Short-range spin-glass model with discrete bonds

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(Received 30 March 1982)

The replica-trick method and an infinite-order summation have been used for the theoretical description of the spin-glass-state model with discrete and chaotic bonds in a simple cubic Ising lattice. A new order parameter defined with the use of the four-spin correlation has been introduced and in this approximation the entropy of the spin-glass state at $T=0$ is zero. The characteristic thermodynamic quantities and the phase diagram have been obtained for different temperature regimes at equal concentrations of the negative and positive bonds.

I. INTRODUCTION

The theoretical treatment of the spin-glass state (SG) has received a great deal of interest in the last few years. The simple case of the system consisting of a spin coupled by a random infinite-range interaction, distributed with a Gaussian probability, has been treated by Edwards and Anderson[1] using a new order parameter. The problem has been reconsidered by Sherrington and Kirkpatrick,[2] Thouless, Anderson, and Palmer,[3] and other authors.[4] The stability of the spin-glass model treated in Ref. 2 has been analyzed by Almeyda and Thouless,[5] Pytte and Rudnick,[6] and Chen and Lubenski,[7] and in order to overcome the difficulties which appeared the idea of the replica symmetry breaking has been introduced. The new models proposed by Parisi,[8] Bray and Moore,[9] and other authors[10,11] present other inconsistencies in spite of the sophisticated mathematical methods used.

On the other hand, the experimental investigations on some compounds suggested the existence of the spin-glass state, which appears due to the short-range discrete interaction between the magnetic moments. The attempt to describe the spin-glass state with the use of the Sherrington and Kirkpatrick method gives rise to real mathematical difficulties.[12]

In this paper we try to explain the spin-glass behavior of the compounds $Co(S_xSe_{1-x})_2$ and $CrTe_{1-x}Sb_x$ observed by Adachi *et al.*[13] and Lotgering and Goster.[14] The main idea of the model is the existence of the competitive ferro- and antiferromagnetic interactions between the nearest-neighbor magnetic atoms. Indeed, in $Co(S_xSe_{1-x})_2$ the Co atoms situated in the fcc lattice sites have six metalloid nearest neighbors which form a nearly octahedral ligand. Between all adjacent Co atoms are intercalated a nonmagnetic atom, which can be S or Se. These nonmagnetic atoms mediate a superexchange, and the Co-S-Co interaction is ferromagnetic, but the second interaction Co-Se-Co is antiferromagnetic. Thus we have competition between two different interactions, which may give rise to the spin-glass state. A simple model which will describe our spin-glass state can be imagined as consisting of a lattice which contains two kinds of nonmagnetic atoms that mediates a ferromagnetic and an antiferromagnetic interaction between the magnetic ions. We will denote one of these interactions by I_A (which will be called bond), and let us consider that the concentration of the I_A bonds is $n_1/n=1-c$. The other type of interaction will be described by the n_2 coupling constants I_B and will have the concentration $c=n_2/n$. If I_A and I_B have different signs, the system is frustrated, and for a lattice with y sites the frustration probability is given by the following equation[15] if $y<5$:

$$p=yc(1-c)^{y-1}+\frac{y}{6}(y-1)(y-2)c^3(1-c)^{y-3}\;. \qquad (1)$$

We consider that between the nearest-neighbor magnetic atoms which are responsible for the magnetic behavior of such compounds as $Co(S_xSe_{1-x})$ and $CrTe_{1-x}Sb_x$, with competitive ferromagnetic and antiferromagnetic interactions, the density of probability for two kinds of bonds I_A and I_B is

$$P(J_{ij})=(1-c)\delta(J_{ij}-I_A)+c\delta(J_{ij}-I_B)\;, \qquad (2)$$

where $J_{ij}=J(R_{ij})_i$ and $R_{ij}=|R_i-R_j|\sim a$, where a is the lattice constant. In this model the disorder is given by the bond distribution, which is chaotic, and there are no problems with the equivalence between this model and the model with the site disorder.

Such problems appear for the long-range cases.[11] The occurrence of the spin-glass state in a system with short-range interactions can be treated by using the interactions between nearest-neighbor atoms, but using for this interaction a Gaussian density of probability. In the critical region there are no differences between these two models,[16] but far from the critical region there are essential differences[17] as at the low temperatures.

Before presenting our model we will discuss the main results obtained by different authors for the problem of the magnetic order given by the short-range discrete interaction. In the first papers treating the disordered ferromagnet with short-range interaction, Katsura *et al.* and Veno and Oguch[18] and later Matsubara and Sakata[19] did not use the spin-glass and frustration concepts.

Important results have been obtained by Grinstein *et al.*[20] by solving the one-dimensional Ising model and by Veno and Oguchi[21] for the random Ising model with $I_A = |I_B|$. They predicted the occurrence of the spin-glass phase for the intermediate range of concentrations. Katsura[22] also obtained an analytical result for $I_A = |I_B|$ but in Ref. 22 the magnetic susceptibility presents a singularity in the zero-temperature limit. The model with $I_A \neq |I_B|$ has been treated by Medvedev[23] in the molecular field approximation, and a critical temperature was obtained (similar to the freezing temperature of Ref. 2), which is different from zero for $I_A = I_B$, thus in absence of frustration, indicating an incorrect result.

Medvedev[24] started with a density of probability given by Eq. (2), but all his calculations have been performed with different supplementary suppositions about the quantities that have to be calculated, in spite of the fact that all averages must be performed for this model using Eq. (2).

The two-dimensional Ising model with random bonds have been studied by Jayaprahash *et al.*[25] using the Migdal-Kadanoff[26] recursion relation and a maximum in the specific heat above the ferromagnetic critical temperature was obtained; this maximum can be caused by the short-range order.

Grinstein, Jayaprakash, and Wortis[27] reconsidered the analysis from Ref. 28, and using an expansion as a function of the concentration, obtained for $T = 0$ and $I_A = |I_B|$ a spin-glass state, above a critical concentration. Different attempts concerning this problem are contained in Refs. 29 and 30.

The theoretical treatment of the three-dimensional model is poor and does not contain any relevant results. For $T \neq 0$ the majority of the results have been obtained for $I_A = |I_B|$; even if these results are interesting, they are not enough to obtain the phase diagram with the parameter I_A/I_B. The calculations performed by Medvedev[23,24] in order to obtain the phase diagram contained too many approximations and it is considered a very difficult solution to this problem.

The Monte Carlo simulations have been extensively used in order to study the spin-glass state given by the short-range discrete interactions. These simulations reproduce generally the experimental results, but we must note that these results reflect an obvious ambiguity.[31] All the theoretical descriptions[32,33] try to demonstrate the correctness of a model by comparing the results obtained by the Monte Carlo simulations. The common feature of these simulations is contained in Refs. 17 and 34; the main result consists in the fact that the spin-glass phase defined in Ref. 17 can appear above a critical concentration. However, recently Morgenstein and Binder,[35] performing a static and dynamic average, obtained an interesting result, namely, that the order parameter defined by Edwards and Anderson[1] vanishes below the freezing temperature for the models in two and three dimensions. This result can be explained as follows: For a finite time of the simulation the system will remain near a metastable minimum. For small simulation time the metastable minimum will give a nonzero value for the order parameter, but the average order parameter given by these metastable minima gives a zero value in two or three dimensions.

Kirkpatrick and Young,[36] using the results from Ref. 35, introduced a new order parameter related to the four-spin correlation $\langle S_i^\alpha S_j^\beta S_i^\gamma S_j^\delta \rangle$, where $\alpha, \beta, \gamma, \delta$ are the replica indices. With the use of the Monte Carlo simulation it was shown that a spin-glass phase characterized by the new order parameter can appear. In spite of the fact that this idea seems to be useful in the theory of the spin-glass state, Kaplan,[37] performing analytical calculations, obtained interesting results that the number of the metastable states in the one-dimensional Heisenberg model is zero, and concluded that a large number of low-lying minima in certain vector-spin models are without physical foundation. All these results, which have been considered in this short review of our paper, demonstrate that the results obtained by the Monte Carlo simulation can be a basis for a discussion of some analytical results, but cannot be the decisive test of the validity of one model or of a method.

In Sec. II we will use the replica-trick formalism for a short-range model with $I_A + I_B > 0$, but the summation will be performed considering an infinite number of terms. The calculation performed in Sec. III following the Edwards and Anderson[1] method will reproduce even the unphysical Sherrington and Kirkpatrick[2] result. In Sec. IV we will use the new order parameter introduced by Kirkpatrick and

Young[36] in order to describe the new spin-glass phase. Section V contains the discussions of these results.

II. THE MODEL

We start with the Hamiltonian

$$\mathscr{H}=-\sum_{ij}{}' J_{ij}S_iS_j-H\sum_i S_i,\quad S_i=\pm 1 \tag{3}$$

which describes the Ising cubic lattice of spins, which are randomly distributed and which interact by the exchange integral J_{ij}. The summations in (3) denoted by $\sum'$ mean that we consider the spin-spin interaction at the distance $|R_i-R_j|=a$, where a is the lattice constant. Then we have $\sum'_{ij}1=Nz$, where N is the number of sites and z the number of the nearest-neighbor bonds per site, ν will be the number of the nearest-neighbor bond for a magnetic atom; we will call ν the number of active bonds. In the Hamiltonian (3) H is the external field and J_{ij} the random coupling constant distributed according to the density of probability

$$P(J_{ij})=(1-c)\delta(J_{ij}-I_A)+c\delta(J_{ij}-I_B)\ . \tag{4}$$

In the thermodynamic limit, the free energy of the system can be written in the replica-trick formalism as

$$f=-k_BT\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{nN}\left[\mathrm{Tr}_n\int\prod_{ij}{}'[P(J_{ij})dJ_{ij}]\exp\left[\sum_\alpha \mathscr{H}^\alpha_\beta\right]-1\right], \tag{5}$$

where

$$\mathscr{H}^\alpha=-\sum_{ij}{}' J_{ij}S_i^\alpha S_j^\alpha-H\sum_i S_i^\alpha,\quad \beta=\frac{1}{k_BT}\ . \tag{6}$$

α is the replica index and Tr_n denotes the trace, which will be performed separately in each of the n replicas. Using the results given by Eqs. (A1), (A10), and (A11), we get for (5) the equation

$$f=-k_BT\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{nN}\left\{\mathrm{Tr}_n\exp\left[\beta H\sum_{i\alpha}S_i^\alpha+\sum_{ij}{}'\sum_{k=1}^{\infty}a_k\left[\beta\sum_\alpha^n S_i^\alpha S_j^\alpha\right]^k\right]-1\right\}, \tag{7}$$

where

$$a_1=(1-c)I_A+cI_B,\quad a_k\,|_{k\geq 2}=\frac{c(1-c)f_k(c)}{k!}(I_A-I_B)^k\ . \tag{8}$$

From (A11) we can see that the function $f_k(c)$ is a polynomial of a $(k-2)$ order in c. Another important observation is that in the three limiting cases $c=0$, $c=1$, and $I_A=I_B$ the two or the superior replica interaction terms in the free energy (7) vanish and then the spin-glass state cannot appear.

In this paper we will be interested in obtaining the phase diagram and other thermodynamic quantities at $T\neq 0$ for different values of the ratio I_A/I_B. The phase diagram for the systems, which can be described by "I_A-I_B model,"[13,14] has been obtained for $c=\frac{1}{2}$. This concentration is above the critical threshold[27] obtained for $I_A=|I_B|$ at $T=0$. The spin-glass phase defined in the Edwards and Anderson sense may appear for any favorable values of the parameters T and I_A/I_B. It is clear that it is easier to study this problem if we fix $c=\frac{1}{2}$; using (A16), we get for the free energy

$$f=-k_BT\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{nN}\left\{\mathrm{Tr}_n\exp\left[\beta H\sum_{ai}S_i^\alpha+a_1\beta\sum_{ij}{}'\sum_\alpha S_i^\alpha S_j^\alpha+\sum_{ij}{}'\sum_{k=1}^{\infty}a_{2k}\left[\beta\sum_\alpha^n S_i^\alpha S_j^\alpha\right]^{2k}\right]-1\right\}. \tag{9}$$

The interaction within the same replica gives rise to the magnetization[38] $m=\langle S_i\rangle$ and

$$\sum_{ij}{}' S_i^\alpha S_j^\alpha\cong 2\sum_{ij}{}'(\langle S_i^\alpha\rangle S_j^\alpha-\tfrac{1}{2}\langle S_i^\alpha\rangle\langle S_j^\alpha\rangle)\ . \tag{10}$$

If we define

$$T_{2k}=\sum_{ij}{}'\left[\sum_\alpha^n S_i^\alpha S_j^\alpha\right]^{2k}, \tag{11}$$

then, Eq. (9) becomes

$$f=-k_BT\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{nN}\left[\exp(-zNna_1\beta m^2)\mathrm{Tr}_n\exp\left[\beta(H+2a_1zm)\sum_{i\alpha}S_i^\alpha+\sum_{k=1}^{\infty}a_{2k}\beta^{2k}T_{2k}\right]-1\right]. \quad (12)$$

From this equation we can see that in order to calculate the free energy we have to calculate explicitly the term T_{2k}. Next, we will consider the contribution of this term up to infinite order. Before performing such a calculation with the new order parameter introduced in Ref. 36, we will present the results obtained using the Edwards-Anderson approximation, but for the short-range model.

III. EDWARDS AND ANDERSON APPROXIMATION

We obtain the Edwards and Anderson[1] approximation if the term T_{2k} given by Eq. (11) is written as

$$T_{2k}=\sum_{ij}{}'\sum_{\alpha_1\cdots\alpha_{2k}}S_i^{\alpha_1}\cdots S_i^{\alpha_{2k}}S_j^{\alpha_1}\cdots S_j^{\alpha_{2k}}$$

$$=2\sum_{ij}{}'\sum_{\alpha_1\cdots\alpha_{2k}}(\langle S_i^{\alpha_1}\cdots S_i^{\alpha_{2k}}\rangle S_j^{\alpha_1}\cdots S_j^{\alpha_{2k}}-\tfrac{1}{2}\langle S_i^{\alpha_1}\cdots S_i^{\alpha_{2k}}\rangle\langle S_j^{\alpha_1}\cdots S_j^{\alpha_{2k}}\rangle) \quad (13)$$

and the $2k$ replicated average can be expressed as

$$\langle S_i^{\alpha_1}\cdots S_i^{\alpha_{2k}}\rangle=\prod_{l=1}^{k}(\delta_{\alpha_{2l-1}\alpha_{2l}}+\tilde{\delta}_{\alpha_{2l-1}\alpha_{2l}}q), \quad (14)$$

where

$$\tilde{\delta}_{\alpha_i\alpha_j}=1-\delta_{\alpha_i\alpha_j},\quad q=\lim_{n\to 0}\langle S_i^\alpha S_i^\beta\rangle\,|_{\alpha\neq\beta} \quad (15)$$

is the Edwards and Anderson order parameter.[1] After some algebra we get from Eqs. (13)–(15)

$$T_{2k}=\nu\sum_i\left[n(1-q)+q\left[\sum_\alpha S_i^\alpha\right]^2\right]^k-Nz[n+(n-1)nq^2]^k \quad (16)$$

and from (A14)–(A19)

$$\exp\left[\nu\sum_i\sum_{k=1}^{\infty}\frac{h_{2k}(\frac{1}{2})}{(2k)!}\left[\beta(I_A-I_B)\sqrt{q}\sum_\alpha S_i^\alpha\right]^{2k}\right]=\int_{(\nu)}\tilde{P}_1\{J\}d\{J\}\exp\left[\{J\}\,|I_A-I_B|\,\frac{\beta\sqrt{q}}{2}\sum_{i\alpha}S_i^\alpha\right], \quad (17)$$

where $\tilde{P}_1(J)$ has been given by (A19) and

$$\int_{(\nu)}\tilde{P}_1\{J\}d\{J\}f(\{J\})\equiv\int\prod_{i=1}^{\nu}[\tilde{P}_1(J_i)dJ_i]f\left[\sum_{i=1}^{\nu}J_i\right]. \quad (18)$$

On the other hand, in Eq. (12) the contributions containing n^p with $p\geq 2$ vanishes for $n\to 0$ and we obtain for the free energy the equation

$$f=-k_BT\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{nN}\left\{\exp[zNna_2\beta^2(1-q)^2-zNna_1\beta m^2]\right.$$

$$\left.\times\mathrm{Tr}_n\int_{(\nu)}\tilde{P}_1\{J\}d\{J\}\exp\left[\beta\left[H+2a_1zm+\{J\}\frac{|I_A-I_B|}{2}\sqrt{q}\right]\sum_{i\alpha}S_i^\alpha\right]-1\right\}. \quad (19)$$

In this case the average of the configurations reduced all the problems to a one-site problem. In fact, if one spin in the I_A-I_B model interacts only with ν nearest-neighbor bonds we have for one spin only ν active bonds, which can randomly take the value I_A or I_B. This means that in this model, and using the Edwards-Anderson concept of the order parameter, the average of the configurations can be performed using Eq. (4) over all ν active bonds.

From the free energy given by (19) we obtain in the usual way[1,2] the following equations:

$$f = zI_0 m^2 - z\frac{I_1^2(1-q)^2}{2k_BT} - k_BT\int_{(\nu)} \widetilde{P}_1\{J\}d\{J\}\ln(2\cosh\Sigma)\ , \tag{20}$$

$$q = 1 - \frac{k_BT}{\nu I_1\sqrt{q}}\int_{(\nu)} \widetilde{P}_1\{J\}d\{J\}(\tanh\Sigma)\{J\}\ , \tag{21}$$

$$m = \int_{(\nu)} \widetilde{P}_1\{J\}d\{J\}\tanh\Sigma\ , \tag{22}$$

where

$$I_0 = \frac{I_A+I_B}{2},\quad I_1 = \frac{|I_A-I_B|}{2},\quad \Sigma = \frac{1}{k_BT}(\nu m I_0 + H + \{J\}I_1\sqrt{q})\ . \tag{23}$$

From (20)—(23) we obtain the internal energy U and the entropy S of the system,

$$U = -\left[zm^2I_0 + mH + \frac{zI_1^2}{k_BT}(1-q^2)\right]\ , \tag{24}$$

$$S = -\frac{m(\nu m I_0 + H)}{T} - \frac{I_1^2 z}{2k_BT^2}(1-q)(3q+1) + k_B\int_{(\nu)} \widetilde{P}_1\{J\}d\{J\}\ln(2\cosh\Sigma)\ . \tag{25}$$

With these results and using (B5)—(B7) we can calculate the magnetic susceptibility in the high-temperature limit. The phase diagram obtained in this way is given in Fig. 1. The order parameter q can be calculated at the transition from the phase with $q\neq 0$ and $m=0$ (the spin-glass phase) in the paramagnetic phase with $m=0$, $q=0$. In this approximation we get

$$q \cong \frac{160}{141}\left[1-\frac{T_f}{T}\right],\quad k_BT_f = \frac{4I_1}{\sqrt{3}}\ . \tag{26}$$

The occurrence of the cusp in the magnetic susceptibility will be given by the following equations:

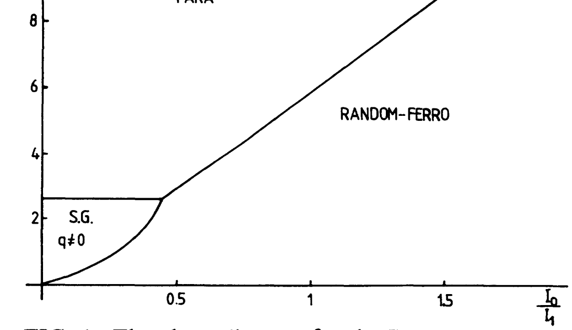

FIG. 1. The phase diagram for the Edwards-Anderson approximation. $I_0/I_1 = (I_A+I_B)/|I_A-I_B|$.

$$\chi = \frac{\chi_0}{k_BT - \nu I_0\chi_0}\ ,\qquad \chi_0 = \int_{(\nu)} \frac{\widetilde{P}_1\{J\}d\{J\}}{\cosh^2\Sigma}\bigg|_{m=H=0}\ . \tag{27}$$

At the transition from the paramagnetic phase to the random ferromagnetic phase ($q\neq 0$, $m\neq 0$) we obtain

$$m^2 \cong 3\frac{\left[\frac{T}{T_f}\right]^2 - 1}{\left[\frac{T}{T_f}\right]^2 + \frac{19}{8}}\left[1-\frac{T}{T_c}\right],\quad T_c = \frac{\nu I_0}{k_B}\ , \tag{28}$$

$$q \cong m^2\left[\frac{T}{T_f}\right]^2\left[\left[\frac{T}{T_f}\right]^2 - 1\right]^{-1}\ . \tag{29}$$

From Eq. (27) we can see that at the transition point between the spin-glass and random ferromagnet the magnetic susceptibility is divergent.

Using Eqs. (B8)—(B10) we obtain

$$q \cong 1 - \frac{15}{48}\frac{k_BT}{I_1\sqrt{q}},\quad m \cong \tfrac{5}{16} + U\exp\left[-\frac{1}{T}\right],\quad T\to 0 \tag{30}$$

and the entropy becomes

$$\left.\frac{S}{k_B}\right|_{T=0} = -\frac{75}{128} .$$

It can be proved that the heat capacity presents linear temperature dependence in the low-temperature domain. The heat capacity showed a cusp at T_f, but in this case this behavior can be considered as a characteristic feature of a concentrated spin-glass.[39]

Thus, in this section we showed that the Edwards and Anderson[1] description gives similar results with the Sherrington-Kirkpatrick[1,2] mean-field solution for the long-range case. If we analyze the Edwards-Anderson method applied to this model, we must note that in the explicit calculation of the T_{2k} terms of Eq. (13) and $2k$-order replicated average, given by Eqs. (14) and (15), we assumed that only the Edwards-Anderson one-site averages are different from zero and all the other spin correlations vanish. The reason for this approach is the tradition of the spin-glass theory, and in fact this approach is supported by the results presented in Refs. 1–7, which seem to be overcome.[35,36] In Sec. IV we will try to solve the difficulties that appear in the traditional theory, using a new order parameter that will give zero entropy for $T=0$. This important result is in agreement with the Monte Carlo calculation, but it has been obtained using an infinite summation; with this approximation we will obtain better results than the mean-field approximation.

IV. DESCRIPTION WITH THE NEW ORDER PARAMETER

The T_{2k} terms from Eq. (11) can be treated in such a way that the introduction of the two-site—four-spin average becomes possible:

$$T_{2k}=2\sum_{ij}{}' \sum_{\alpha_1 \cdots \alpha_{2k}} [\langle S_i^{\alpha_1} S_j^{\alpha_2} \cdots S_i^{\alpha_{2k-1}} S_j^{\alpha_{2k}} \rangle S_j^{\alpha_1} S_i^{\alpha_2} \cdots S_j^{\alpha_{2k-1}} S_i^{\alpha_{2k}} - \tfrac{1}{2} \langle S_i^{\alpha_1} S_j^{\alpha_2} \cdots S_i^{\alpha_{2k-1}} S_j^{\alpha_{2k}} \rangle \langle S_j^{\alpha_1} S_i^{\alpha_2} \cdots S_j^{\alpha_{2k-1}} S_i^{\alpha_{2k}} \rangle] . \tag{31}$$

To make the $2k$-order replicated correlations explicit, we take in consideration the following:

(a) In agreement with the Monte Carlo simulations[35,36] the Edwards-Anderson-type average vanishes.

(b) Without the one-replica average, from Eq. (10), which gives the bulk magnetization, the only nonvanishing correlation is

$$Q=\lim_{n\to 0} \langle S_i^\alpha S_j^\alpha S_i^\beta S_j^\gamma \rangle \,|_{\substack{\alpha\neq\beta \\ \alpha\neq\gamma}} , \tag{32}$$

where Q is the new order parameter. In this situation, Eq. (14) becomes

$$\langle S_i^{\alpha_1} S_j^{\alpha_2} \cdots S_i^{\alpha_{2k-1}} S_j^{\alpha_{2k}} \rangle = \delta(k,2p) \prod_{i=1}^{p} (\delta_{\alpha_i \alpha_{i+2}} \delta_{\alpha_{i+1}\alpha_{i+3}} \tilde{\delta}_{\alpha_i \alpha_{i+1}} + Q \tilde{\delta}_{\alpha_i \alpha_{i+2}} \tilde{\delta}_{\alpha_{i+1}\alpha_{i+3}} \delta_{\alpha_i \alpha_{i+1}}) , \tag{33}$$

where

$$\delta(k,2p)=\begin{cases} 1 & \text{if } k=2p, \\ 0 & \text{if } k=2p+1; \end{cases}$$

and p is an arbitrary integer. Using Eqs. (32) and (33), the T_{2k} term from (31) becomes

$$T_{2k}=2\delta(k,2p)\sum_{ij}{}' \left[\left[n(n-1)+Q \sum_{\substack{\alpha\neq\beta \\ \alpha\neq\gamma}} S_i^\alpha S_j^\alpha S_i^\beta S_j^\gamma \right]^p - \tfrac{1}{2}[n(n-1)+Q^2(n^3-2n^2+n)]^p \right] . \tag{34}$$

In the approximation of the four-spin coefficient in (34) we take into account that $\sum_{\alpha\neq\beta,\alpha\neq\gamma} = \sum_{\alpha\beta\gamma} \tilde{\delta}_{\alpha\beta} \tilde{\delta}_{\alpha\gamma}$ and that

$$\sum_{\alpha\beta\gamma} S_i^\alpha S_j^\alpha S_i^\beta S_j^\gamma \equiv 4 \left[\sum_{(\alpha\beta)} S_i^\alpha S_i^\beta \right] \left[\sum_{(\gamma\delta)} S_j^\gamma S_j^\delta \right] + 4n \sum_{(\alpha\beta)} S_i^\alpha S_j^\beta + n^2 - \sum_{\alpha\neq\delta,\beta,\gamma} S_i^\alpha S_j^\delta S_i^\beta S_j^\gamma, \ (\alpha\beta) \equiv \alpha\neq\beta \Lambda \alpha<\beta \tag{35}$$

and neglecting the irrelevant two- and four-spin terms, we obtain

$$\sum_{\substack{\alpha\neq\beta\\ \alpha\neq\gamma}} S_i^\alpha S_j^\alpha S_i^\beta S_j^\gamma \cong n+4\left[\sum_\alpha S_i^\alpha\right]^2\left[\sum_\beta S_j^\beta\right]^2 . \tag{36}$$

In this way from Eqs. (12), (34), and (36) we get

$$f=-k_BT\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{nN}\left\{\exp[-zNna_1\beta m^2-zNna_4\beta^4(1-Q)^2]\right.$$
$$\times \mathrm{Tr}_n\exp\left[\beta(H+2a_1zm)\sum_{i\alpha}S_i^\alpha\right.$$
$$\left.\left.+\,2\sum_{ij}{}'\sum_{k=1}^{\infty}a_{4k}\beta^{4k}(4Q)^k\left[\sum_\alpha S_i^\alpha\right]^{2k}\left[\sum_\beta S_j^\beta\right]^{2k}\right]-1\right\} . \tag{37}$$

From Eqs. (A10)—(A14) and (A19)—(A22) we have

$$\exp\left[2z\sum_{k=1}^{\infty}\frac{h_{4k}(\frac{1}{2})}{(4k)!}\left[\beta(I_A-I_B)(4Q)^{1/4}\left|\sum_\alpha S_i^\alpha\right|^{1/2}\left|\sum_\beta S_j^\beta\right|^{1/2}\right]^4\right]$$
$$=\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}\exp\left[\{J\}I_1\beta(4Q)^{1/4}\left|\sum_\alpha S_i^\alpha\right|^{1/2}\left|\sum_\beta S_j^\beta\right|^{1/2}\right]d\{J_1\}d\{J_2\} , \tag{38}$$

where

$$\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}f(\{J\})\equiv\int\prod_{ij=1}^{z}[\widetilde{P}_1(J_1^i)\widetilde{P}_2(J_2^j)dJ_1^idJ_2^j]f\left(\sum_{i=1}^{z}J_1^i+\sum_{j=1}^{z}J_2^j\right) . \tag{39}$$

Now we can use (A10) and (A11) for a_1 and a_4, and the free energy equation (37) becomes

$$f=-k_BT\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{nN}\left[\exp\left[-zNn\beta I_0m^2+\frac{I_1{}^4}{12}\beta^4nNz(1-Q)^2\right.\right.$$
$$+N\ln\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}$$
$$\times\mathrm{Tr}_n\exp\left\{\beta(H+2I_0zm)\sum_\alpha S_i^\alpha\right.$$
$$\left.\left.\left.+\,\{J\}I_1\beta(4Q)^{1/4}\left[\left[\sum_\alpha S_i^\alpha\right]^2\left[\sum_\beta S_{i+a}^\beta\right]^2\right]^{1/4}\right\}\right]-1\right] . \tag{40}$$

Performing the trace separately in all the n replicas, and using the approximation $[(n-2k)^2(n-2p)^2]^{1/2}\simeq n-k-p$ for $n>k,p$, $n\to 0$, we obtain

$$\mathrm{Tr}_n\exp\left\{A\sum_\alpha S_i^\alpha+B\left[\left[\sum_\alpha S_i^\alpha\right]^2\left[\sum_\beta S_{i+a}\right]^2\right]^{1/4}\right\}$$
$$=\sum_{k=0}^{n}C_n^k\exp\left[A(n-2k)+\frac{B}{2}(n-2k)\right]\sum_{p=0}^{n}C_n^p\exp\left[\frac{B}{2}(n-2p)\right] , \tag{41}$$

where we consider C_n^m defined in (B1), and A and B as two spin-independent quantities. With these approximations the free energy and the equations for the order parameter and magnetization are

$$f=zI_0m^2-\frac{I_1^4}{12}z\beta^3(1-Q)^2-k_BT\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}\times\ln 4\cosh\beta\left[H+2I_0mz+\frac{\{J\}}{2}I_1(4Q)^{1/4}\right]\cosh\left[\frac{\{J\}}{2}I_1\beta(4Q)^{1/4}\right],\tag{42}$$

$$Q=1-\frac{1}{(4Q)^{3/4}(I_1\beta)^3}\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}\{J\}\times\left[\tanh\left[\frac{\{J\}}{2}I_1\beta(4Q)^{1/4}\right]+\tanh\beta\left[H+2I_0mz+\frac{\{J\}}{2}I_1(4Q)^{1/4}\right]\right],\tag{43}$$

$$m=\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}\tanh\beta\left[H+2I_0mz+\frac{\{J\}}{2}I_1(4Q)^{1/4}\right].\tag{44}$$

From Eqs. (42)–(44) we obtain the internal energy and the entropy of the system:

$$U=-[I_0zm^2+mH+I_1^4\beta^3(1-Q^2)],\tag{45}$$

$$\frac{S}{k_B}=-\beta m(H+2I_0mz)-\frac{\beta^4I_1^4}{4}(1-Q)(5Q+3)+\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}\ln 4\cosh\beta\left[H+2I_0mz+\frac{\{J\}}{2}I_1(4Q)^{1/4}\right]\cosh\left[\frac{\{J\}}{2}I_1\beta(4Q)^{1/4}\right].\tag{46}$$

The magnetic susceptibility is given by Eq. (27) with

$$\chi_0=\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}\times\frac{1}{\cosh^2[\beta(\{J\}/2)I_1(4Q)^{1/4}]}.\tag{47}$$

The new phase diagram (Fig. 2) has been obtained following the procedure described in Sec. III. Near the transition line from the paramagnetic state ($m=0$, $Q=0$) to the spin-glass state ($m=0$, $Q\neq 0$) we obtain from (B22) and (B23)

$$Q=\bar{a}\left[1-\frac{T}{T_f}\right],$$

where (48)

$$k_BT_f=I_1\left[\frac{17\times 197}{180}\right]^{1/4},$$

where $\bar{a}=3.924$.

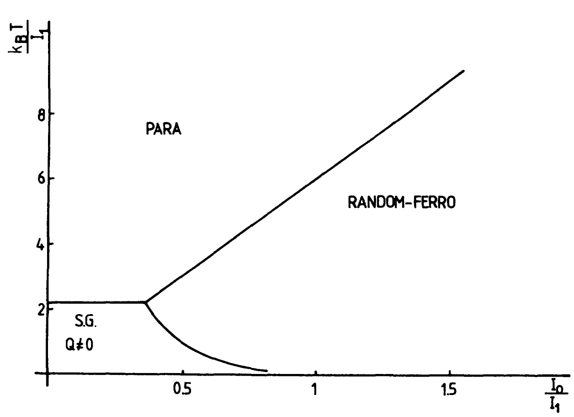

FIG. 2. The phase diagram for the theory with the new order parameter. $I_0/I_1=(I_A+I_B)/|I_A-I_B|$.

The Curie temperature T_C, which is the critical temperature, for the transition from the paramagnetic state to the random ferromagnet is identical with the value obtained from Eq. (28). The linear temperature dependence of the order parameter Q given by (48) and Eqs. (27) and (47) for the magnetic susceptibility implies the occurrence of the cusp in $\chi(T)$ at the freezing temperature T_f. At $T=0$, the model does not present negative entropy. Using (B27), we obtain for $T\to 0$

$$Q\cong 1-\frac{z}{(I_1\beta)^3}(4Q)^{-3/4}\tag{49}$$

and using (49) in (46), we get

$$S/k_B=0 \text{ at } T=0.$$

We mention that the zero-entropy result is not a fortunate accident of some well-chosen coefficients in the free energy (43). It can be proved that independently of the numerical coefficients in the free energy, the entropy of the system will vanish at $T=0$.

Another characteristic of this model is that at the transition from the paramagnetic to the spin-glass state, the free energy variation is negative, and at the transition point the ordered phase is stable energetically compared to the paramagnetic one:

$$\delta f = f\,|_{Q\neq 0} - f_{Q=0} = -\frac{I_1{}^4\beta^3}{4}Q^2 < 0 \; . \tag{50}$$

At T_c we have $\delta f < 0$ and

$$\delta f = f\,|_{\substack{Q\neq 0\\ m\neq 0}} - f\,|_{\substack{Q=0\\ m=0}} = zI_0 m^2\left[1-\frac{T_c}{T}\right] - \frac{I_1{}^4\beta^3 Q^2}{4} < 0 \; , \quad \text{for } T \lesssim T_c \; . \tag{51}$$

The validity of these results for the theory of the spin-glass needs more accurate experimental data on compounds which may be described by the $I_A - I_B$ model. This model can be improved and the calculations can be generalized for the $c \neq \frac{1}{2}$ case, and taking into consideration the occurrence of the clusters.

V. DISCUSSIONS

We presented an analytic description for the spin-glass state with discrete and chaotic bonds. In order to simplify the mathematical aspects, we treated only the case of the equal concentrations of the negative and positive bonds. The model consists of the Ising spins in a simple cubic lattice. We treated in detail the case $I_A + I_B > 0$ case with $I_A > 0$ and $I_B < 0$ bonds. The replica-trick method and the infinite-order summation have been used in order to obtain the thermodynamic quantities. First, we showed that in this model the Edwards and Anderson[1] results can be reobtained, in spite of the fact that the density of probability in our case differs from the Gaussian one, and although the calculations were not performed using a steepest-descent procedure (and then the interchange of the $N\to\infty$ and $n\to 0$ limits), the Sherrington and Kirkpatrick[2] results with negative entropy have been reobtained. It is interesting to mention that this conclusion remains true if the system is frustrated as well, as in the case, if at $T=0$ we have $m\neq 0$ and $Q\neq 0$. However, if the system is not frustrated ($I_A + I_B > |I_A - I_B|$) the entropy becomes zero at $T=0$. This result seems to confirm the fact that the actual difficulties of the actual stage of the spin-glass theory is due to the Edwards-Anderson[1] parameter in the frustrated system.[6] Furthermore, recent Monte Carlo simulation[35,36] indicated that the Edwards and Anderson[1] order parameter vanishes below the freezing temperature.

In our paper, following the Kirkpatrick and Young[36] suggestion, we have described a model in which the order parameter is given by four-spin correlation, and we obtained at $T=0$ the zero value for the entropy. These "ordered phases" just below the transition temperatures are stable from an energetical point of view. In our model the heat capacity (C_p) presents a cusp at the freezing temperature and gives a T^2 dependence in the limit $T\to 0$. The cusp from C_p can be removed above T_f by clustering effects, but the low-temperature dependence is characteristic for this model. The results concerning the heat capacity C_p are not essentially connected with the model because the concentrated spin-glass presents such a behavior. The definition of the order parameter is not *a priori* fixed, and we can treat it using this new order parameter as well as the long-range model.

This paper takes into consideration the results obtained by the Monte Carlo simulations, and in order to get reasonable agreement with the numerical simulations and the experimental data we defined a new order parameter that seems to be appropriate for this model of the spin-glass. An important conclusion of this paper is that the average of the configurations for the short-range discrete bond model, from the new point of view, was changed from the average of the nearest-neighbor bonds to an average over all nearest-neighbor atom pairs per one site. This average presents some advantages in performing the calculation at $T=0$. If this definition for the order parameter is maintained for the other systems that are in the spin-glass state, such an average will be useful for the $I_A - I_B$ model, giving zero value for the entropy at $T=0$.

APPENDIX A

The coefficients a_k from the relation

$$\int P(J)dJ \exp\left[\beta J \sum_\alpha S_i^\alpha S_j^\alpha\right] = \exp\left[\sum_{k=1}^{\infty} a_k \left[\beta \sum_\alpha S_i^\alpha S_j^\alpha\right]^k\right] , \tag{A1}$$

where

$$P(J) = (1-c)\delta(J-I_A) + c\delta(J-I_B) \; , \tag{A2}$$

will be determined as follows: The integral from (A1) can be written in the form

$$\int P(J)dJ \exp\left[\beta J \sum_\alpha S_i^\alpha S_j^\alpha\right] = \sum_{l=0}^{\infty}\left[\beta\sum_\alpha S_i^\alpha S_j^\alpha\right]^l \frac{(1-c)I_A^l+cI_B^l}{l!} . \tag{A3}$$

For the exponential term from (A1) we use

$$\exp\left[\sum_{k=1}^{\infty} a_k t^k\right] = \sum_{l=0}^{\infty} t^l A_l(a_1,a_2,\ldots,a_i,\ldots) , \tag{A4}$$

where

$$t=\beta\sum_\alpha S_i^\alpha S_j^\alpha . \tag{A5}$$

The coefficient $A_l(a_1,a_2,\ldots,a_i,\ldots)$ can be expressed in the following way:

$$\exp\left[\sum_{k=1}^{\infty} a_k t^k\right] = \sum_{p=0}^{\infty}\frac{1}{p!}\left[\sum_{k=1}^{\infty} a_k t^k\right]^p = \sum_{p=0}^{\infty}\frac{t^p}{p!}\left[\sum_{k=1}^{\infty} a_k t^{k-1}\right]^p = \sum_{p=0}^{\infty}\frac{t^p}{p!}\sum_{k=0}^{\infty} d_k^p t^k = \sum_{k,p=0}^{\infty} t^{k+p}\left[\frac{1}{p!}d_k^p\right] . \tag{A6}$$

The coefficients d_k^p (for d, the indices p do not mean a power) satisfy the following recurrence relations[40]:

$$d_k^p=\frac{1}{ka_1}\sum_{j=1}^{k}(jp-k+j)a_{j+1}d_{k-j}^p . \tag{A7}$$

From Eqs. (A4), (A6), and (A7), using coefficient identification, we obtain

$$A_l(a_1,a_2,\ldots,a_i,\ldots)=\sum_{j=0}^{l}\frac{d_j^{l-j}}{(l-j)!} . \tag{A8}$$

Now it is possible to express a_k from (A3), (A4), (A5), and (A8) as

$$\begin{aligned}
&(1-c)I_A+cI_B=A_1(a_1,a_2,\ldots,a_i,\ldots)=a_1 ,\\
&\frac{(1-c)I_A{}^2+cI_B{}^2}{2!}=A_2(a_1,a_2,\ldots,a_i,\ldots)=\frac{a_1{}^2}{2}+a_2 ,\\
&\frac{(1-c)I_A{}^3+cI_B{}^3}{3!}=A_3(a_1,a_2,\ldots,a_i,\ldots)=\frac{a_1{}^3}{6}+a_1a_2+a_3 ,\\
&\frac{(1-c)I_A{}^4+cI_B{}^4}{4!}=A_4(a_1,a_2,\ldots,a_i,\ldots)=\frac{a_1{}^4}{24}+\frac{a_2a_1{}^2+a_2{}^2}{2}+a_1a_3+a_4 ,
\end{aligned} \tag{A9}$$

etc. From (A9) we get

$$\begin{aligned}
&a_1=(1-c)I_A+cI_B \quad \text{for } k=1 ,\\
&a_k=\frac{c(1-c)f_k(c)}{k!}(I_A-I_B)^k \quad \text{for } k\geq 2 ,
\end{aligned} \tag{A10}$$

where

$$f_k(c)=\begin{cases} 1 \quad \text{if } k=2 \\ (-1)^k+\displaystyle\sum_{m=2}^{k}\left[\sum_{k_m=1}^{\Theta_m^k}\sum_{k_{m-1}=1}^{\Theta_{m-1}^k}\cdots\sum_{k_2=1}^{\Theta_2^k} m^{k_m}(m-1)^{k_{m-1}}\cdots 3^{k_3}2^{k_2}\right] \\ (-1)^{k-m+1}c^{m-1} \quad \text{if } k\geq 3 \end{cases} \tag{A11}$$

where

$$\Theta_{m-p}^k=k-m+p-\sum_{j=m-p+1}^{m} k_j .$$

For example, $f_3(c)=2c-1$, $f_4(c)=6c^2-6c+1$, $f_5(c)=24c^3-36c^2+14c-1$, etc. Equation (A1) with the coefficients (A10) and (A11) are correct for arbitrary values of the $\beta J\sum_\alpha S_i^\alpha S_j^\alpha$ factor, because in the calculations of these coefficients we used series expansions for the exponential function, which has an infinite radius of convergence.

In order to make simpler the $f_k(c)$ coefficient expressions we can use (A10) and (A1),

$$(1-c)e^{I_A t}+ce^{I_B t}=e^{t[(1-c)I_A+cI_B]}\exp\left[\sum_{k=2}^{\infty} c(1-c)f_k(c)\frac{t^k(I_A-I_B)^k}{k!}\right] . \tag{A12}$$

From (A12) we obtain a Fourier expansion

$$\ln(1-c\{1-\exp[-t(I_A-I_B)]\})=\sum_{k=1}^{\infty}\frac{h_k(c)}{k!}[t(I_A-I_B)]^k , \tag{A13}$$

where

$$h_k(c)=\begin{cases}-1 & \text{if } k=1\\ c(1-c)f_k(c) & \text{if } k\geq 2 .\end{cases} \tag{A14}$$

Then

$$f_k(c)\,|_{k\geq 2}=\frac{1}{c(1-c)}\left[\frac{\partial^k}{\partial x^k}\ln[1-c(1-e^{-x})]\right]\Bigg|_{x=0} . \tag{A15}$$

It is interesting to point out that for $c=\frac{1}{2}$, $f_{2k+1}(C)=0$ for $k\geq 1$. Then

$$f_{2k+1}(\tfrac{1}{2})\,|_{k\geq 1}=0 . \tag{A16}$$

Equation (A16) is satisfied because $(\partial^2/\partial x^2)\ln(1+e^{-x})=1/4\cosh^2(x/2)$, and then the higher-order derivative of $\ln(1+e^{-x})$ does not contain an odd power of x in the series expansion around $x=0$.

For the $c=\frac{1}{2}$ situation, from (A12) we obtain

$$\tfrac{1}{2}(e^{t(I_A-I_B)/2}+e^{-t(I_A-I_B)/2})=\exp\left[\sum_{k=1}^{\infty} h_{2k}(\tfrac{1}{2})\frac{[t(I_A-I_B)]^{2k}}{(2k)!}\right] . \tag{A17}$$

Introducing the notation $x=t(I_A-I_B)/2$ we have

$$\int \tilde{P}_1(J)e^{Jx}dJ=\exp\left[\sum_{k=1}^{\infty} h_{2k}(\tfrac{1}{2})\frac{(2x)^{2k}}{(2k)!}\right] , \tag{A18}$$

where

$$\tilde{P}_1(J)=\tfrac{1}{2}[\delta(J+1)+\delta(J-1)] . \tag{A19}$$

Using $t\rightarrow it$ in (A17), we obtain

$$\tfrac{1}{2}(e^{it(I_A-I_B)/2}+e^{-it(I_A-I_B)/2})=\exp\left[\sum_{k=1}^{\infty} h_{2k}(\tfrac{1}{2})(-1)^k\frac{[t(I_A-I_B)]^{2k}}{(2k)!}\right] . \tag{A20}$$

Now, if we multiply (A17) with (A20), we obtain

$$\int\int \tilde{P}_1(J_1)\tilde{P}_2(J_2)dJ_1dJ_2\exp[(J_1+J_2)x]=\exp\left[\sum_{k=1}^{\infty} h_{4k}(\tfrac{1}{2})\frac{2(2x)^{4k}}{(4k)!}\right] , \tag{A21}$$

where

$$\tilde{P}_2(J)=\tfrac{1}{2}[\delta(J+i)+\delta(J-i)] . \tag{A22}$$

APPENDIX B

In this appendix we calculate the integrals that occur in the analyzed models. For the Edwards and Anderson description, three different configurational integrals are necessary. Every one of these can be calculated with the following equation:

$$\int_{(\nu)}\tilde{P}_1\{J\}d\{J\}f(\{J\})\equiv\frac{1}{2^\nu}\sum_{k=0}^{\nu}C_\nu^k f(\nu-2K)\;, \tag{B1}$$

where $C_\nu^k=\nu(\nu-1)\cdots(\nu-k+1)/k!$ and $f(x)$ is an arbitrary function. Using (B1) one obtains for $\Sigma=a+\{J\}b$:

$$\begin{aligned}\mathcal{J}_1&=\int_{(\nu)}\tilde{P}_1\{J\}d\{J\}\tanh\Sigma\\&=\frac{1}{2^6}[\tanh(a+6b)+6\tanh(a+4b)+15\tanh(a+2b)+20\tanh a+15\tanh(a-2b)\\&\qquad+6\tanh(a-4b)+\tanh(a-6b)]\;,\end{aligned} \tag{B2}$$

$$\begin{aligned}\mathcal{J}_2&=\int_{(\nu)}\tilde{P}_1\{J\}\cdot\{J\}\tanh\Sigma d\{J\}\\&=\frac{6}{2^6}[\tanh(a+6b)+4\tanh(a+4b)+5\tanh(a+2b)-5\tanh(a-2b)-4\tanh(a-4b)\\&\qquad-\tanh(a-6b)]\;,\end{aligned} \tag{B3}$$

$$\begin{aligned}\mathcal{J}_3&=\int_{(\nu)}\tilde{P}_1\{J\}\ln 2\cosh\Sigma d\{J\}\\&=\frac{1}{2^6}[\ln 2\cosh(a+6b)+6\ln 2\cosh(a+4b)+15\ln 2\cosh(a+2b)+20\ln 2\cosh a\\&\qquad+15\ln 2\cosh(a-2b)+6\ln 2\cosh(a-4b)+\ln 2\cosh(a-6b)]\;.\end{aligned} \tag{B4}$$

In the concrete equations of Sec. III, $a=A/T$ and $b=B/T$. For the case $T\to\infty$, from (B2)–(B4) up to T^{-3}-order terms we obtain

$$\mathcal{J}_1\cong a-\frac{a^3}{3}-6ab^2+O(T^{-5})\;, \tag{B5}$$

$$\mathcal{J}_2\cong 6b-32b^3+\frac{2^5\times 47}{5}b^5-6ba^2+O(T^-5)\;, \tag{B6}$$

$$\mathcal{J}_3\cong\ln 2+3b^2+\frac{a^2}{2}+O(T^{-4})\;. \tag{B7}$$

We examine the $T\to 0$ approximation for the $a<2b$ case:

$$\mathcal{J}_1\cong\tfrac{5}{16}+O(e^{-1/T})\;, \tag{B8}$$

$$\mathcal{J}_2\cong\tfrac{15}{8}+O(e^{-1/T})\;, \tag{B9}$$

$$\mathcal{J}_3\cong\tfrac{5}{16}a+\tfrac{15}{8}b+O\exp\left[-\frac{1}{T}\right]\;, \tag{B10}$$

For the model with the new order parameter the configurational integrals can be calculated with the following equations:

$$\int\int_{(z)}\tilde{P}_1\{J_1\}\tilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}f(\{J\})\equiv\frac{1}{2^{2z}}\sum_{k=0}^{z}\sum_{l=0}^{z}C_z^kC_z^l f[(z-2k)+i(z-2l)]\;, \tag{B11}$$

where $\{J\}=\{J_1\}+\{J_2\}$ and $f(x)$ is an arbitrary function.

For $\Sigma=a+\{J\}b$ we obtain from (B11)

$$\overline{\mathscr{F}}_1=\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}\tanh\Sigma=\frac{1}{2^6}(\Theta^{3,3}_{(a,b)}+3\Theta^{3,1}_{(a,b)}+3\Theta^{1,3}_{(a,b)}+9\Theta^{1,1}_{(a,b)}) , \quad \text{(B12)}$$

where

$$\Theta^{n,m}_{(a,b)}=F^{n,m}_{(a,b)}-F^{n,m}_{(-a,b)},\quad F^{n,m}_{(a,b)}=\frac{\sinh 2(nb+a)}{\cosh^2(nb+a)-\sin^2 mb} , \quad \text{(B13)}$$

$$\overline{\mathscr{F}}_2=\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}\{J\}\tanh\Sigma=\frac{1}{2^6}(\phi^{3,3}_{(a,b)}+3\phi^{3,1}_{(a,b)}+3\phi^{1,3}_{(a,b)}+9\phi^{1,1}_{(a,b)}) , \quad \text{(B14)}$$

where

$$\phi^{n,m}_{(a,b)}=E^{n,m}_{(a,b)}+E^{n,m}_{(-a,b)} \text{ and } E^{n,m}_{(a,b)}=\frac{n\sinh 2(nb+a)-m\sin 2mb}{\cosh^2(nb+a)-\sin^2 mb} , \quad \text{(B15)}$$

$$\overline{\mathscr{F}}_3=\int\int_{(z)}\widetilde{P}_1\{J_1\}\widetilde{P}_2\{J_2\}d\{J_1\}d\{J_2\}\ln 2\cosh\Sigma=\frac{1}{2^6}(\varphi^{3,3}_{(a,b)}+3\varphi^{3,1}_{(a,b)}+3\varphi^{1,3}_{(a,b)}+9\varphi^{1,1}_{(a,b)}) , \quad \text{(B16)}$$

where

$$\varphi^{n,m}_{(a,b)}=H^{n,m}_{(a,b)}+H^{n,m}_{(-a,b)},\quad H^{n,m}_{(a,b)}=\ln 2[\cosh 2(nb+a)+\cos 2mb] . \quad \text{(B17)}$$

For the $a=A/T$ and $b=B/T$, in the $T\to\infty$ case we obtain

$$\Theta^{n,m}_{(a,b)}+\Theta^{m,n}_{(a,b)}=8\left[a-\frac{a^3}{3}+\frac{2}{15}a^5\right]-16\xi(n,m)ab^4+O(T^{-7}) , \quad \text{(B18)}$$

$$\phi^{n,m}_{(a,b)}+\phi^{m,n}_{(a,b)}=8\xi(n,m)b^3-32\xi(n,m)a^2b^3+\eta(n,m)b^7+\zeta(n,m)b^{11}+O(T^{-9}) , \quad \text{(B19)}$$

$$\varphi^{n,m}_{(a,b)}+\varphi^{m,n}_{(a,b)}=4a^2-\frac{2a^4}{3}+2b^4\xi(n,m)+4\ln 4+O(T^{-6}) , \quad \text{(B20)}$$

where

$$\xi(n,m)=\tfrac{2}{3}(n^4+m^4)-(n^2-m^2)^2 , \quad \text{(B21)}$$

$$\eta(n,m)=8\left[\frac{4}{9\times 35}(n^8+m^8)-\tfrac{2}{9}(n^4+m^4)-(n^2-m^2)^4-\tfrac{8}{45}(n^2-m^2)(n^6-m^6)+\tfrac{4}{3}(n^2-m^2)^2(n^4+m^4)\right] , \quad \text{(B22)}$$

$$\begin{aligned}\zeta(n,m)=4\Bigg[&\frac{2^{11}}{11!}(n^{12}+m^{12})-\frac{6\times 2^{10}}{10!}(n^{10}-m^{10})(n^2-m^2)+\frac{2^8}{8!}(n^8+m^8)(n^2-m^2)^2\\&+\left[\frac{2^3}{4!}(n^4+m^4)(n^2-m^2)-\frac{2^5}{6!}(n^6-m^6)\right]\left[\frac{2^5}{5!}(n^6-m^6)+2(n^2-m^2)^3-\frac{3\times 2^4}{4!}(n^2-m^2)(n^4+m^4)\right]\\&+2\xi(n,m)\left[\frac{2^5}{6!}(n^6-m^6)(n^2-m^2)-\frac{2^7}{8!}(n^8+m^8)\right]\\&+\frac{\xi(n,m)}{4}\left[(n^2-m^2)^2-\frac{8}{4!}(n^4+m^4)\right]\Bigg] . \end{aligned} \quad \text{(B23)}$$

From Eqs. (B12)–(B23) we obtain

$$\overline{\mathscr{F}}_1\cong a-\frac{a^3}{3}+\frac{2}{15}a^5-\frac{20}{3}ab^4+O(T^{-7}) , \quad \text{(B24)}$$

$$\overline{\mathscr{F}}_2\cong 4b^3-16a^2b^3-\frac{197\times 17\times 4b^7}{45}+O(T^{-9}) , \quad \text{(B25)}$$

$$\bar{\mathscr{J}}_3 \cong \ln 2 + \frac{a^2}{2} - \frac{a^4}{12} + b^4 + O(T^{-6}) \,. \tag{B26}$$

For $T \to 0$ we have $(a < b)$:

$$\tilde{\mathscr{J}}_1 \cong O(e^{-1/T}), \;\; \bar{\mathscr{J}}_2 \cong \tfrac{3}{2} + O(e^{-1/T}), \;\; \bar{\mathscr{J}}_3 \cong \tfrac{3}{2} b + O(e^{-1/T}) \,. \tag{B27}$$

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