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The One-Dimensional Ising Model with a Transverse Field

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The one-dimensional Ising model with a transverse field is solved exactly by transforming the set of Pauli operators to a new set of Fermi operators. The elementary excitations, the ground-state energy and the free energy are found. The instantaneous correlation function between any two spins is calculated and this model shows a finite long-range order in the ground state when the transverse field is less than a critical value.

I. INTRODUCTION

The Ising model with a transverse field is of some physical interest, because it corresponds to the pseudospin formulation of several phase transition problems and may be used to study order disorder ferroelectrics with a tunnelling effect [1], or the magnetic ordering in materials with singlet crystal field ground state [2]. This anisotropic spin system in one dimension with nearest neighbour interactions is shown to correspond to the Ising Heisenberg antiferromagnetic chain treated by Lieb, Schultz, and Mattis [3]. The ground-state energy, the elementary excitations and the correlation functions are calculated and compared with the results of a perturbation treatment [4]. As with the Ising model with nearest neighbour interactions, this model shows no phase transition occurring at finite temperature. At zero temperature when the system is in the ground state there is long-range order but this disappears when the transverse field exceeds a critical value.

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II. Formulation

A. *Transformation into a system of noninteracting Fermions*

The model consists of N spins, one-half arranged in a row and having only nearest neighbour interactions. The Hamiltonian is written as:

$$H = -\Gamma \sum_i S_i^z - J \sum_i S_i^x S_{i+1}^x . \tag{2.1}$$

In the ferroelectric problem [1], Γ corresponds to the tunnelling energy and J is the short range proton proton interaction. The ends of the chain may be treated in two different ways:

(a) as free ends in which case $1 \leqslant i \leqslant N$ for the first term and $1 \leqslant i \leqslant N-1$ for the second term;

(b) as a cyclic chain in which case $1 \leqslant i \leqslant N$, $S_{N+1}^x = S_1^x$.

We shall mainly consider case (b) where for N large calculations are more tractable. For N small case (a) gives interesting results about the degeneracy of the ground state when Γ varies—but this point will not be developed here.

The Ising model and the free-spin system correspond respectively to $\Gamma = 0$ and $J = 0$. The effect of J is to order the spins along x (the order is defined by $\langle 0 \mid S_i^x \mid 0 \rangle = M_x$, where $\mid 0 \rangle$ is the ground state of H) while Γ tends to destroy this order by flipping the spins. When Γ varies from zero to infinity, the system goes from a completely ordered to a completely disordered system. We shall see later than the order in the ground state disappears for $\Gamma \geqslant J/2$.

After using the following set of transformations [3]

$$\left.\begin{aligned} a_i^+ &= S_i^x + iS_i^y \\ a_i &= S_i^x - iS_i^y \end{aligned}\right\} \tag{2.2}$$

$$\left.\begin{aligned} c_i &= \exp\left(\pi i \sum_{j=1}^{i-1} a_j^+ a_j\right) a_i \\ c_i^+ &= a_i^+ \exp\left(-\pi i \sum_{j=1}^{i-1} a_j^+ a_j\right) \end{aligned}\right\} \tag{2.3}$$

(where the c_i and c_i^+ are Fermi operators), the Hamiltonian (2.1) is transformed into

$$\begin{aligned} H = \frac{\Gamma N}{2} - \Gamma \sum_{i=1}^{N} c_i^+ c_i - \frac{J}{4} \sum_{i=1}^{N} (c_i^+ - c_i)(c_{i+1}^+ + c_{i+1}) \\ + \frac{J}{4} [(c_N^+ - c_N)(c_1^+ + c_1)](\exp(i\pi L) + 1) \end{aligned} \tag{2.4}$$

with

$$L = \sum_{j=1}^{N} c_j^+ c_j = \sum_{j=1}^{N} (S_j^z + \tfrac{1}{2}). \tag{2.5}$$

As in [3] we may neglect for a large system the last correction term in (2.4) and the Hamiltonian is a quadratic form in Fermi operators identical to (3.10) of [3]. For a more detailed calculation, the reader is referred to reference [3] from which we get

$$H = \Gamma \sum_k \Lambda_k \eta_k^+ \eta_k - \frac{\Gamma}{2} \sum_k \Lambda_k \tag{2.6}$$

with

$$\eta_k = \sum_i \left\{ \left(\frac{\varphi_{ki} + \psi_{ki}}{2} \right) c_i + \left(\frac{\varphi_{ki} - \psi_{ki}}{2} \right) c_i^+ \right\} \tag{2.7}$$

Defining $\lambda = J/2\Gamma$, we find that for $\lambda \neq 1$ the normal modes are given by

$$\varphi_{kj} = \begin{cases} (2/N)^{1/2} \sin(kj) & k > 0 \\ (2/N)^{1/2} \cos(kj) & k \leqslant 0 \end{cases} \tag{2.9a}$$

$$\psi_{kj} = -\Lambda_k^{-1}[(1 + \lambda \cos k)\, \varphi_{kj} + \lambda \sin(k)\, \varphi_{-kj}] \tag{2.9b}$$

with

$$\Lambda_k^2 = (1 + \lambda^2 + 2\lambda \cos k) \tag{2.10}$$

and

$$\begin{aligned} k = 2\pi m/N \qquad & m = -\tfrac{1}{2}N, \ldots, 0, \ldots, \tfrac{1}{2}N - 1 && (N \text{ even}) \\ & m = -\tfrac{1}{2}(N-1), \ldots, 0, \ldots, \tfrac{1}{2}(N-1) && (N \text{ odd}). \end{aligned} \tag{2.11}$$

For $\lambda = 1$ and $m = -\frac{1}{2}N$,

$$\Lambda_k = 0, \qquad \varphi_{kj} = N^{-1/2}, \qquad \psi_{kj} = \pm N^{-1/2}. \tag{2.12}$$

We get a system of noninteracting fermions of energy $\Gamma\Lambda_k$. The ground state energy of the system is:

$$E_0 = -\frac{\Gamma}{2} \sum_k \Lambda_k \tag{2.13}$$

and the free energy is

$$F = -NkT \left\{ Ln\, 2 + \frac{1}{\pi} \int_0^{\pi} dk\, Ln \cosh \left(\frac{1}{2} \beta \Gamma \Lambda_k \right) \right\} \qquad \text{with} \quad \beta = \frac{1}{kT}. \tag{2.14}$$

B. *Correlation Functions*

Even in the ordered state, the order parameter $M_x = \langle 0 \mid S_i^x \mid 0 \rangle$ cannot be obtained because of the invariance of the Hamiltonian when S_i^x is changed into $-S_i^x$. On the contrary $M_z = \langle 0 \mid S_i^z \mid 0 \rangle$ and the correlation functions $\rho_n{}^x = \langle 0 \mid S_i^x S_{i+n}^x \mid 0 \rangle$, $\rho_n{}^y = \langle 0 \mid S_i^y S_{i+n}^y \mid 0 \rangle$ and $\rho_n{}^z = \langle 0 \mid S_i^z S_{i+n}^z \mid 0 \rangle - M_z{}^2$ can be calculated following the method used by Lieb *et al.* [3]. We get the following results

$$M_z = \tfrac{1}{2} G(0) \tag{2.15}$$

$$\rho_n{}^z = -\tfrac{1}{4} G(n)\, G(-n) \tag{2.16}$$

$$\rho_n{}^x = \frac{1}{4} \begin{bmatrix} G(-1) & G(-2) & \cdots & G(-n) \\ G(0) & G(-1) & \cdots & G(-n+1) \\ \vdots & \vdots & & \vdots \\ G(n-2) & G(n-1) & \cdots & G(-1) \end{bmatrix} \tag{2.17}$$

$$\rho_n{}^y = \frac{1}{4} \begin{bmatrix} G(1) & G(0) & \cdots & G(2-n) \\ G(2) & G(1) & \cdots & G(3-n) \\ \vdots & \vdots & & \vdots \\ G(n) & G(n-1) & \cdots & G(1) \end{bmatrix} \tag{2.18}$$

with

$$G(n) = L(n) + \lambda L(n+1) \tag{2.19}$$

and

$$L(n) = \frac{1}{\pi} \int_0^\pi dk\, \Lambda_k^{-1} \cos(kn). \tag{2.20}$$

For different values of λ, the following values of G are obtained:

$$\lambda = 1 \qquad G(n) = \frac{2}{\pi} \frac{(-1)^n}{2n+1}, \tag{2.21}$$

$$\lambda = \infty (\Gamma = 0) \qquad G(n) = \delta_{n,-1}, \tag{2.22}$$

$$\lambda = 0 (J = 0) \qquad G(n) = \delta_{n,0}. \tag{2.23}$$

III. Discussion of the Results

A. *Elementary Excitations*

The energy of the elementary excitations given by (2.10) is shown in Fig. 1 as a function of $k' = \pi - k$ for different values of λ. To each k corresponds an eigenstate which can be expressed in terms of c operators through (2.7). If we suppose

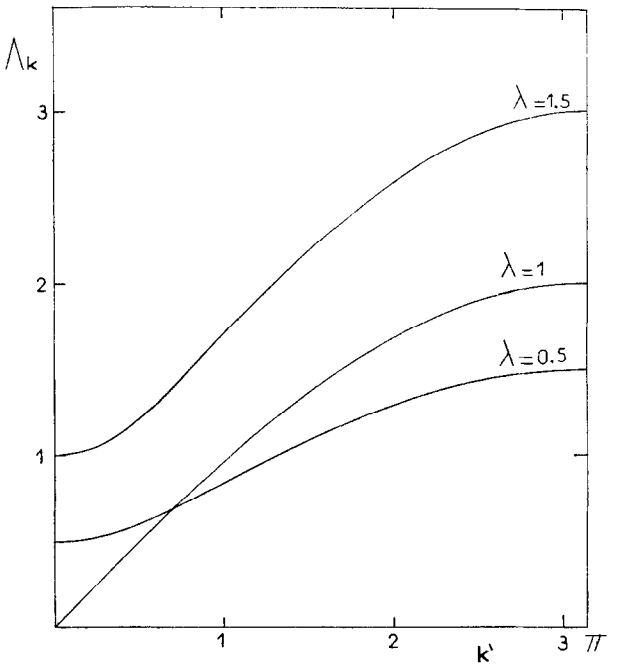

FIG. 1. Energy of elementary excitations as a function of k' for three different values of $\lambda = J/2\Gamma$.

that the ground state is not far from the Ising model ground state, $c_i \sim a_i(-1)^i$ (2.3) and $k' = \pi - k$ is the pseudo wave vector of the excitations. The $k' = 0$ excitation corresponds to the excited state whose configuration is closest to the ground state configuration. For $\lambda = 1$ ($\Gamma = J/2$) the gap in the excitation spectrum disappears. The $k' = 0$ mode energy drops to zero and rises again when Γ is $\neq J/2$. Contrary to the two- or three-dimensional case these excitations are noninteracting Fermion excitations. If $|0\rangle$ is the ground state of H (2.1) with energy E_0, $\eta_k^+ |0\rangle$ is an eigenstate of H with energy $E_0 + \Gamma\Lambda_k$. However, as shown by Lieb *et al.* [3], if we do not neglect the correction factor in (2.4) then the elementary excitations are not independent because of the dependence on the evenness and oddness of the total number of excitations. This correction term cancels for states with an even number of excitations. When Γ goes to zero (Ising model) the excitation energy goes to $J/2$ which corresponds to the first excited state for a free end chain but to only half the first excited state for a cyclic chain. All the cyclic chain excited states can only be described by an even number of excitations. The first excited state energy has also been calculated by n-th order perturbation theory as an expansion in λ [4]. The first few terms obtained so far agree with the first terms

in the power series expansion in λ of the excitation energy $\Gamma\Lambda_k$ (2.10). For $\lambda = 1$ $\Lambda_{k'=0} = 0$; thus, we expect certain quantities to become singular at that point. We shall show later that in fact the long range order $\rho_n{}^x$ in the limit as $n \to \infty$ vanishes for $\lambda < 1$. It is also interesting to note that, as shown by Lieb *et al.* [3], this excitation spectrum is identical to the excitation spectrum of the xy model with the Hamiltonian

$$H = -2\Gamma \sum_{i=1}^{N} S_i{}^z S_{i+1}^z - J \sum_{i=1}^{N} S_i{}^x S_{i+1}^x \tag{3.1}$$

but the correlation functions $\rho_n{}^x$ and $\rho_n{}^z$ are quite different.

B. *Ground State Energy and Free Energy*

The ground state energy given by (2.13) (2.10) is expressed by an elliptic integral of the second kind

$$\frac{-E_0}{\Gamma N} = \frac{2}{\pi}(1+\lambda)\, E\left(\frac{\pi}{2}, \theta\right) \qquad \text{with} \quad \theta^2 = \frac{4\lambda}{(1+\lambda)^2}. \tag{3.2}$$

This function is nonanalytic for $\theta = 1$ ($\lambda = 1$). The quantity $-E_0/NJ$ is plotted in Fig. 2 as a function of Γ/J.

The free energy given by (2.14) has not been explicitly calculated. For $T \neq 0$ this function does not show any singularity in T.

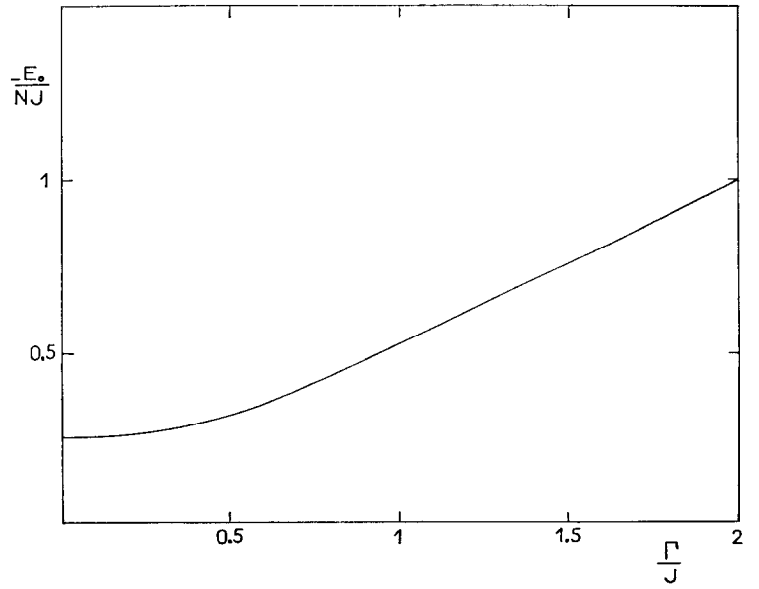

FIG. 2. Ground state energy as a function of Γ/J.

C. *M_z, M_x and the correlation functions $\rho_n{}^x$, $\rho_n{}^y$, $\rho_n{}^z$*

M_z given by (2.15) is equal to an elliptic integral of the first kind and is thus deduced directly from tables [5]. When Γ/J varies from zero to infinity M_z varies from zero to $\frac{1}{2}$ as shown in Fig. 3. The point $\lambda = 1$ ($\Gamma = J/2$) is nonanalytic.

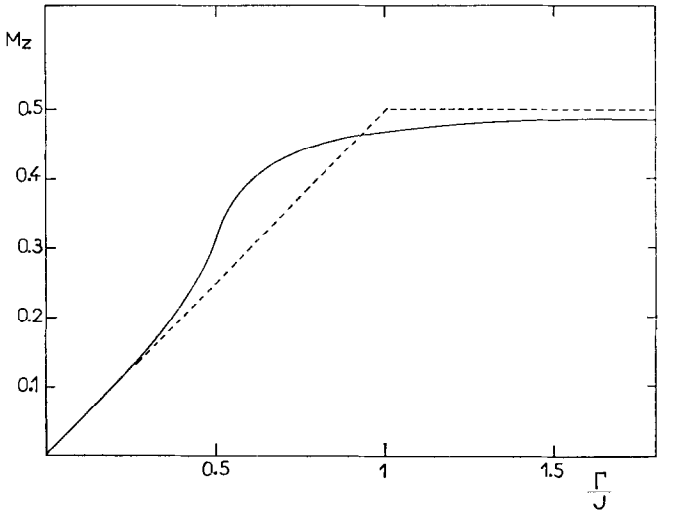

FIG. 3. $M_z = \langle 0 \mid S_i^z \mid 0 \rangle$ as a function of Γ/J. The dotted line corresponds to the molecular field result.

On the same figure the molecular field result [6] is shown for comparison. The difference between these two results becomes important for $0.4 < \Gamma/J < 1$, where, as we shall show later, $\rho_n{}^z$ is large and cannot be neglected as in the molecular field approximation.

The correlation functions given by (2.16) (2.17) (2.18) depend only on $G(n)$. As a function of λ, $G(n)$ is nonanalytic for $\lambda = 1$ and so are the correlation functions. The short range order correlation functions $\rho_1{}^x$, $\rho_1{}^y$, $\rho_1{}^z$ are plotted in Fig. 4 as functions of Γ. The quantity $\rho_1{}^x$ is taken from the tables [5] while $\rho_1{}^y$ and $\rho_1{}^z$ are only approximated and would have to be computed. $\rho_1{}^x$ is much larger than $\rho_1{}^y$ and $\rho_1{}^z$ because of the strong anisotropy in the interaction between neighbouring spins.

The critical case $\lambda = 1$ can be studied more easily because of the simple form of $G(n)$ (2.21). We get from (2.16)

$$\rho_n{}^z = \frac{1}{\pi^2} \cdot \frac{1}{4n^2 - 1} \tag{3.3}$$

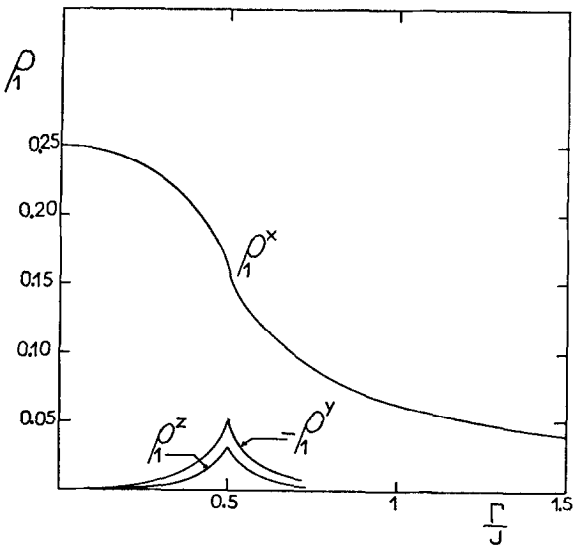

FIG. 4. Short range correlation functions as functions of Γ/J.

and the Toeplitz determinants $\rho_n{}^x$ and $\rho_n{}^y$ (2.17) (2.18) can be calculated, following McCoy [7]. $\rho_n{}^x$ corresponds to R_n of reference [7] and $\rho_n{}^y$ is closely related.

We then get

$$\rho_n{}^x = \frac{1}{4} \cdot \left(\frac{2}{\pi}\right)^n \cdot 2^{2n(n-1)} \cdot \frac{H(n)^4}{H(2n)} \tag{3.4}$$

$$\rho_n{}^y = -\frac{1}{4n^2 - 1} \times \rho_n{}^x \tag{3.5}$$

with

$$H(n) = 1^{n-1} \cdot 2^{n-2} \cdots (n-1). \tag{3.6}$$

The values of $\rho_n{}^x$, $\rho_n{}^y$, $\rho_n{}^z$ given in Table I for $1 \leqslant n \leqslant 12$ are plotted in Fig. 5 They all go to zero when n goes to infinity. For large n

$$\rho_n{}^x \sim \frac{1}{4} e^{1/4} 2^{1/12} A^{-3} n^{-1/4} \left(1 - \frac{1}{64} n^{-2} + \cdots\right) \tag{3.7a}$$

$$\rho_n{}^y \sim -\frac{1}{16} e^{1/4} 2^{1/12} A^{-3} n^{-9/4} \left(1 + \frac{15}{64} n^{-2} + \cdots\right) \tag{3.7b}$$

$$\rho_n{}^z \sim \frac{1}{4\pi^2} n^{-2} \left(1 + \frac{1}{4} n^{-2} + \cdots\right) \tag{3.7c}$$

with $A \simeq 1.2824$.

TABLE I
Correlation Functions for $\lambda = 1$ ($\Gamma = J/2$).

n	$4\rho_n{}^x$	$-4\rho_n{}^y$	$4\rho_n{}^z$
1	0.6366	0.2122	0.13509
2	0.5404	0.0360	0.02702
3	0.4893	0.01398	0.01158
4	0.4556	0.00723	0.00643
5	0.4311	0.00435	0.00409
6	0.4119	0.00288	0.00283
7	0.3964	0.00203	0.00208
8	0.3834	0.00150	0.00159
9	0.3723	0.00115	0.00125
10	0.3627	0.00091	0.00102
11	0.3541	0.00073	0.00084
12	0.3465	0.00060	0.00070

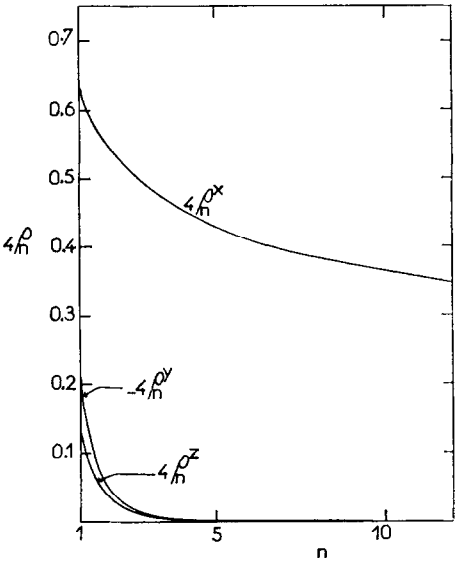

FIG. 5. Correlation functions as functions of n for $\lambda = 1(\Gamma = J/2)$.

We note that $\rho_n{}^y$ and $\rho_n{}^z$ behave in a very similar way. $\rho_n{}^x$ goes to zero for n large but nevertheless is not integrable. The quantity $\sum_n \langle 0 \mid S_i{}^x S_{i+n}^x \mid 0 \rangle$ diverges at $\lambda = 1$ when order appears in the system. We are essentially interested in the long-range order correlation function $\rho_n{}^x$ as $n \to \infty$ when λ varies from 0 to ∞. Fortunately this quantity has been worked out by McCoy [7].

For $\lambda < 1$ and n large we deduce from (4.26) of [7] that

$$\rho_n{}^x \simeq \tfrac{1}{4}(1 - \lambda^2)^{-1/4}\, \pi^{-1/2} n^{-1/2} \lambda^n [1 - \tfrac{1}{8} n^{-1}(1 + \lambda^2)(1 - \lambda^2)^{-1} + 0(n^{-2})] \quad (3.8)$$

and thus for $\lambda < 1$,

$$\lim \rho_n{}^x = 0 \qquad \text{as} \qquad n \to \infty. \quad (3.9)$$

For $\lambda > 1$ we deduce[1] from (3.36) of (7) that

$$\lim \rho_n{}^x = \tfrac{1}{4}(1 - \lambda^{-2})^{1/4} \qquad \text{as} \qquad n \to \infty. \quad (3.10)$$

The long-range order correlation function vanishes for $\lambda \leqslant 1$. At $T = 0$ in the ground state the system is ordered when $\Gamma < J/2$ and disordered for $\Gamma \geqslant J/2$ and $M_x = \langle 0 \mid S_i{}^x \mid 0 \rangle$ should vanish for $\Gamma \geqslant \Gamma_c = J/2$. Again the molecular field result $\Gamma_c = J$, [6] is quite wrong.

In the limit as $n \to \infty$

$$\rho_n{}^x = M_x{}^2 \quad (3.11)$$

and from (3.9), (3.10), and (3.11)

$$M_x = \tfrac{1}{2}(1 - \lambda^{-2})^{1/8} \qquad \text{for} \quad \lambda > 1 \quad (3.12a)$$

and

$$M_x = 0 \qquad \lambda \leqslant 1. \quad (3.12b)$$

The same result has been obtained by a perturbation method [4]. In this n-th order perturbation treatment, the transverse field part of the Hamiltonian is considered as a perturbation and the ground state and thus $\langle 0 \mid S_i{}^x \mid 0 \rangle$ is then expanded as a power series in λ^{-2}. The first three terms have been calculated and correspond exactly to the first three terms in the power series expansion of the exact result for M_x (3.12).

For the free end chain (case a), following Lieb *et al.* [3] similar results are obtained. The excitation spectrum is given by (2.10) with k solution of the equation:

$$\frac{\sin k(N + 1)}{\sin kN} = -\lambda \quad (3.13)$$

for $\lambda > 1$ one of the N roots becomes complex.

$$k_0 = \pi + iv, \quad (3.14)$$

[1] Equations (3.4), (3.7a), (3.8), and (3.10) were first obtained by T. T. Wu [8] as a special case for the two spin correlation function of the two dimensional Ising model. In fact $\rho_n{}^x$ of this paper corresponds to $S_n^{(0)}$ of [8] with λ replaced by α_2^{-1}. $S_n^{(0)}$ is also equal to R_n (taken in the limit $T \to 0$) introduced by B. McCoy [7] with α_2 replaced by α. Equations (5.2) of [8] and (4.26) of [7] give similar results leading to Eq. (3.8) of this paper. Equations (5.5) of [8] and (5.15a) of [7] give the asymptotic behaviour of $\rho_n{}^x$ leading to Eq. (3.10) of this paper.

where v satisfies the equation

$$\frac{\sinh(N+1)v}{\sinh Nv} = \lambda. \tag{3.15}$$

The excitation k_0 carries the energy

$$\Gamma\Lambda_{k_0} = \frac{J}{2}\lambda^{-N}[1 - \lambda^{-2} + \cdots + a_p\lambda^{-2p} + \cdots]. \tag{3.16}$$

For $\lambda > 1$ Eq. (3.16) shows an asymptotic degeneracy of the ground state leading to the appearance of order in the system when $N \to \infty$ (the gap of order λ^{-N} tends to zero when $N \to \infty$ more rapidly than $1/N$). Let us suppose that N is finite; the Ising model ($\Gamma = 0$) ground state is doubly degenerate thus

$$\langle 0 \mid S_i^x \mid 0\rangle = \pm\tfrac{1}{2}. \tag{3.17}$$

When a transverse field is added this degeneracy is removed. The new ground state $\mid 0\rangle$ is symmetric and remains unchanged when S^x is changed into $-S^x$, while the first excited state $\mid 1\rangle$ is antisymmetric and is changed into $-\mid 1\rangle$. Thus, we get

$$\langle 0 \mid S_i^x \mid 0\rangle = 0. \tag{3.18}$$

If N tends to infinity with $\lambda > 1$, the ground state becomes degenerate with the state carrying the k_0 excitation and $\langle 0 \mid S^x \mid 0\rangle \neq 0$. On the contrary, if $\lambda < 1$ the ground state remains nondegenerate and no order appears.

Let us now consider the end-to-end correlation function ρ_{1N}^x for a free end chain. We get

$$\rho_{1N}^x = \tfrac{1}{4}(1 - \lambda^{-2}) + 0(1/N) \qquad \lambda > 1 \tag{3.19a}$$

and

$$\rho_{1N}^x = 0(1/N) \qquad \lambda \leqslant 1 \tag{3.19b}$$

The difference with the result (3.10) may be due to end effects. To avoid these we should have to calculate $\rho_{l,l+m}^x$ as $m \to \infty$. This quantity is more difficult to calculate than ρ_{1N}^x, and has not as yet been done.

At finite temperature, following either Lieb *et al.* [3] or McCoy [7], the long-range order $\rho_n{}^x$ as $n \to \infty$ vanishes for all values of λ and as expected there is no finite temperature phase transition. However, as for the Ising model [9], when $J(r)$ ($r = i - j$) is long range, we expect a phase transition if $J(r)$ satisfies certain conditions to be determined.

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