Exact Thermodynamic Behavior of a Generalized Spin–Isospin Ising System on the Bethe Lattice

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We study a generalized Ising system consisting of a Bethe lattice on every site of which two spin-1/2 and two isospin-1/2 (or atomic species A) states can be realized, the spin-species interacting with appropriate nearest neighbor couplings. The system is equivalent to that of four states per site and we obtain its exact thermodynamic behavior. The case of a fixed concentration of species is the annealed or liquid magnetic binary alloy. The temperature dependence of the short-range-order (SRO) parameter of such systems is obtained as an application of the theory and discussed in connection with relevant material from the literature. When fixing both the concentration and the nearest neighbor spatial correlation of the species, we obtain Eggarter's formulas for the "frozen-in" species problem, which therefore are only approximately valid even on the Bethe lattice.

KEY WORDS: Ising; Bethe; binary alloy.

1. INTRODUCTION

Magnetic binary alloys are a particular class of two-component Ising systems and a method introduced by Eggarter[1] produces approximately their thermodynamic behavior when the atoms are "frozen in." The method and its straightforward extensions have been applied to investigate several aspects of such systems,[2,3] including the influence of atomic clustering interactions in them.[4]

A more general class of two-component Ising systems can be defined by considering two kinds of states that can be realized on every lattice site, both of the "spin-1/2" type. Such kinds can be the usual $\mu = \sigma \mu_0$ magnetic

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moment ($\sigma = \pm 1$) and any other two-state site variable X, such as the isospin 1/2 or more realistically the atomic species A or B variable ($X = $ A or B). A configuration-dependent Hamiltonian of the Ising type is considered and when the nearest neighbor interaction $u(X_i, \sigma_i, X_j, \sigma_j)$ is the sum of two terms $G(\sigma_i, \sigma_j) + U(X_i, X_j)$ each involving one kind of variables only, the system trivially splits into two independent subsystems of the usual Ising type. The case of coupled such subsystems is studied here and more specifically the case where magnetic coupling between two neighboring sites depends on the "species" states A or B being realized on the sites.

The system is equivalent to that of four states per site and when all possible configurations are allowed, this can be a model for the magnetic binary alloy in equilibrium with a heat and particle A, B reservoir as for systems undergoing magnetic and chemical interactions. Further models can be realized by successively imposing conditions on the unconstrained ensemble. When restricting to particle A (B)-conserving configurations, this can be a model for the annealed magnetic alloy,[5,6] the magnetic liquid alloy,[7] or the magnetic lattice gas. The annealed behavior of the Ising model has been studied in the case of bond-disordered systems.[8–10]

Finally, when restricting the accessible configurations further so that a neighbor-site species SRO parameter $P_{A/B}$ is also conserved, the thermodynamic behavior of our system should approach that of the "frozen-in" species system but it should not coincide with it, since farther-neighbor species correlations (beyond $P_{A/B}$) in our system remain temperature dependent in general. In spite of these expected differences, we obtain in this case a thermodynamic behavior that coincides with the one produced by Eggarter's treatment[1] of the magnetic binary alloy with "frozen-in" species.

Our method, which is similar in structure to the one introduced by Eggarter,[1] produces on the Bethe lattice the exact thermodynamic behavior of all three cases discussed above and at the same time reveals fully the limitations of Eggarter's treatment, namely that it remains approximate even on the Bethe lattice.

We present in Section 2 the formalism and in Section 3 we present and discuss the behavior of appropriate thermodynamic probabilities in relation to cases already presented in the literature.

2. FORMALISM

We consider an Ising spin system on a Bethe lattice of coordination z with spin carrying atoms of two kinds, called species A and B, randomly

distributed on the lattice sites. The Hamiltonian of such a system is given by

$$\mathscr{H} = - \sum_{(i,j)} [J(X_i, X_j)\, \sigma_i \sigma_j + U(X_i, X_j)] - H \sum_i \mu(X_i)\, \sigma_i \qquad (1)$$

where we consider only nearest neighbor interactions and $\sigma_i = \pm 1$ indicate the spin orientations. $J(X_i, X_j) > 0$ are ferromagnetic coupling constants for the neighboring X_i, X_j species and $U(X_i, X_j)$ are neighboring species interactions, with $U(A, A) > 0$, $U(B, B) > 0$, $U(A, B) < 0$. Here H is the external magnetic field and $\mu(X_i)$ the magnetic moment of the species occupying site i.

We introduce the spin species pair probabilities $P(X_i, \sigma_i; X_j, \sigma_j)$ between neighboring sites i and j as well as the single-site probabilities $P(X_i, \sigma_i)$, where (X_i, σ_i) is any of the four states $(A, \uparrow) \equiv 1$, $(A, \downarrow) \equiv 2$, $(B, \uparrow) \equiv 3$, or $(B, \downarrow) \equiv 4$ that can be realized on lattice site i. The pair and single-site probabilities can therefore be expressed by $P(l, k)$ and $P(l)$, respectively (where l, k label those four states), and they obey the relations

$$\sum_{k=1}^{4} P(l, k) = P(l) \qquad (2)$$

$$\sum_{l=1}^{4} P(l) = 1 \qquad (3)$$

The probability for every configuration $P(k_0, k_1, k_2,..., k_z)$ where a lattice site O is occupied by state k_0 and its z neighboring lattice sites are occupied by states $k_1, k_2,..., k_z$ can be expressed as a product of single and pair probabilities

$$P(k_0, k_1, k_2,..., k_z) = P(k_0)^{1-z} \prod_{i=1}^{z} P(k_0, k_1) \qquad (4)$$

due to the Bethe lattice topology.[1,3]

2.1. Case A. Unconstrained Case

We extend the basic thermodynamic relations used originally by Eggarter[1]:

$$\frac{P(k_0, k_1, k_2,..., k_z)}{P(k_0', k_1, k_2,..., k_z)} = \exp[\beta\, \Delta E(k_1, k_2,..., k_z, k_0 \rightarrow k_0')] \qquad (5)$$

where the state of site O is "flipped" from k_0 to k_0' with the states k_1, $k_2,..., k_z$ on the z nearest neighboring sites of the central site O kept fixed.

This relation is exact in thermodynamic equilibrium due to the Cayley tree topology of the Bethe lattice.

The basic thermodynamic relations (5) can be expressed in terms of pair probabilities due to (2) and (4). Taking $k_0 = l$, $k'_0 = k$ in (5) with the neighboring sites in state m, $(l, \{m\}) \to (k, \{m\})$, we obtain a system of equations of the form

$$\left(\frac{P(l)}{P(k)}\right)^{1-z} \left(\frac{P(m, l)}{P(m, k)}\right)^{z} = e^{\beta \, \Delta E(\{m\}, l \to k)} \tag{6}$$

For $m = 1$ and $l \to k$ the ΔE are given by

(a) $l = 1 \to k = 2$: $\Delta E(\{1\}, 1 \to 2) = 2\mu_A H + 2zJ_{AA}$ \hfill (7a)

(b) $l = 3 \to k = 4$: $\Delta E(\{1\}, 3 \to 4) = 2\mu_B H + 2zJ_{BB}$ \hfill (7b)

(c) $l = 1 \to k = 3$: $\Delta E(\{1\}, 1 \to 3)$

$$= (\mu_A - \mu_B)H + z(J_{AA} - J_{AB}) + \tilde{z}(U_{AA} - U_{AB}) \tag{7c}$$

and using (7a)–(7c), we obtain from (6) a system of three equations corresponding to cases (a)–(c).

Statistical homogeneity in the bulk of the lattice gives six relations $P(X_i, \sigma_i; X_j, \sigma_j) = P(X_i, \sigma_j; X_i, \sigma_i)$ [or   equivalently $P(l, k) = P(k, l)$], which reduce the number of independent pair probabilities $P(l, k)$ from 16 to 10.

Dividing by parts two of equations (6) that differ on the peripheral site states only ($\{m\}$ on one and $\{n\}$ on the other), we obtain nine more equations ($m \to n$, $l \to k$ are three "flips" each) of the form

$$\frac{P(m, l)}{P(m, k)} \frac{P(n, k)}{P(n, l)} = e^{\beta \, \Delta E(m, n, k, l)} \tag{8}$$

where

$$\Delta E(m, n, k, l) = U_{ml} + U_{nk} - U_{mk} - U_{nl}$$
$$+ \mathscr{J}_{ml} + \mathscr{J}_{nk} - \mathscr{J}_{mk} - \mathscr{J}_{nl}, \qquad \mathscr{J}_{ml} \equiv \sigma_m \sigma_l J_{ml}$$

The subscripts in U and J denote the "species" part and those in σ denote the spin part of the state (i.e., $m \equiv X_m$, σ_m; $X_m = A$ or B; $\sigma_m = \pm 1$). Of these, only six are independent, because ($m \to n$, $l \to k$) and ($l \to k$, $m \to n$) give the same equations due to statistical homogeneity. Table I shows the (m, n, k, l) of the six independent equations (8) and the corresponding equation number assigned to each case.

Equations (6), (7a)–(7c), and (8a)–(8f), along with the normalization condition [relations (2) and (3)], are the ten algebraic equations needed to completely determine the pair probabilities of the system.

Table I

m	n	k	l	Equation number
1	2	1	2	(8a)
1	3	1	2	(8b)
1	4	1	2	(8c)
3	1	3	4	(8d)
3	4	3	4	(8e)
1	3	1	3	(8f)

2.2. Case B. The Magnetic Binary Alloy

We consider the number of magnetic species A and B in the system to be fixed with a concentration of the A "atoms" c_A. This implies

$$\sum_{\sigma_i, \sigma_j} \sum_{X_j} P(A, \sigma_i; X_j, \sigma_j) = c_A \tag{9}$$

Of the nine equations (6)–(8), only two are derived from transitions that do not conserve the species concentration, namely Eq. (6), case (c), and Eq. (8f). Equation (8f), though, is acceptable in the present case where species concentration is the only condition imposed, since it can be derived by considering a double cluster consisting of two neighboring "central" sites occupied by different species (e.g., states A↑, B↑) and their other $2(z-1)$ nearest neighbors. By mutually "flipping" the states in the two "central" sites (A↑ → B↑, B↑ → A↑) in the cluster, a concentration-preserving "flip," we obtain a thermodynamic relation similar to (5), which with proper choice of the states in the perimeter of the cluster gives again Eq. (8f).

Consequently, the system that determines the $P(k, l)$ in the present case differs from the one in case A, in that Eq. (6), case (c), is replaced by the fixed-concentration condition, Eq. (9).

2.3. Case C. The Magnetic Alloy with Fixed Short-Range Order

In this case we further restrict the magnetic binary alloy case by requiring both the concentration and nearest neighbor correlation of the magnetic species to remain fixed. This extra restriction is expressed as

$$\sum_{\sigma_i, \sigma_j} P(A, \sigma_i; B, \sigma_j) = c_A P_{B/A} \tag{10}$$

where $P_{B/A}$ is the correlation parameter.

This relation replaces Eq. (8f) of the two preceding cases, since it is obtained from species exchange (see Section 2.2), which does not conserve species correlation. Note that in this case the neighboring species interactions $U(X_i, X_j)$ are not included in the equations that determine the pair probabilities.

The ten equations that determine here the pair probabilities [Eqs. (6), cases (a) and (b), Eqs. (8a)–(8e), (9), and (10), along with the normalization condition, relations (2) and (3)] are identical to those obtained by Eggarter[1] for the case of "frozen-in" magnetic species A and B on the system.

Since our treatment is exact for the Bethe lattice, we conclude that Eggarter's treatment of the "frozen-in" case is approximate even for the Bethe lattice, a negative feature not shared by the usual Bethe–Peierls approximation. Indeed, one can easily verify from the ten equations of the present subsection that Eggarter's theory gives temperature-dependent probabilities for any species configuration containing more than just two neighboring species, in violation of the "frozen-in" hypothesis. This violation may be very strong in certain cases.[11]

2.4. Reduction of Cases A and B to the Case C Formalism

In this section we show that the pair probabilities $P(l, k)$ pertaining to cases A and B can be obtained from the solution of the set of equations of case C as follows:

Case B: In this case, the pair probabilities $P(l, k)$ satisfy the same equations as in case C with the exception of Eq. (8f), which in case C is replaced by Eq. (10). Since these probabilities substituted in Eq. (10) give the (then) temperature-dependent parameter $P_{A/B}$, there is a one-to-one correspondence between $P_{A/B}$ and $(R_A + R_B)$, where

$$R_A = U_{AA} - U_{AB}, \qquad R_B = U_{BB} - U_{AB} \qquad (11)$$

as the U_{AA}, U_{BB}, U_{AB} appear in the $(R_A + R_B)$ form in Eq. (8f). The $R_A + R_B$ and $P_{A/B}$ are related in terms of the $P(k, l)$ as follows:

$$P_{A/B} = [P(1, 3) + P(1, 4) + P(2, 3) + P(2, 4)]/[P(3) + P(4)] \qquad (12)$$

[where $P(3) = \sum_{l=1}^{4} P(3, l)$ and $P(4) = \sum_{l=1}^{4} P(4, l)$, according to Eq. (3)] and then the $P(k, l)$ of case B coincide with those of case C for the appropriate value $P_{A/B}$ obtained from Eq. (12).

Case A. In this case the pair probabilities $P(k, l)$ satisfy the same equations as in case B with the exception of Eq. (6), case (c), which in case B is replaced by Eq. (9). Since these probabilities substituted in Eq. (9) give

the (then) temperature-dependent concentration c_A, there corresponds one c_A for the pair (R_A, R_B) [see Eq. (11)] that is used in case A. The c_A is related to R_A, R_B as follows:

$$c_A = \sum_{l=1}^{4} [P(1, l) + P(2, l)] \tag{13}$$

and then the $P(k, l)$ of case A coincide with those of case B, with the appropriate value of c_A obtained from Eq. (13). Obviously, case A can subsequently be reduced to case C also.

The reduction of cases A and B to case C gives in general different correspondences of parameters at different values of T.

3. RESULTS AND DISCUSSION

The parameter space in cases A, B, and C studied in Section 2 is very large, containing quantities such as J_{AA}, J_{BB}, J_{AB}, U_{AA}, U_{BB}, U_{AB}, c_A, etc.
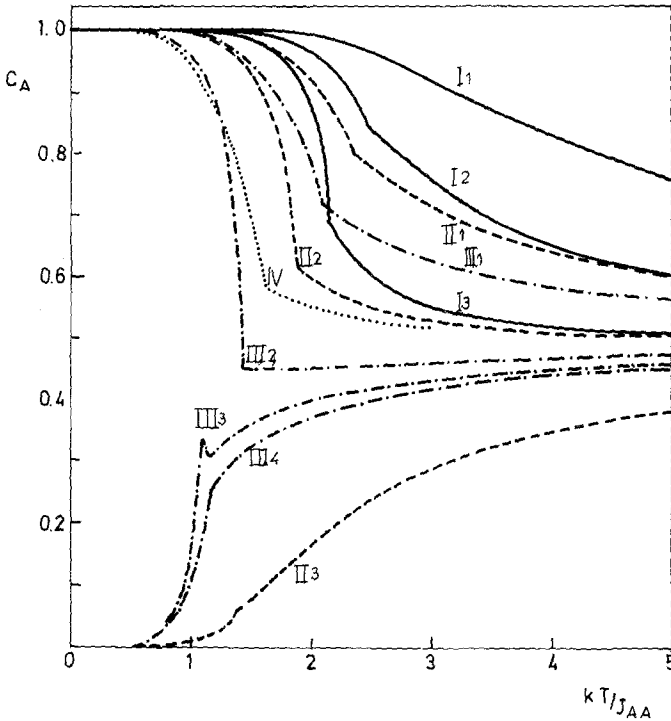

Fig. 1. Concentration of A-type "atoms" c_A versus temperature kT/J_{AA} for four different values of $R_A + R_B$: (I) $R_A + R_B = 2$ for $R_A = 1.9$ (1), 1.3 (2), 1.0 (3); (II) $R_A + R_B = 1$ for $R_A = 0.9$ (1), 0.5 (2), 0.0 (3); (III) $R_A + R_B = 0.5$ for $R_A = 0.5$ (1), 0.1 (2), 0.0293 (3), and 0.0 (4); (IV) $R_A + R_B = 0.0$ for $R_A = 0.0$; where R_A and R_B are in units of J_{AA}.

The behavior of basic thermodynamic quantities such as energy and
magnetization in case C, on the other hand, coincides, as discussed in the
introduction, to the "frozen-in" species case as studied in the literature (in
the framework of Eggarter's method) both for ferromagnetic[1] and
antiferromagnetic[2,3] systems. Therefore, since at every T, cases A and B
can be reduced to case C (see Section 2.4), one can obtain the ther-
modynamic behavior of all three cases by using the already published
corresponding "frozen-in" results mentioned above. For that purpose, the
relations of c_A, $P_{A/B}$ of that method to the R_A, R_B involved in cases A and
B is needed, and we present in Figs. 1 and 2 these relations for represen-
tative choices of (R_A, R_B) for a $z = 4$ neighbor Bethe lattice system with
$J_{AA} = 2J_{BB} = 10J_{AB} > 0$ in the absence of magnetic field.

In these figures we present $c_A(R_A, R_B)$ and $P_{A/B}(R_A, R_B)$ in a way that
is convenient for use in both cases A and B. Then, since in case B, c_A
depends on $R_A + R_B$, we have chosen our (R_A, R_B) pairs required for the
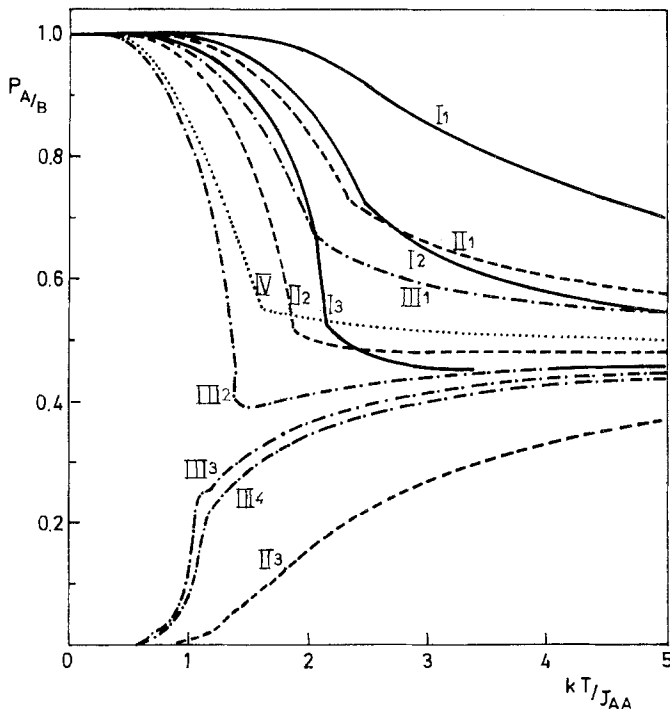reduction A → C, at different values of $R_A + R_B$, namely $R_A + R_B = 2$, 1,

Fig. 2.   Correlation $P_{A/B}$ versus temperature/J_{AA} for the same cases as in Fig. 1.

0.5, and 0 (in units of J_{AA}), so that Fig. 1 can be used for the reduction B → C as well.

Some interesting features emerge from Figs. 1 and 2, namely that the roles of A and B are not interchangeable due to $J_{AA} \neq J_{BB}$ considered here, but at the same time B dominates over A when R_B is sufficiently larger than R_A. There are also interesting marginal cases (see, for example, cases III2, III3 in Figs. 1 and 2) between which the system is passing from A domination to B domination and structure emerges in the curves (see Fig. 1, case III3) pertinent to that passage. The possibility of two, dominant A and dominant B, phases at low T, depending on initial or boundary conditions, also exists in the marginal cases. Slope discontinuities are present in all cases presented in Figs. 1 and 2, relating to phase transitions of the corresponding systems.

In order to illustrate the use of Figs. 1 and 2 in studying systems belonging to case A or case B, we have produced the T dependence of the SRO parameter $P_{A/B}$ for a system belonging to case B. Considering this system as a model for liquid or annealed magnetic alloys,[5-7] we have
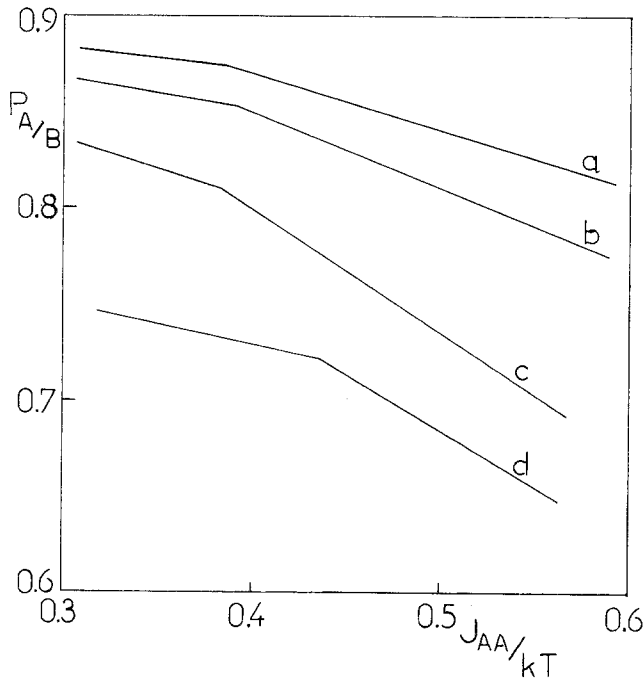

Fig. 3. Correlation $P_{A/B}$ versus J_{AA}/temperature for concentration $c_A = 0.9$ and three values of $R_A + R_B$: (a) 0.5, (b) 1.0, and (c) 2.0, as well as (d) for concentration $c_A = 0.8$ and $R_A + R_B = 1.0$; deduced from Figs. 1 and 2.

obtained, using Figs. 1 and 2, a behavior of $P_{A/B}$ (see Fig. 3) qualitatively the same as in ref. 5 (see Fig. 12 therein).

A study that would span the whole parameter space referred to above should treat the cases of "antiferromagnetic"-type spin or species coupling by introducing sublattices.[3]

REFERENCES

1. T. P. Eggarter, *J. Stat. Phys.* **11**:363 (1974).
2. E. Eggarter and T. P. Eggarter, *Phys. Rev. B* **15**:2804 (1977).
3. C. E. Paraskevaidis and C. T. Papatriantafillou, *J. Phys. C: Solid State Phys.* **16**:3947 (1983).
4. C. T. Papatriantafillou and C. E. Paraskevaidis, *J. Phys. C: Solid State Phys.* **16**:3963 (1983).
5. V. Pierron-Bohnes, M. C. Codeville, and F. Gautier, *J. Phys. F: Met. Phys.* **13**:1689 (1983).
6. V. Pierron-Bohnes, M. C. Codeville, A. Bieher, and F. Gautier, *J. Mag. Mag. Mat.* **54–57**:1027 (1986).
7. M. Takahashi, F. Sato, and S. Ishio, *J. Mag. Mag. Mat.* **49**:145 (1985).
8. D. C. Rapaport, *J. Phys. C: Solid State Phys.* **5**:1830 (1972).
9. M. F. Thorpe and D. Beeman, *Phys. Rev. B* **14**:188 (1976).
10. J. A. Blackman and J. Poulter, *J. Phys. C: Solid State Phys.* **17**:1095 (1984).
11. C. E. Paraskevaidis and C. T. Papatriantafillou, to be published.