

EXACT SOLUTION OF A ONE-DIMENSIONAL SPIN SYSTEM*

By R. W. GIBBERD†

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Abstract

A one-dimensional spin system with the following Hamiltonian is considered.

$$H = - \sum_{j=1}^N J(1+\gamma) S_j^x S_{j+1}^x + J(1-\gamma) S_j^y S_{j+1}^y + \hbar S_j^z - (J_1/N) \sum_{i=1}^N \sum_{j=1}^N S_i^z S_j^z.$$

The partition function and the Gibb's free energy are calculated exactly in the thermodynamic limit, using techniques which are well known in the theory of superconductivity. This calculation illustrates explicitly the similarity between the phase transition in superconductivity and the molecular field transitions in spin systems. The model is a generalization of the molecular field Ising model and it is shown that the presence of the x - y interaction reduces the critical temperature. It is conjectured that this is a general result, i.e. adding a perpendicular interaction to the Hamiltonian of the Ising model tends to disorder the spins and hence lower the critical point.

I. INTRODUCTION

The study of the phenomena of phase transitions can be approximately divided into two categories. The first category deals with "classical theories" or "molecular field theories" and includes such studies as the Van der Waal's theory of liquid-gas transitions, the Weiss theory of ferromagnetism, and the BCS theory of superconductivity. These apparently different physical phenomena can be classified together, since their solutions are found to have many common properties at the critical point. In fact Brout (1965) has discussed these phenomena by looking at the formal similarities that exist amongst them. The second category of models can be regarded as those that can be solved exactly, or those models whose critical-point properties can be obtained by series expansions (for reviews of these results see Fisher 1967 and Lebowitz 1968). These models have made it clear that the molecular or mean field theories of magnetism are quantitatively inaccurate near the critical point.

In this paper we are concerned with studying a model that belongs to the molecular field theory category. The model is a one-dimensional spin $\frac{1}{2}$ system with long-range z - z interactions and short-range x - y interactions. We show that by transforming the spin operators into Fermi operators the Hamiltonian resembles the reduced Hamiltonian of superconductivity. The thermodynamic properties can then be obtained exactly in the thermodynamic limit using the Bogoliubov, Zubarev, and Tserkovnikov (BZT) technique.

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† Center for Statistical Mechanics and Thermodynamics, The University of Texas at Austin, Austin, Texas 78712, U.S.A.

Although molecular field models are not quantitatively correct at the critical point, the model which we are studying is useful for several reasons. Firstly, we can show explicitly the similarity between the BCS mechanisms of superconductivity and the molecular field model of ferromagnetism. Emch (1967) has given a discussion of the similarity between the mean field Heisenberg model and the BCS model. The present work can be regarded as an explicit example of the general ideas discussed by Emch. Secondly, this model has interest as it can be regarded as an extension of the X - Y model, discussed first by Lieb, Schultz, and Mattis (1961) and Katsura (1962). The X - Y model has attracted a great deal of attention recently through its time-dependent properties (Niemeijer 1967; Barouch and Dresden 1969; Girardeau 1969) and its analogies to the two-dimensional Ising model (Barouch and McCoy, personal communication). It is hoped in the future to extend the X - Y calculations to the model considered here. Finally, this model is of interest because of its relation to recent inequalities demonstrated by Griffiths (1967). Griffiths has shown rigorously that if one increases the z - z interactions of the Ising model the new critical temperature will be equal to or greater than the original critical temperature. From this model, the present paper calculates what happens to the critical temperature of the Ising model if x - x or y - y interactions are also present. The critical point is lowered and it is conjectured that perhaps this is a general result for all Ising models.

II. CALCULATION OF THE PARTITION FUNCTION

We consider a one-dimensional spin $\frac{1}{2}$ system with the Hamiltonian

$$H = H_0 + H_1, \quad (1)$$

where

$$H_0 = - \sum_{j=1}^N J(1+\gamma) S_j^x S_{j+1}^x + J(1-\gamma) S_j^y S_{j+1}^y + h S_j^z,$$

$$H_1 = -(J_1/N) \sum_{i=1}^N \sum_{j=1}^N S_i^z S_j^z.$$

The symbols S_j^x , S_j^y , and S_j^z are the Pauli spin operators, h is the external magnetic field, and N is the number of spins. The part of the Hamiltonian in the single summation H_0 corresponds to the X - Y model, which has been solved exactly by Lieb, Schultz, and Mattis (1961) and Katsura (1962). The terms in the double summation H_1 represent infinite long-range z - z interactions, which correspond to the Weiss model of ferromagnetism. We shall see that the addition of the term H_1 does not make the model impossible to solve, although if there were only finite range interactions the problem would be insoluble.

We write H_1 as

$$H_1 = -(J_1/N) \left(\sum_{i=1}^N S_i^z \right)^2 + \frac{1}{4} J_1. \quad (2)$$

To calculate the partition function of this model, it is necessary to write the spin operators in terms of Fermi operators. The required transformations have been well developed (e.g. Katsura 1962) and we use the following results, which hold for a cyclic chain with an even number of spins:

$$\sum_{i=1}^N S_i^x S_{i+1}^x + S_i^y S_{i+1}^y = \sum_{k=1}^{\frac{1}{2}N} (b_k^\dagger b_k + b_{-k}^\dagger b_{-k}) \cos(2\pi k/N), \quad (3a)$$

$$\sum_{i=1}^N S_i^x S_{i+1}^y - S_i^y S_{i+1}^x = i \sum_{k=1}^{\frac{1}{2}N} (b_k^\dagger b_{-k}^\dagger + b_k b_{-k}) \sin(2\pi k/N), \quad (3b)$$

$$\sum_{i=1}^N S_i^z = \sum_{k=1}^{\frac{1}{2}N} b_k^\dagger b_k + b_{-k}^\dagger b_{-k} - \frac{1}{2}N, \quad (3c)$$

where $b_k^\dagger$ and b_k are Fermi creation and annihilation operators. Substituting equations (3) into (2) and (1), we obtain

$$\begin{aligned} H = & \sum_{k=1}^{\frac{1}{2}N} [\{J_1 - h - J \cos(2\pi k/N)\} (b_k^\dagger b_k + b_{-k}^\dagger b_{-k}) - iJ\gamma \sin(2\pi k/N) (b_k^\dagger b_{-k}^\dagger + b_k b_{-k})] \\ & - (J_1/N) \sum_{k_1=1}^N \sum_{k_2=1}^N b_{k_1}^\dagger b_{k_1} b_{k_2}^\dagger b_{k_2} - \frac{1}{4}J_1(N-1) + \frac{1}{2}Nh. \end{aligned} \quad (4)$$

The transformed Hamiltonian is now similar in appearance to the reduced Hamiltonian of superconductivity, and we shall calculate the partition function by the BZT technique (for a good review of this technique see Blatt 1964, Ch. 6). The BZT technique consists of introducing constants ω_k and then rewriting the quartic part of the Hamiltonian H as

$$\begin{aligned} & - (J_1/N) \sum_{k_1, k_2} b_{k_1}^\dagger b_{k_1} b_{k_2}^\dagger b_{k_2} \\ & = - (J_1/N) \sum_{k_1, k_2} (b_{k_1}^\dagger b_{k_1} - \omega_{k_1})(b_{k_2}^\dagger b_{k_2} - \omega_{k_2}) - 2\Delta \sum_k b_k^\dagger b_k + (N/J_1)\Delta^2, \end{aligned} \quad (5)$$

where

$$\Delta = (J_1/N) \sum_k \omega_k.$$

If the first term on the right-hand side (the double summation) of equation (5) is ignored, the resulting Hamiltonian is quadratic and the partition function can be calculated. The aim of the BZT method is to adjust the constants ω_k in such a way that the correction arising from the neglected term becomes completely negligible in the thermodynamic limit. Bogoliubov (1960) has shown that this is possible if we define ω_k by equation (7) below. The partition function Z is defined as

$$Z = \text{Trace}\{\exp(-\beta\tilde{H})\},$$

where, using equations (5) and (4), $\tilde{H}$ is given by

$$\begin{aligned} \tilde{H} = & \frac{1}{2}Nh - \frac{1}{4}J_1(N-1) + (N/J_1)\Delta^2 \\ & + \sum_{k=1}^{\frac{1}{2}N} [\{J_1 - h - J \cos(2\pi k/N) - 2\Delta\} (b_k^\dagger b_k + b_{-k}^\dagger b_{-k}) \\ & - iJ\gamma \sin(2\pi k/N) (b_k^\dagger b_{-k}^\dagger + b_k b_{-k})] \end{aligned} \quad (6)$$

and ω_k is given by

$$\omega_k = \text{Tr}\{b_k^\dagger b_k \exp(-\beta \tilde{H})\} Z^{-1}. \quad (7)$$

To calculate the partition function we diagonalize $\tilde{H}$, using the Bogoluibov-Valatin transformation. Defining new Fermi operators by

$$\left. \begin{aligned} b_k &= u_k a_k + v_k a_{-k}^\dagger, & b_k^\dagger &= u_k a_k^\dagger - v_k a_{-k}, \\ b_{-k} &= u_k a_{-k} - v_k a_k^\dagger, & b_{-k}^\dagger &= u_k a_{-k}^\dagger + v_k a_k, \end{aligned} \right\} \quad (8)$$

we substitute equations (8) into the expression for $\tilde{H}$ and choose u_k and v_k such that the coefficients of the non-diagonal elements are zero. We obtain after some standard algebraic manipulations

$$\begin{aligned} \tilde{H} &= \frac{1}{2}Nh - \frac{1}{4}J_1(N-1) + (N/J)\Delta^2 + \sum_{k=1}^{\frac{1}{2}N} (a_k^\dagger a_k + a_{-k}^\dagger a_{-k} - 1)A_k + A_k \\ &= \frac{1}{2}Nh - \frac{1}{4}J_1(N-1) + (N/J)\Delta^2 + \sum_{k=-\frac{1}{2}N}^{\frac{1}{2}N} (a_k^\dagger a_k - \frac{1}{2})A_k + \frac{1}{2}A_k, \end{aligned} \quad (9)$$

where

$$\begin{aligned} v_k^2 &= -\frac{1}{2} + \frac{1}{2}A_k/A_k, & u_k^2 &= \frac{1}{2} + \frac{1}{2}A_k/A_k, \\ A_k &= J_1 - h - 2\Delta - J \cos(2\pi k/N), \\ B_k &= -iJ\gamma \sin(2\pi k/N), & A_k &= (A_k^2 - B_k^2)^{\frac{1}{2}}. \end{aligned}$$

Now that the Hamiltonian is diagonalized we can evaluate the partition function trivially to give

$$\begin{aligned} Z &= C \prod_{k=-\frac{1}{2}N}^{\frac{1}{2}N} \{\exp(\frac{1}{2}\beta A_k) + \exp(-\frac{1}{2}\beta A_k)\} \exp(-\frac{1}{2}\beta A_k) \\ &= 2^N C \prod_{k=-\frac{1}{2}N}^{\frac{1}{2}N} \cosh(\frac{1}{2}\beta A_k) \exp(-\frac{1}{2}\beta A_k), \end{aligned}$$

where

$$C = \exp[-\beta\{\frac{1}{2}Nh - \frac{1}{4}J_1(N-1) + (N/J)\Delta^2\}].$$

This expression is only exact in the thermodynamic limit and so we define the thermodynamic free energy as

$$\begin{aligned} F &= \lim_{N \rightarrow \infty} N^{-1} \log Z \\ &= (2\pi)^{-1} \int_{-\pi}^{\pi} d\theta \log[\cosh\{\frac{1}{2}\beta A(\theta)\}] + \log 2 - \frac{1}{4}\beta J_1 + \beta\Delta - \beta\Delta^2/J, \end{aligned} \quad (10)$$

where

$$\begin{aligned} A(\theta) &= \{A(\theta)^2 - B(\theta)^2\}^{\frac{1}{2}}, \\ A(\theta) &= J_1 - h - 2\Delta - J \cos \theta, & B(\theta) &= -iJ\gamma \sin \theta. \end{aligned}$$

We note the similarity of the expression (10) to the solution of the X - Y model, the main difference being that $\Delta(\theta)$ in this case is a function of θ , as yet undetermined, constant Δ . It is also intriguing to note the similarity of (10) with Onsager's (1944) solution of the two-dimensional Ising model.

To obtain an expression for the constant Δ , we use equations (5) and (7) and the diagonal representation for $\tilde{H}$. We obtain

$$\omega_k = -(\frac{1}{2}A_k/\Delta_k)\tanh(\frac{1}{2}\beta\Delta_k) + \frac{1}{2}.$$

Substituting in equation (7) and taking the thermodynamic limit gives

$$\Delta = -\frac{1}{2}(J_1/2\pi) \int_{-\pi}^{\pi} d\theta \{A(\theta)/\Delta(\theta)\} \tanh\{\frac{1}{2}\beta\Delta(\theta)\} + \frac{1}{2}J_1. \quad (11)$$

Thus Δ is determined by an integral equation (since $\Delta(\theta)$ is a function of Δ) and, as would be expected, it closely resembles the integral equation for the energy gap parameter obtained in the solution of the superconductivity problem. Unfortunately there does not exist a solution to this equation. However, it can be studied in several limiting cases. Firstly, in the X - Y model limit ($J_1 = 0$), we obtain $\Delta = 0$ and the solution in equation (10) reduces to that given by Katsura (1962). Secondly, in the Weiss model limit ($J = 0$), we obtain

$$B(\theta) = 0 \quad \text{and} \quad A(\theta) = \Delta(\theta) = J_1 - h - 2\Delta.$$

Thus equation (11) becomes a simple transcendental equation, typical of molecular field models,

$$\Delta = -\frac{1}{2}J_1 \tanh\{\frac{1}{2}\beta(J_1 - h - 2\Delta)\} + \frac{1}{2}J_1. \quad (12)$$

In the theory of superconductivity, Δ is often called the energy gap parameter. For our model it is easily shown that Δ is related to the z component of the magnetization of the spin system. We define the magnetization M as

$$M = N^{-1} \sum_{j=1}^N \langle S_j^z \rangle = N^{-1} \sum_{k=1}^N \langle b_k^\dagger b_k - \frac{1}{2} \rangle = \Delta/J_1 - \frac{1}{2}, \quad (13)$$

where

$$\langle \dots \rangle = \text{Tr}\{\dots \exp(-\beta\tilde{H})\} Z^{-1}.$$

This same relation between M and Δ can be obtained by defining $M = \beta^{-1} \partial F / \partial h$. Substituting (13) into (11) we obtain

$$M = -\frac{1}{2}(2\pi)^{-1} \int_{-\pi}^{\pi} d\theta \{A(\theta)/\Delta(\theta)\} \tanh\{\frac{1}{2}\beta\Delta(\theta)\}, \quad (14)$$

where $A(\theta)$ can now be written as

$$A(\theta) = -h - J \cos \theta - 2J_1 M.$$

We also note that equation (12) can be written as

$$M = \frac{1}{2} \tanh\{\frac{1}{2}\beta(J_1 M + h)\}.$$

which is the well-known molecular field result (Brout 1965).

III. EVALUATION OF THE CRITICAL POINT

Although the integral equation (14) makes it difficult to calculate the thermodynamic quantities, we can calculate the critical point for a few special cases. For the system to have a critical point, we first require that the external field h be zero. To determine the critical point β_c , we assume that M tends to zero as $\beta \rightarrow \beta_c$ from above ($\beta = 1/kT$). Thus we can take M arbitrarily small as $\beta \rightarrow \beta_c$ and can expand the integrand of (14) in powers of M . This will give us a relation which determines β_c . We shall do the calculations for the explicit case when $\gamma = 0$ as it simplifies the algebra. In this case, equation (14) becomes

$$M = -\frac{1}{2}(2\pi)^{-1} \int_{-\pi}^{\pi} d\theta \tanh\{\frac{1}{2}\beta(J \cos \theta + 2J_1 M)\}. \quad (15)$$

Retaining only the terms of order M we obtain

$$\begin{aligned} M &= -\frac{1}{2}(2\pi)^{-1} \int_{-\pi}^{\pi} d\theta \{ \tanh(\frac{1}{2}\beta J \cos \theta) + \beta J_1 M \} \\ &\quad \times \{ 1 - \beta J_1 M \tanh(\frac{1}{2}\beta J \cos \theta) \} \\ &= -\frac{1}{2}(2\pi)^{-1} \int_{-\pi}^{\pi} d\theta \beta J_1 M \{ 1 - \tanh^2(\frac{1}{2}\beta J \cos \theta) \}. \end{aligned}$$

Hence, we obtain the relation determining β_c ,

$$(\beta_c J_1)^{-1} = \frac{1}{2}(2\pi)^{-1} \int_{-\pi}^{\pi} d\theta \operatorname{sech}^2(\frac{1}{2}\beta_c J \cos \theta). \quad (16)$$

If $J = 0$, we obtain $(J_1 \beta_c)^{-1} = \frac{1}{2}$, which is the molecular field result. With a negative or positive J , we obtain $(J_1 \beta_c)^{-1} < \frac{1}{2}$, since $\operatorname{sech}^2 x \leq 1$. Thus, the critical temperature T_c decreases when the X - Y interaction is present. From equation (16) one can calculate the dependence of the critical temperature on J and show that T_c is a monotonically decreasing function of J . As $J \rightarrow \infty$, $T_c \rightarrow 0$ which corresponds to the absence of a critical point in the X - Y model.

One can calculate the critical temperature for all values of γ , and the result for $\gamma = 1$ is worth noting as this corresponds to the addition of only the x - x interaction. The critical temperature is again lowered, but not so quickly as in the case $\gamma = 0$. Thus, the disordering effect of the x - x and y - y interaction is greater than just the x - x interaction. If this were a general result, we would expect the Ising, X - Y , and Heisenberg models in two and three dimensions to have critical temperatures T_I , T_{X-Y} , and T_H such that $T_I \geq T_{X-Y} \geq T_H$. According to series expansion results (Fisher 1967; Stanley 1967, Betts, Elliot, and Lee, personal communication) this appears to be the case.

Griffiths (1967) has shown that for Ising ferromagnets the correlation function is a monotonic increasing function of the interactions. Hurst and Sherman (1969, 1970) have enquired whether the corresponding assertion is correct for the Heisenberg ferromagnet. They have shown that the correlations are not monotonic increasing for a three-spin Heisenberg system. In the present model, we are able to produce a direct counter-example of the extension of the Griffiths inequality to Heisenberg-like systems with an infinite number of spins. Using equation (15) we can show that

$$\frac{\partial M}{\partial J} = \frac{1}{N} \sum_i \frac{\partial}{\partial J} \langle S_i^z \rangle \leq 0 \quad \text{for} \quad T \leq T_c.$$

Although the straightforward generalization of the Griffiths inequalities to more general systems is not correct, this model may be fruitful in suggesting whether additional conditions can be imposed to restore the inequalities.

IV. CONCLUSIONS

The present paper has introduced a model of a spin system which has allowed an exact solution. This model has intrinsic interest not only because it is exactly soluble, but also because it can be used to study the effect of non-commuting operators in the Ising spin Hamiltonian. We have seen that the critical temperature is lowered although the critical indices remain the same as the molecular field values. In particular, it provides a convenient example of how the generalization of the Griffiths (1967) inequalities does not hold. In the future it is hoped to produce some calculations of time-dependent properties of this model.

V. REFERENCES

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