond distribution functions is thus given by

$$g(h, l) = \int \delta(h - H(h_2^{(z-1)}, l_2^{(z-1)}, J, U)) \delta(l - L(h_2^{(z-1)}, l_2^{(z-1)}, J, U)) \times \Phi(J, U) dJ dU g^{(z-1)}(h_2^{(z-1)}, l_2^{(z-1)}) dh_2^{(z-1)} dl_2^{(z-1)} , \quad (3.1)$$

where we have neglected the correlations between $(z-1)$ -bond distribution functions and the random distribution for J and U .

Now we assume a general M -bond distribution function,²⁵ which is expressed in terms of the single-bond distribution functions as

$$g^{(M)}(h, l) = \int \delta\left(h - \sum_{j=1}^M h_j\right) \delta\left(l - \sum_{j=1}^M l_j\right) \prod_{j=1}^M g(h_j, l_j) dh_j dl_j . \quad (3.2)$$

Then (3.1) and (3.2) with $M = z-1$, constitute a fundamental set of integral equations for g and $g^{(z-1)}$.

Eliminating $g^{(z-1)}$ from (3.1) and (3.2) with $M = z-1$, we have an integral equation for g alone given by

$$g(h, l) = \int \delta(h - H(h_2^{(z-1)}, l_2^{(z-1)}, J, U)) \delta(l - L(h_2^{(z-1)}, l_2^{(z-1)}, J, U)) \Phi(J, U) dJ dU \prod_{m=1}^{z-1} g(h_{2m}, l_{2m}) dh_{2m} dl_{2m} . \quad (3.3)$$

We have introduced the general relations

$$h_i^{(M)} = \sum_{m=1}^M h_{im} \quad (i=1, 2) \quad (3.4)$$

and

$$l_i^{(M)} = \sum_{m=1}^M l_{im} \quad (i=1, 2) . \quad (3.5)$$

In (3.3) we have used (3.4) or (3.5) with $M = z-1$. The fields h_{im} are shown in Fig. 4. Using (3.4) with $M = z-1$, we see immediately that Figs. 3 and 4 are equivalent. Using (3.1) and (3.2) with $M = z-1$, we find that the integral equation for $g^{(z-1)}$ is given by

$$g^{(z-1)}(h, l) = \int \delta\left(h - \sum_{j=1}^{z-1} H(h_j, l_j, J_j, U_j)\right) \delta\left(l - \sum_{j=1}^{z-1} L(h_j, l_j, J_j, U_j)\right) \prod_{j=1}^{z-1} [\Phi(J_j, U_j) dJ_j dU_j g^{(z-1)}(h_j, l_j) dh_j dl_j] . \quad (3.6)$$

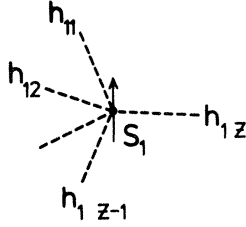


FIG. 4. Spin S_1 and the z single-bond fields. Figure 4 is equivalent to Fig. 3, for $h_1^{(z-1)} = \sum_{j=1}^{z-1} h_{1j}$ and $h_{1z} \equiv h_1$.

Using the Fourier-integral representation of the δ functions in (3.6), we obtain

$$g^{(z-1)}(h, l) = \frac{1}{(2\pi)^2} \int \exp[-i(ph + sl)] \times [G(p, s)]^{z-1} dp ds, \quad (3.7)$$

$$\langle \langle A(S_1) \rangle \rangle_{12} = \int \frac{\text{Tr}[A(S_1)\rho_{12}]}{\text{Tr}\rho_{12}} \mathcal{P}(J, U) dJ dU g^{(z-1)}(h_1^{(z-1)}, l_1^{(z-1)}) dh_1^{(z-1)} dl_1^{(z-1)} \times g^{(z-1)}(h_2^{(z-1)}, l_2^{(z-1)}) dh_2^{(z-1)} dl_2^{(z-1)}, \quad (3.9)$$

where the bracket with indices 12 on the left-hand side of (3.9) means the thermal average by ρ_{12} ; the bold angular brackets with a subscript R mean the configurational average over the randomness which is calculated here by integrating over the probability distribution for J and U and the two distribution functions for the $(z-1)$ -bond fields and potentials at both ends of the pair sites. The thermal and configurational average of $A(S_1)$ by ρ_1 is likewise given by

$$\langle \langle A(S_1) \rangle \rangle_1 = \int \frac{\text{Tr}[A(S_1)\rho_1]}{\text{Tr}\rho_1} g^{(z-1)}(h_1^{(z-1)}, l_1^{(z-1)}) dh_1^{(z-1)} dl_1^{(z-1)} g(h_1, l_1) dh_1 dl_1, \quad (3.10)$$

where we have used the expression for ρ_1 given by (2.23). Substituting (3.3) for $g(h_1, l_1)$ in (3.10), we have

$$\langle \langle A(S_1) \rangle \rangle_1 = \int \frac{\text{Tr}[A(S_1) \exp\beta\{(B + h_1^{(z-1)} + H)S_1 + (\mu + l_1^{(z-1)} + L)S_1^2\}]}{\text{Tr} \exp\beta\{(B + h_1^{(z-1)} + H)S_1 + (\mu + l_1^{(z-1)} + L)S_1^2\}} g^{(z-1)}(h_1^{(z-1)}, l_1^{(z-1)}) dh_1^{(z-1)} dl_1^{(z-1)} \times \mathcal{P}(J, U) dJ dU g^{(z-1)}(h_2^{(z-1)}, l_2^{(z-1)}) dh_2^{(z-1)} dl_2^{(z-1)}. \quad (3.11)$$

Using (2.19), the first factor incorporating the traces in the integrand of (3.11) becomes

$$\frac{\text{Tr}_1[A(S_1)(\text{Tr}_2\rho_{12})]}{\text{Tr}_1(\text{Tr}_2\rho_{12})} = \frac{\text{Tr}[A(S_1)\rho_{12}]}{\text{Tr}\rho_{12}}. \quad (3.12)$$

We now have the equality for the two kinds of averages for $A(S_1)$,

$$\langle \langle A(S_1) \rangle \rangle_{12} = \langle \langle A(S_1) \rangle \rangle_1. \quad (3.13)$$

This shows that the pair approximation, which we have used in our formulation, is a natural generalization of the Bethe-Peierls-Weiss approximation for the

where

$$G(p, s) = \int \exp[ipH(h, l, J, U) + isL(h, l, J, U)] \times \mathcal{P}(J, U) dJ dU g^{(z-1)}(h, l) dh dl. \quad (3.8)$$

Equations (3.7) and (3.8) are in a convenient form to allow numerical calculations to be readily carried out.

Now we will show that the integral equation (3.3) ensures that the density matrices ρ_1 and ρ_{12} give the same value of the thermal and configurational average for $A(S_1)$, where $A(S_1)$ is an arbitrary function of S_1 . The thermal and configurational average of $A(S_1)$ by ρ_{12} is given by

regular spin system to that of the disordered magnetic system.

IV. THERMODYNAMIC POTENTIAL AND STATIONARITY

The thermodynamic potential per bond in the pair approximation is given by²⁴⁻²⁶

$$\phi = \phi_{12} - 2 \left(1 - \frac{1}{z} \right) \phi_1, \quad (4.1)$$

where

$$\begin{aligned} \phi_{12} = & -\beta^{-1} \int \ln(\text{Tr}\rho_{12}) \mathcal{P}(J, U) dJ dU \\ & \times \prod_{k=1}^{z-1} g(h_{1k}, l_{1k}) dh_{1k} dl_{1k} \\ & \times \prod_{m=1}^{z-1} g(h_{2m}, l_{2m}) dh_{2m} dl_{2m} \quad , \quad (4.2) \end{aligned}$$

with $\text{Tr}\rho_{12}$ given by (2.20), and with $h_i^{(z-1)}$ and $l_i^{(z-1)}$ given by (3.4) and (3.5) with $M = z - 1$, respectively, and

$$\phi_1 = -\beta^{-1} \int \ln(\text{Tr}\rho_1) \prod_{k=1}^z g(h_{1k}, l_{1k}) dh_{1k} dl_{1k} \quad , \quad (4.3)$$

with $\text{Tr}\rho_1$ given by (2.5), and with $h_1^{(z)}$ and $l_1^{(z)}$ given by (3.4) and (3.5) with $i=1$ and $M=z$. For notation purposes we have defined $h_{1z} \equiv h_1$ and $l_{1z} \equiv l_1$, with h_1 and l_1 as used in Sec. II. The physical meaning of

the factor $2(1-1/z)$ in (4.1) is most readily understood by employing an argument specifically involving the limit of absolute zero. In the limit of absolute zero, ϕ_{12} gives the energy of the pair which contains $2(z-1)$ single-bond interaction energies between the pair and the surrounding medium. The integral in (4.3) contains z single-bond interaction energies between the single site and the medium. Therefore, the $2(z-1)$ single-bond energies in ϕ_{12} must be canceled by subtracting the term $2(z-1)z^{-1}\phi_1$, where ϕ_1 is the sum of z single-bond energies at absolute zero.

Now we show that ϕ is stationary with respect to the variation of the single-bond distribution function. Consider an arbitrary variation preserving the normalization condition of the single-bond distribution function,

$$\int \delta g(h, l) dh dl = 0 \quad . \quad (4.4)$$

The variation of ϕ_{12} gives

$$\begin{aligned} \delta\phi_{12} = & -2(z-1)\beta^{-1} \int \ln(\text{Tr}\rho_{12}) \mathcal{P}(J, U) dJ dU \prod_{k=2}^{z-1} g(h_{1k}, l_{1k}) dh_{1k} dl_{1k} \\ & \times \prod_{m=1}^{z-1} g(h_{2m}, l_{2m}) dh_{2m} dl_{2m} \delta g(h_{11}, l_{11}) dh_{11} dl_{11} \quad , \quad (4.5) \end{aligned}$$

and that of ϕ_1 gives

$$\delta\phi_1 = -z\beta^{-1} \int \ln(\text{Tr}\rho_1) \prod_{k=2}^k g(h_{1k}, l_{1k}) dh_{1k} dl_{1k} \delta g(h_{11}, l_{11}) dh_{11} dl_{11} \quad . \quad (4.6)$$

Inserting (2.20) into (4.5), we can write the variation of ϕ as

$$\begin{aligned} \delta\phi = & -2(z-1)\beta^{-1} \int \delta g(h_{11}, l_{11}) dh_{11} dl_{11} \\ & \times \prod_{k=2}^{z-1} g(h_{1k}, l_{1k}) dh_{1k} dl_{1k} \\ & \times \left\{ \int \ln \left[Z_1 \left[\sum_{m=1}^{z-1} h_{2m}, \sum_{m=1}^{z-1} h_{2m} \right] \right] \mathcal{P}(J, U) dJ dU \prod_{m=1}^{z-1} g(h_{2m}, l_{2m}) dh_{2m} dl_{2m} \right. \\ & + \int \ln \left[Z_1 \left[\sum_{k=1}^{z-1} h_{1k} + H, \sum_{k=1}^{z-1} l_{1k} + L \right] \right] \mathcal{P}(J, U) dJ dU \prod_{m=1}^{z-1} g(h_{2m}, l_{2m}) dh_{2m} dl_{2m} \\ & \left. - \int \ln \left[Z_1 \left[\sum_{k=1}^z h_{1k}, \sum_{k=1}^z l_{1k} \right] \right] g(h_{1z}, l_{1z}) dh_{1z} dl_{1z} \right\} \quad . \quad (4.7) \end{aligned}$$

The first term in the braces is independent of the variables h_{11} and l_{11} and thus the contribution from this term vanishes because of the preservation of the normalization, (4.4). Stationarity then gives the following identity for the g function of h_{11} and l_{11} :

$$\begin{aligned} \int \prod_{k=2}^{z-1} g(h_{1k}, l_{1k}) dh_{1k} dl_{1k} \left\{ \int \ln \left[Z_1 \left[\sum_{k=1}^{z-1} h_{1k} + H, \sum_{k=1}^{z-1} l_{1k} + L \right] \right] \mathcal{P}(J, U) dJ dU \prod_{m=1}^{z-1} g(h_{2m}, l_{2m}) dh_{2m} dl_{2m} \right. \\ \left. - \int \ln \left[Z_1 \left[\sum_{k=1}^z h_{1k}, \sum_{k=1}^z l_{1k} \right] \right] g(h_{1z}, l_{1z}) dh_{1z} dl_{1z} \right\} = 0 \quad . \quad (4.8) \end{aligned}$$

It is easily seen that the substitution of the integral equation (3.3) for $g(h_{1z}, l_{1z})$ in the above equation assures the vanishing of the right-hand side of (4.8). Thus the integral equation (3.3) is a sufficient condition for the stationarity of the thermodynamic potential.²⁵

The thermodynamic potential is also expressed in terms of the $(z-1)$ -bond and z -bond distribution functions. Using (3.2) with $M = z-1$, (4.2) is rewritten as

$$\phi_{12} = -\beta^{-1} \int \ln [Z_1(h_2^{(z-1)}, l_2^{(z-1)}) Z_1(h_1^{(z-1)} + H, l_1^{(z-1)} + L)] \mathcal{P}(J, U) dJ dU \\ \times g^{(z-1)}(h_1^{(z-1)}, l_1^{(z-1)}) dh_1^{(z-1)} dl_1^{(z-1)} g^{(z-1)}(h_2^{(z-1)}, l_2^{(z-1)}) dh_2^{(z-1)} dl_2^{(z-1)}, \quad (4.9)$$

and using (3.2) with $M = z$, (4.3) is rewritten as

$$\phi_1 = -\beta^{-1} \int \ln Z_1(h_1^{(z)}, l_1^{(z)}) g^{(z)}(h_1^{(z)}, l_1^{(z)}) dh_1^{(z)} dl_1^{(z)} \quad (4.10)$$

These expressions are particularly useful for taking the limit of infinitely-long-ranged interactions, which we will study in detail in the following paper.²⁷

V. LIMITING CASE $\mu \rightarrow \infty$

We now consider the limiting case where particles occupy all the lattice sites and are not allowed to change sites. We call this case the standard disordered spin system. This case corresponds formally to the limit where the chemical potential $\mu \rightarrow \infty$. In this limit, it can readily be demonstrated that the effective potentials $l_i^{(z)}$ and $l_i^{(z-1)}$ along with the nonmagnetic interaction U no longer appear in the normalized density matrix. Therefore, the standard disordered spin system reduces to an appropriate spin- $\frac{1}{2}$ system. We now present this appropriate spin- $\frac{1}{2}$ system and use it to make detailed connection with the works of previous authors, as qualitatively discussed in the Introduction.

We find that

$$\frac{\rho_1}{\text{Tr} \rho_1} \xrightarrow{\mu \rightarrow \infty} \frac{\hat{\rho}_1}{\text{Tr} \hat{\rho}_1}, \quad (5.1)$$

where

$$\hat{\rho}_1 = \exp(-\beta \hat{\mathcal{K}}_1) \quad (5.2)$$

and

$$\hat{\mathcal{K}}_1 = -(h_1 + h_1^{(z-1)}) \sigma_1 - B \sigma_1 \quad (\sigma_1 = \pm 1), \quad (5.3)$$

along with

$$\frac{\rho_{12}}{\text{Tr} \rho_{12}} \xrightarrow{\mu \rightarrow \infty} \frac{\hat{\rho}_{12}}{\text{Tr} \hat{\rho}_{12}}, \quad (5.4)$$

where

$$\hat{\rho}_{12} = \exp(-\beta \hat{\mathcal{K}}_{12}) \quad (5.5)$$

and

$$\hat{\mathcal{K}}_{12} = -J \sigma_1 \sigma_2 - (B + h_1^{(z-1)}) \sigma_1 - (B + h_2^{(z-1)}) \sigma_2 \\ (\sigma_i = \pm 1, \quad i = 1, 2). \quad (5.6)$$

Equations (2.16) and (2.17) become in the limit $\mu \rightarrow \infty$,

$$H \rightarrow \hat{H} \equiv \hat{H}(h_2^{(z-1)}, J) \\ = \beta^{-1} \tanh^{-1} [\tanh \beta (B + h_2^{(z-1)}) \tanh \beta J], \quad (5.7)$$

and

$$L \rightarrow \hat{L} \equiv \hat{L}(h_2^{(z-1)}, J, U) = U + \frac{1}{2\beta} \ln \left[\frac{\cosh \beta (B + h_2^{(z-1)} + J) \cosh \beta (B + h_2^{(z-1)} - J)}{[\cosh \beta (B + h_2^{(z-1)})]^2} \right]. \quad (5.8)$$

It is to be noted that L is now independent of $l_2^{(z-1)}$. We define the magnetic single-bond distribution function by

$$g_M(h) = \int g(h, l) dl. \quad (5.9)$$

Integrating Eq. (3.3) with respect to l and remember-

ing L is independent of $l_2^{(z-1)}$, we obtain

$$g_M(h) = \int \delta(h - \hat{H}(h_2^{(z-1)}, J)) P(J) dJ \\ \times \prod_{k=1}^{z-1} g_M(h_{2k}) dh_{2k}, \quad (5.10)$$

where $P(J)$ is the probability distribution for the

magnetic interaction only and is given by

$$P(J) = \int \mathcal{P}(J, U) dU .$$

Equation (5.10) is the same equation as derived by Morita for the standard disordered spin system.^{25,26} We define the magnetic $(z-1)$ -bond distribution function by

$$g_M^{(z-1)}(h) = \int g^{(z-1)}(h, l) dl . \quad (5.11)$$

Then the integral equation (3.6) leads to

$$g_M^{(z-1)}(h) = \int \delta \left[h - \sum_{j=1}^{z-1} \hat{H}(h_j^{(z-1)}, J_j) \right] \times \prod_{j=1}^{z-1} P(J_j) dJ_j g_M^{(z-1)}(h_{2j}) dh_{2j} , \quad (5.12)$$

which agrees with the integral equation derived by Katsura *et al.*⁶

Introducing a new variable x by

$$x = \tanh \beta(B + h) , \quad (5.13)$$

which represents the fictitious thermal average for a spin subject to both the $(z-1)$ -bond field h and the external magnetic field B . Using (5.13), the $(z-1)$ -bond distribution function is converted to a distribution function for the fictitious thermal average for a spin, i.e.,

$$f(x) = g_M^{(z-1)}(h) \left(\frac{dx}{dh} \right)^{-1} . \quad (5.14)$$

The integral equation for $f(x)$ is obtained from (5.7) and Eqs. (5.12)–(5.14) as

$$f(x) = \int \delta \left[x - \tanh \beta \left(B + \beta^{-1} \sum_{j=1}^{z-1} \tanh^{-1}(x \tanh \beta J) \right) \right] \times \prod_{j=1}^{z-1} P(J_j) dJ_j f(x_j) dx_j , \quad (5.15)$$

where we have used a formula for the δ function,

$$\delta(h - a) = \frac{dx}{dh} \delta(x - \tanh \beta(B + a)) . \quad (5.16)$$

The integral equation (5.15) is equivalent to the integral equation derived by Matsubara²¹ and by Katsura and Fujiki.²³

The free energy, up to an additive constant, for the standard disordered spin system is easily obtained by replacing ρ_{12} by $\hat{\rho}_{12}$, ρ_1 by $\hat{\rho}_1$ and $g(h, l) dh dl$ by $g(h) dh$ in (4.2) and (4.3).

VI. SUMMARY AND DISCUSSION

A spin-1 model of a disordered magnetic lattice gas with random distribution for both the magnetic and

nonmagnetic interactions has been presented as a natural generalization of the magnetic lattice gas presented in the previous paper.¹¹

We have given a formulation of the problem using the method of the distribution function. The concept of an effective potential is shown to be necessary as well as the usual effective field in order to describe our system. The distribution functions were shown to satisfy appropriate nonlinear integral equations. The thermodynamical potential has been introduced and shown to be stationary when the single-bond distribution functions satisfy these integral equations. We have shown that the pair approximation for the disordered magnetic system can be considered as a natural extension of the Bethe-Peierls-Weiss approximation previously employed for the study of nondisordered magnetic systems.

In the limit where each lattice site is occupied by a single particle, our systems reduces to the standard disordered spin system, and the distribution functions and the integral equations they satisfy become equivalent to those derived by previous authors^{6,21–26} for the standard disordered spin systems.

Having presented a general formulation for the disordered magnetic lattice gas in this paper, we now proceed to solve this system for the specific case of infinitely-long-ranged interactions [i.e., the mean-field approximation (MFA)] with Gaussian distributed coupling constants in the following paper.²⁷ With what we have said above and already shown in this paper, we expect the final solution of that study to reduce to the spin-glass result² in an appropriate limit as well as providing results for these new and most interesting systems, the disordered magnetic lattice gas (DMLG) and the disordered lattice gas (DLG)²⁸ (see the Appendix), respectively.

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APPENDIX

In the case of no magnetic interaction and with $B=0$, our disordered magnetic lattice gas reduces to that of a disordered lattice gas. Apart from the double counting resulting from the degeneracy of the up-down spin labeling, the Hamiltonian (2.1) is now isomorphic to that of the disordered lattice gas, given

by

$$\mathcal{H} = - \sum_{(i,j)} U_{ij} \xi_i \xi_j - \mu \sum_i \xi_i \quad (\xi_i = 0, 1) , \quad (\text{A1})$$

where μ denotes the chemical potential of the system. Using a relation

$$\xi_i = \frac{1}{2}(1 + \sigma_i) \quad (\sigma_i = \pm 1) , \quad (\text{A2})$$

the disordered lattice gas is now readily transformed to an appropriate disordered magnetic system described by

$$\mathcal{H} = - \left(\frac{1}{8} z U_0 + \frac{1}{2} \mu \right) N - \frac{1}{4} \sum_{(i,j)} U_{ij} \sigma_i \sigma_j - \sum_i B_i \sigma_i , \quad (\text{A3})$$

where z denotes the number of interaction bonds for

a single lattice site; U_0 is the average potential defined by

$$U_0 = \frac{1}{Nz} \sum_i \sum_j U_{ij} \quad (\text{A4})$$

and B_i is an effective random magnetic field given by

$$B_i = \frac{1}{2} \mu + \frac{1}{4} \sum_{j=1}^z U_{ij} . \quad (\text{A5})$$

It is to be noted that there exists some correlation between B_i and the interaction bonds at the i th site. This means that the physical behavior of our system is expected to be quite different in general from that of the standard disordered magnetic system^{1,2} displaying the spin-glass state, as will be seen in the following paper.²⁷

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