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PHYSICAL REVIEW B VOLUME 5, NUMBER 9 1 MAY 1972

Formulation of the Constant-Coupling Approximation

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(Received 17 September 1971)

We utilize a Glauber identity to formulate the $S=\frac{1}{2}$ Ising-model problem. This formulation provides a concise view of some connections between the molecular field and the constant-coupling approaches and may provide a useful medium for generating and testing other approximations.

I. INTRODUCTION

The constant-coupling approximation, introduced by Kasteleijn and van Kranendonk,[1-4] provides a method for calculating equilibrium properties of spin systems. The method attempts to deal with correlations which the usual molecular field approximations neglect, and some results of the constant-coupling approximation, e.g., critical-temperature values, represent an improvement over molecular field results.

To gain broader understanding of the constant-coupling approximation seems a worthwhile goal, since the approximation is related to the important general problem[5] of obtaining reliable reduced statistical operators for many-particle systems. It is noteworthy that the constant-coupling approximation is applied to the two-spin reduced statistical operator which has inherited its structure from the exact N-spin statistical operator, whereas the molecular field method hinges on a variational technique[6] in which a *trial* N-spin statistical operator is written as a product of one-spin operators.

In addition to the original work of Kasteleijn and van Kranendonk, general cluster expansions[7] for Heisenberg and Ising systems have been shown to provide a common framework for arriving at both the molecular field and constant-coupling approximations; however, the cluster expansions tend to be rather complicated and do not seem the most efficient route toward the particular goal stated above.

With that in mind we discuss the formulation of the $S=\frac{1}{2}$ Ising-ferromagnet problem in terms of a spin probability identity[8] which Glauber presented. The formulation provides a relatively concise view of some connections between the molecular field and the constant-coupling approaches and may provide a useful medium for generating and testing other approximations.

II. MARGINAL SPIN PROBABILITY

In this section we develop some techniques which are model independent insofar as they apply to any collection of spins of magnitude $\frac{1}{2}$ irrespective of the Hamiltonian or ensemble.

Consider a system of N spins, each of magnitude $\frac{1}{2}$, and let s_i denote the operator for the z projection of the ith spin:

$$s_i=\pm 1, \quad i=1,2,\ldots,N . \tag{2.1}$$

Of the 2^N spin configurations, focus attention on those with a particular value of

$$m=(1/N)\textstyle\sum_i s_i \tag{2.2}$$

and let $\langle\cdots;\ m\rangle_N$ denote a conditional average over the set M of spin states with the same m. Now we utilize the Glauber[8] identity to write the exact two-spin conditional probability in the implicit form

$$p_N(s_i,\ s_j;\ m)=\tfrac{1}{4}(1+\langle s_i;\ m\rangle_N s_i + \langle s_j;\ m\rangle_N s_j+\langle s_i s_j;\ m\rangle_N s_i s_j) , \tag{2.3}$$

where $1\leq i<j\leq N$.

For a homogeneous system

$$m=\langle s_i;\ m\rangle_N, \quad i=1,2,\ldots,N \tag{2.4}$$

so that

$$p_N(s_i,\ s_j;\ m)=\tfrac{1}{4}[1+(s_i+s_j)m+s_i s_j\langle s_i s_j;\ m\rangle_N] . \tag{2.5}$$

From the definition of $\langle s_i + s_j;\ m\rangle_N$, $\langle s_i s_j;\ m\rangle_N$, and the normalization condition

$$\sum_{s_i, s_j} p_N(s_i s_j;\ m) = 1 \ , \tag{2.6}$$

one easily verifies the representation

$$p_N(s_i,\ s_j;\ m)$$

$$= \exp\{-\beta[-A_{ij} - (s_i + s_j) h B_{ij} - s_i s_j J C_{ij}]\} \ , \tag{2.7}$$

where the coefficients A_{ij}, B_{ij}, and C_{ij} satisfy

$$\beta h B_{ij} = -\frac{1}{4} \ln\left[\left(1 - \frac{2m}{1 + \langle s_i s_j;\ m\rangle_N}\right)\Big/\left(1 + \frac{2m}{1 + \langle s_i s_j;\ m\rangle_N}\right)\right] \ , \tag{2.8}$$

or, equivalently,

$$\tanh(2\beta h B_{ij}) = 2m/(1 + \langle s_i s_j;\ m\rangle_N) \tag{2.9}$$

and

$$\beta J C_{ij} = \tfrac{1}{4} \ln\left(1 + \frac{4(\langle s_i s_j;\ m\rangle_N - m^2)}{(1 - \langle s_i s_j;\ m\rangle_N)^2}\right) , \tag{2.10}$$

whereas

$$\beta A_{ij} = -\ln 4 + \tfrac{1}{2} \ln(1 - \langle s_i s_j;\ m\rangle_N{}^2) + \tfrac{1}{4} \ln\left(1 - \frac{4m^2}{(1 + \langle s_i s_j;\ m\rangle_N)^2}\right) . \tag{2.11}$$

The quantities B_{ij}, C_{ij}, and A_{ij} in general depend on N, m, and the undefined parameters β and h. We relate these quantities to the canonical ensemble by interpreting $1/(k_B \beta)$ as the temperature, and regarding hB_{ij} as an effective magnetic field while JC_{ij} is interpreted as an effective coupling parameter for a pair of spins. Notice that the sign of $\beta J C_{ij}$ is the same as the sign of the conditional covariance

$$\langle s_i s_j;\ m\rangle_N - \langle s_i m\rangle_N \langle s_j;\ m\rangle_N \ .$$

The combination

$$-(s_i + s_j) h B_{ij} - s_i s_j J C_{ij}$$

is then interpreted as an effective pair Hamiltonian in the conditional ensemble for a particular m. Irrespective of the interpretation, the above results apply to any uniform system of N spins (each of magnitude $\frac{1}{2}$) with an arbitrary Hamiltonian and an arbitrary ensemble describing the system, and for $1 \leq i < j \leq N$.

We now apply the results to a particular Hamiltonian and use the canonical ensemble.

III. ISING SYSTEM

Consider the Hamiltonian

$$\mathcal{H} = -J \sum_{\{ij\}} s_i s_j - h \sum_i s_i \tag{3.1}$$

$$= -\sum_{\{ij\}} \left(J s_i s_j + \frac{h}{q} (s_i + s_j)\right) , \tag{3.2}$$

where $\{ij\}$ denotes the set of nearest-neighbor pairs on a lattice of coordination number q. The magnetic field parameter h and the coupling parameter J are taken non-negative, and periodic boundary conditions are imposed.

The eigenstates and eigenvalues may be classified according to definite values of m. With $E_N(l_m)$ denoting an eigenvalue associated with a particular m one has the partition function

$$Z_N = \textstyle\sum_m Z_N(m) \ , \tag{3.3}$$

where

$$Z_N(m) = \textstyle\sum_{l_m} \exp[-\beta E_N(l_m)] \ . \tag{3.4}$$

For our N-spin system let $g_N(m)$ denote the number of states with a given m:

$$g_N(m) = N! \Big/ \left[\left(\frac{N + Nm}{2}\right)! \left(\frac{N - Nm}{2}\right)!\right] \tag{3.5}$$

$$= \lim_{\beta \to 0} Z_N(m) \ . \tag{3.6}$$

We thus have the identity

$$\ln Z_N(m) = \ln g_N(m) - \int_0^\beta d\beta' \langle \mathcal{H};\ m\rangle_N \ , \tag{3.7}$$

where the conditional average[9]

$$\langle \mathcal{H};\ m\rangle_N = \frac{1}{Z_N(m)} \sum_{l_m} E_N(l_m)\, e^{-\beta E_N(l_m)} \tag{3.8}$$

$$= -\sum_{\{ij\}} \sum_{s_i s_j} \left(J s_i s_j + \frac{h}{q} (s_i + s_j)\right) \times p_N(s_i,\ s_j;\ m) \tag{3.9}$$

$$= -\sum_{\{ij\}} \left(J \langle s_i s_j;\ m\rangle_N + \frac{2hm}{q}\right) \tag{3.10}$$

$$= -\frac{N}{2}\left(Jq \langle s_1 s_2;\ m\rangle_N + 2hm\right) . \tag{3.11}$$

In reaching the latter result we have utilized the assumption of a uniform system and the notation of Sec. II. The uniformity assumption enables one to write $\langle s_1 s_2;\ m\rangle_N$ where subscripts 1, 2 refer to *any* pair of nearest-neighbor spins s_1, s_2.

Equation (3.7) may be written

$$\ln Z_N(m) = \ln g_N(m) + N\beta h m + \tfrac{1}{2} N \beta J q m^2 + \tfrac{1}{2} N J q \int_0^\beta d\beta' (\langle s_1 s_2;\ m\rangle_N - m^2) \ . \tag{3.12}$$

Now introduce

$$\beta f_N(m,\ \beta,\ h) \equiv -\frac{1}{N} \ln Z_N(m) \ , \tag{3.13}$$

$$\frac{1}{N} \ln \gamma_N \equiv \frac{1}{N}\left[N \ln N - N\left(\frac{1+m}{2}\right) \times \ln N\left(\frac{1+m}{2}\right) - N\left(\frac{1-m}{2}\right) \ln N\left(\frac{1-m}{2}\right)\right]$$

$$= -\left(\frac{1+m}{2}\right)\ln\left(\frac{1+m}{2}\right) - \left(\frac{1-m}{2}\right)\ln\left(\frac{1-m}{2}\right), \tag{3.14}$$

and

$$\beta\phi_N(m,\ \beta,\ h) \equiv \frac{1}{N}\ln\left(\frac{g_N(m)}{\gamma_N(m)}\right) + \tfrac{1}{2}Jq\int_0^{\beta} d\beta'\,(\langle s_1 s_2;\ m\rangle_N - m^2), \tag{3.15}$$

then we have

$$f_N(m,\ \beta,\ h) = -hm - (\tfrac{1}{2}Jq)m^2 + \frac{1}{\beta}\left[\left(\frac{1+m}{2}\right)\ln\left(\frac{1+m}{2}\right) + \left(\frac{1-m}{2}\right)\ln\left(\frac{1-m}{2}\right)\right] - \phi_N(m,\ \beta,\ h)\ . \tag{3.16}$$

The foregoing calculations are all exact and the free energy per spin is

$$f_N(\beta,\ h) = -(1/\beta N)\ln Z_N \tag{3.17}$$

$$= -(1/\beta N)\ln\left[\textstyle\sum_m Z_N(m)\right], \tag{3.18}$$

which is obviously

$$\leqslant -(1/\beta N)\ln Z_N(m) = f_N(m,\ \beta,\ h) \tag{3.19}$$

for any m in the set $\{-1,\ -(N-1)/N,\ -(N-2)/N,\ \cdots 1\}$.

One thus obtains a rigorous upper bound on the exact free energy per spin, and the bound may then be minimized by varying m over the above set.

IV. APPROXIMATIONS

As $N\to\infty$ it is clear that $\ln[g_N(m)/\gamma_N(m)]\to 0$, and it is assumed that limits also exist for P_N, $\langle\cdots;\ m\rangle_N$, $f_N(m,\ \beta,\ h)$, and $\phi_N(m,\ \beta,\ h)$; denote them by p, $\langle\cdots;\ m\rangle$, $f(m,\ \beta,\ h)$, and $\phi(m,\ \beta,\ h)$, respectively, with m regarded as a continuous variable in the interval $(-1,\ 1)$. Then, as $N\to\infty$; i.e., in the thermodynamic limit, we get

$$\lim f_N(\beta,\ h) \equiv f(\beta,\ h) \leqslant f(m,\ \beta,\ h)\ . \tag{4.1}$$

Assume that $\phi(m,\ \beta,\ h)$ is twice differentiable with respect to m and write the minimization conditions:

$$\frac{\partial f(m,\ \beta,\ h)}{\partial m} = 0\ , \tag{4.2}$$

$$\frac{\partial^2 f(m,\ \beta,\ h)}{\partial m^2} > 0\ . \tag{4.3}$$

The first condition and second condition, respectively, require that

$$m = \tanh\left[\beta\left(h + Jqm + \frac{\partial\phi(m,\ \beta,\ h)}{\partial m}\right)\right] \tag{4.4}$$

and

$$\frac{k_B T}{Jq} > (1-m^2)\left(1 + \frac{1}{Jq}\,\frac{\partial^2\phi(m,\ \beta,\ h)}{\partial m^2}\right), \tag{4.5}$$

where

$$\beta\phi(m,\ \beta,\ h) = \tfrac{1}{2}Jq\int_0^{\beta} d\beta'(\langle s_1 s_2;\ m\rangle - m^2). \tag{4.6}$$

It is apparent that to progress one ultimately has to deal with the quantity $\langle s_1 s_2;\ m\rangle$ which is not generally known exactly. A natural approach is to approximate $p(s_1,\ s_2;\ m)$. The advantage of the results in Sec. II is that they contain the exact structure of $p_N(s_i,\ s_j;\ m)$. Thus, one does *not*[7] have to search for consistency conditions for the coefficients A_{ij}, B_{ij}, and C_{ij}; the conditions were already utilized in the derivation of Eqs. (2.8), (2.10), and (2.11). The following examples should help bring the formalism into focus:

A. Molecular Field Results

Select $C_{12} = 0$; then Eq. (2.10) requires that

$$\langle s_1 s_2;\ m\rangle_N = m^2\ , \tag{4.7}$$

which, through Eq. (4.6), requires that

$$\phi(m,\ \beta,\ h) = 0\ . \tag{4.8}$$

The variational equations (4.4) and (4.5) reduce to

$$m = \tanh[\beta(h + Jqm)]\ , \tag{4.9}$$

$$k_B T/Jq > (1-m^2)\ , \tag{4.10}$$

with the approximate free energy per spin

$$f(m,\ \beta,\ h) = -hm - (\tfrac{1}{2}Jq)m^2 + \frac{1}{\beta}\left[\left(\frac{1+m}{2}\right)\ln\left(\frac{1+m}{2}\right) + \left(\frac{1-m}{2}\right)\ln\left(\frac{1-m}{2}\right)\right]. \tag{4.11}$$

These results are the familar ones associated with the molecular field approximation which may be derived directly from a variational method.[6] On the other hand, this formulation does not answer the question[10] "Does the Kasteleijn and van Kranendonk approach, i.e., the selection of C_{ij}, ultimately preserve the variational sense of Eq. (4.1) for physically relevant parameter values?"

B. Constant-Coupling Approximation

Select $C_{12} = 1$. This "constant-coupling" choice which Kasteleijn[3] observed to be the leading term in a high-temperature expansion enables one to obtain a nontrivial approximate form for $\langle s_1 s_2;\ m\rangle_N$ from Eq. (2.10). With $\langle s_1 s_2;\ m\rangle$ expressed in terms of β and m, the quantity $\phi(m,\ \beta,\ h)$ appearing in Eqs. (4.4) and (4.5) may be differentiated with respect to m and integrated with respect to β. The result is a system of generalized relations which resemble Eqs. (4.9) and (4.10), and were noted by

Kasteleijn[3] to be equivalent to the quasichemical approximation.[11]

Rather than explicitly write the constant-coupling equations,[12] we will derive a somewhat general expression for the critical temperature in the context of this discussion. The equation will explicitly yield the molecular field and constant-coupling results as special cases and will serve to further illustrate the unifying nature of the present formulation.

C. Critical Temperature

Let

$$x = e^{2\beta J C_{12}} \tag{4.12}$$

and

$$y = \langle s_1 s_2 ;\ m \rangle . \tag{4.13}$$

The physical solution to Eq. (2.10) is

$$y = [x^2 + 1 - r(m,\ x)]/(x^2 - 1) , \tag{4.14}$$

where

$$r(m,\ x) = [(x^2+1)^2 - (x^2-1)^2 - 4(x^2-1)m^2]^{1/2} . \tag{4.15}$$

Assume, as was done in the molecular field and constant-coupling approximations, that C_{12} is independent of m, then we have

$$\frac{\partial y}{\partial m} = \frac{4m}{r(m,\ x)} \tag{4.16}$$

and

$$\beta \frac{\partial \phi}{\partial m} = \tfrac{1}{2} Jq \int_0^{\beta} d\beta' \left(\frac{\partial y}{\partial m} - 2m \right)$$
$$= \tfrac{1}{2} Jq \int_1^{x} dx' \, \frac{4m/r(m,\ x') - 2m}{2JC_{12}x'} . \tag{4.17}$$

The equation for the critical temperature is obtained from Eq. (4.4) by seeking a nontrivial solution in the zero-field limit, and noting that $r(0,\ x) = 2x$:

$$1 = \beta_c \cdot 0 + \beta_c Jq + \frac{q}{2C_{12}} \int_1^{x_c} dx' \, \frac{1/x' - 1}{x'} . \tag{4.18}$$

Thus we have

$$\beta_c Jq = -(2C_{12}/q)^{-1} \ln[1 - (2C_{12}/q)] , \tag{4.19}$$

and as $C_{12}/q \to 0$, one recovers the molecular field result

$$\beta_c Jq = 1 , \tag{4.20}$$

whereas, as $C_{12} \to 1$, one recovers the constant-coupling result[2,11]

$$\beta_c Jq = -(2/q)^{-1} \ln[1 - (2/q)] ; \tag{4.21}$$

the latter giving a critical temperature of $T_c = 0$ for the linear chain, i.e., the exact result.

ACKNOWLEDGMENT

It is a pleasure to thank Dr. M. Blume for directing my attention to the constant-coupling approximation.

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[9] An explicit prescription for the conditional probability $p_N(s_i,\ s_j;\ m)$ is as follows: Note the N-spin configuration and energy $E_N(l_m)$ for each state in the set M, then, e.g., $p_N(-1,\ -1;\ m)$ is the sum of $\{\exp[-\beta E_N(l_m)]\}/Z_N(m)$ over all those states which are in M and for which s_i and s_j are equal to -1. This is equivalent to Eq. (2.3).

[10] In Ref. 4 it is asserted without proof that for the Heisenberg spin interaction the constant-coupling approximation is in no sense variational.

[11] See, e.g., T. L. Hill, *Statistical Mechanics* (McGraw-Hill, New York, 1956), Sec. 46, for discussion and reference to the earlier work of Bethe and Guggenheim. For transcription purposes note that Hill's w and Kasteleijn's J both correspond to $2J$ in the present paper.

[12] See Ref. 3, Eq. (8) for the magnetic equation of state which follows from our Eqs. (4.4), (4.15), and (4.17).