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THEORY OF THE ISING MODEL

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A system of equations for the correlation functions for an Ising model of arbitrary dimensionality in an external field is derived by the spectral density method. A solution of the equations obtained for a one-dimensional Ising model is considered and explicit expressions for all the correlation functions and the thermodynamic characteristics of the system are obtained.

1. INTRODUCTION

THE nomenclature "Ising model" is used to denote a system of interacting localized dipoles (spins) each of which interacts only with its nearest neighbors and with an external magnetic field. The Hamiltonian for this model has the form

$$H = -J \sum_{(i)} S^z_{(i)} + g \sum_{(i);(j)} S^z_{(i)} V_{(i);(j)} S^z_{(j)}, \tag{1.1}$$

where J is the external field, g is the coupling constant, $S^z_{(i)}$ is the z-component of the spin operator located at the (i) site, (i) is the location index. The potential for the interaction is defined by

$$V_{(i);(j)} = \sum_{m=0}^{t} \delta_{i_1, j_1} \cdots \frac{1}{2} (\delta_{i_m, j_m+1} + \delta_{j_m, i_m+1}) \cdots \delta_{i_t, j_t}, \tag{1.2}$$

where t is the dimensionality of the lattice. Introducing in the usual manner the Fermi-field operators $a^+_{(i)}$ and $a_{(i)}$ and introducing the correspondence

$$S^z_{(i)} = n_{(i)} - 1/2, \quad n_{(i)} = \overset{+}{a}_{(i)} a_{(i)}, \tag{1.3}$$

we rewrite the Hamiltonian for the system (cf., (1.1)) in terms of the new operators. After straightforward transformations we obtain the following expression:

$$H = C + \sum_{(i)} \varepsilon n_{(i)} + g \sum_{(i);(j)} n_{(i)} V_{(i);(j)} n_{(j)}, \tag{1.4}$$

where we have introduced the notation

$$C = \frac{N^t}{2} \left(J + t \frac{g}{2} \right), \quad \varepsilon = -(J + tg). \tag{1.5}$$

Thus, the problem reduces to finding the correlation functions and the thermodynamic characteristics of the system the Hamiltonian of which has the form (1.4). Starting with the well-known paper by Onsager[1] the most complete investigation of this problem has been carried out in the two-dimensional case in the absence of an external field. But the basic methods of the investigation, both the matrix method and the combinatorial method (cf., for example,[2]), in one form or another reduce the problem of finding the thermodynamic potential of the two-dimensional Ising model to the solution of a problem with a different (quadratic) Hamiltonian, but yielding the same thermodynamic potential, and are therefore poorly suited for finding the correlation functions. Moreover, the methods referred to above have not been successfully generalized to the case of a two-dimensional Ising model in an external field, and in the three-dimensional case even in the absence of an external field. Further, so far no one has succeeded in obtaining an exact solution by means of the usual method of the temperature Green's functions even in the case of the one-dimensional Ising model. This is due primarily to the fact that in order to solve the problem within the framework of this method it is necessary to consider along with the single-time correlation functions also the multi-time correlation functions.

The present paper is devoted to a systematic study of the Ising model by means of the method of spectral densities[3]. In this model one has to deal only with the single-time correlation functions, and this considerably simplifies the solution of the problem stated above. In this paper we have obtained a system of equations for the correlation functions of an Ising model of arbitrary dimensionality, and here we restrict ourselves to an exact solution of this system in the simplest case of the one-dimensional Ising model. In this case we have obtained an expression not only for the thermodynamic potential, but also for all the correlation functions in an external field.

2. THE THERMODYNAMIC CHARACTERISTICS OF THE SYSTEM

The properties of the system can be conveniently investigated with the aid of the first spectral density defined in the usual manner:

$$\Lambda_{(i)}(\tau) = \langle [\overset{+}{a}_{(i)}; a_{(i)}(\tau)]_+ \rangle. \tag{2.1}$$

Since the operator $n_{(i)}$ commutes with H then the equation of motion for the operator $a_{(i)}(\tau)$ can be easily integrated, and, therefore, we can write the following expression for the spectral density:

$$\Lambda_{(i)}(\tau) = \left\langle \exp\left\{ -i \left(\varepsilon + 2g \sum_{(j)} V_{(i);(j)} n_{(j)} \right) \tau \right\} \right\rangle. \tag{2.2}$$

Using the definitions of $V_{(i);(j)}$ (cf., (1.2)) we can write the infinite system of moments for $\Lambda_{(i)}(\tau)$ in the form of a single recurrence relation

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (\omega - \varepsilon)^\nu \Lambda_{(i)}(\omega) = g^\nu \sum_{m=0}^{2t} m^\nu d_{(i)}\Big|_m^{2t}, \quad \nu = 0, 1, \ldots, \tag{2.3}$$

where we have introduced the definitions

$$d_{(i)}\Big|_m^{2t} = \sum_{p=m}^{2t} (-1)^{m+p} \binom{p}{m} \langle \Pi_p^{2t}(i) \rangle; \quad \binom{p}{m} = \frac{p!}{m!(p-m)!} \tag{2.4}$$

and $\Pi_p^{2t}(i)$ is the sum over p of all possible combinations (of the particle number density operators) of 2t of the nearest neighbors of the lattice point (i). The spectral density satisfying the whole infinite system of moments has the form

$$\Lambda_{(i)}(\omega) = \sum_{m=0}^{2t} d_{(i)}|_m^{2t} 2\pi\delta(\omega - \varepsilon - mg). \qquad (2.5)$$

In virtue of translational invariance $d_{(i)}|_m^{2t}$ evidently do not depend on the number of the lattice point (i), and if these quantities are known, then the first spectral density is completely determined, and then the investigation of the thermodynamic characteristics of the system presents no difficulties. For example, the average occupation numbers and the thermodynamic potential for the system are respectively given by:

$$\bar{n} = \sum_{m=0}^{2t} \frac{d_m{}^{2t}}{1 + \exp[\beta(\varepsilon + mg)]};$$

$$\frac{\Omega - \Omega_0}{N^t} = t\frac{g}{4} + \frac{1}{2}\int_0^g dg_1 \sum_{m=0}^{2t} \frac{d_m{}^{2t}(m - 2t)}{1 + \exp[\beta(\varepsilon + mg_1)]}, \qquad (2.6)$$

where Ω_0—the thermodynamic potential of the system for g = 0—is usually an easily calculable quantity.

3. THE SYSTEM OF EQUATIONS FOR THE CORRELATION FUNCTIONS

In order to study the correlation functions it is necessary to consider the μ-particle spectral density defined in the following manner:

$$A_{(i_\mu)\dots(i_1)}(\tau) = \langle [n_{i_\mu} \dots n_{(i_2)} a^+_{(i_1)}; a_{(i_1)}(\tau)]_+ \rangle, \qquad (3.1)$$

where for what follows it is essential that $(i_1) \neq \{(i_\mu) \dots (i_2)\}$. In analogy with the first spectral density the infinite system of moments for the spectral function (3.1) can be written in the form of a single recurrence relation:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}(\omega - \varepsilon)^\nu A_{(i_\mu)\dots(i_1)}(\omega) = g^\nu \sum_{m=0}^{2t} m^\nu d_{(i_\mu)\dots(i_1)}|_m^{2t}. \qquad (3.2)$$

By means of a direct check we verify that the solution of the system (3.2) is given by a spectral density of the form

$$A_{(i_\mu)\dots(i_1)}(\omega) = \sum_{m=0}^{2t} d_{(i_\mu)\dots(i_1)}|_m^{2t} 2\pi\delta(\omega - \varepsilon - mg), \qquad (3.3)$$

where $d_{(i_\mu)\dots(i_1)}|_m^{2t}$ are the natural generalizations of expression (2.4) and are equal to

$$d_{(i_\mu)\dots(i_1)}|_m^{2t} = \sum_{p=m}^{2t} (-1)^{m+p} \binom{p}{m} \langle n_{(i_\mu)} \dots n_{(i_2)} \Pi_p^{2t}(i_1) \rangle. \qquad (3.4)$$

Now, utilizing the spectral properties of the function (3.1) we define the μ-particle correlation function by the expression

$$W_{(i_\mu)\dots(i_1)} \equiv \langle n_{(i_\mu)} \cdots n_{(i_1)} \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A_{(i_\mu)\dots(i_1)}(\omega)}{1 + \exp(\beta\omega)}. \qquad (3.5)$$

On the basis of the explicit form for the highest spectral density (cf., (3.3)) the integral on the right hand side of equation (3.5) can be evaluated, and we obtain a system of equations for the correlation functions

$$W_{(i_\mu)\dots(i_1)} = \sum_{m=0}^{2t} \frac{d_{(i_\mu)\dots(i_1)}|_m^{2t}}{1 + \exp[\beta(\varepsilon + mg)]}. \qquad (3.6)$$

In this paper we restrict ourselves to a detailed solution of the system of equations obtained above in the one-dimensional case.

4. THE ONE-DIMENSIONAL ISING MODEL

We now obtain the complete solution for the one-dimensional Ising model, i.e., we determine the thermodynamic properties and all the correlation functions for the system. In order to determine the latter we write equation (3.6) in explicit form. Since the model is one-dimensional (t = 1) with the topology of a closed ring, then the number of nearest neighbors is equal to two, and (i) is an ordinary index. Then it is easy to write an explicit expression for the coefficients $d_{(i_\mu)\dots(i_1)}|_m^2$ (cf., the definition (3.4)):

$$\begin{aligned} d_{i_\mu\dots i_1}|_0^2 &= W_{i_\mu\dots i_2, i_1-1, i_1+1} + W_{i_\mu\dots i_2} \\ &\quad - (W_{i_\mu\dots i_2, i_1-1} + W_{i_\mu\dots i_2, i_1+1}), \\ d_{i_\mu\dots i_1}|_1^2 &= (W_{i_\mu\dots i_2, i_1-1} + W_{i_\mu\dots i_2, i_1+1}) - 2W_{i_\mu\dots i_2, i_1-1, i_1+1}, \\ d_{i_\mu\dots i_1}|_2^2 &= W_{i_\mu\dots i_2, i_1-1, i_1+1}. \end{aligned} \qquad (4.1)$$

Substituting the explicit form of the coefficients $d_{i_\mu\dots i_1}|_m^2$ into equation (3.6) we obtain after straightforward transformations a system of equations for the correlation functions in explicit form:

$$\begin{aligned} &W_{i_\mu\dots i_1} + s(W_{i_\mu\dots i_2, i_1-1} + W_{i_\mu\dots i_2, i_1+1}) \\ &= \frac{W_{i_\mu\dots i_2}}{1 + \exp(\beta\varepsilon)} + rW_{i_\mu\dots i_2, i_1-1, i_1+1}, \end{aligned} \qquad (4.2)$$

where s and r are known functions of the form

$$s = \left(\frac{1}{1 + \exp(\beta\varepsilon)} - \frac{1}{1 + \exp[\beta(\varepsilon + g)]}\right);$$

$$r = \left(\frac{1}{1 + \exp(\beta\varepsilon)} - \frac{2}{1 + \exp[\beta(\varepsilon + g)]} + \frac{1}{1 + \exp[\beta(\varepsilon + 2g)]}\right). \qquad (4.3)$$

We note that Eq. (4.2) is valid if $i_1 \neq (i_\mu \dots i_2)$ and is the basic equation for the one-dimensional Ising model.

If the external field is switched off, i.e., if J = 0, then r = 0 (one can easily verify this utilizing the explicit form (4.3) and the notation of (1.5)). Then the system of equations (4.2) is simplified and decomposes into closed equations of the form

$$W_0|_{i_\mu\dots i_1} + s_0(W_0|_{i_\mu\dots i_2, i_1-1} + W_0|_{i_\mu\dots i_2, i_1+1}) = \frac{W_0|i_\mu \dots i_2}{1 + \exp(-\beta g)}, \qquad (4.4)$$

where s_0 is the value of s for J = 0 and where in future we shall everywhere denote by the subscript zero quantities corresponding to a switched-off external field. Further, without reducing the degree of generality, we can assume that $i_\mu > i_{\mu-1} > \dots > i_1$ since the particle number density operators (cf., (3.5)) commute, and in future this condition is essential. In virtue of translational invariance the correlation function depends only on the difference between subscripts i.e., $W_0|_{i_\mu \dots i_1} = W_0(\gamma_{\mu-1} \dots \gamma_1)$, where $\gamma_e = i_{e+1} - i_e$, and one can easily verify that the solution which has the correct behavior for $N \to \infty$ has the form

$$W_0(\gamma_{\mu-1}\ldots\gamma_1)=\bar{n}_0\sigma_0(\gamma_{\mu-1})\ldots\sigma_0(\gamma_1), \tag{4.5}$$

i.e., in the limit N → ∞ the μ-particle correlation function is represented in multiplicative form, where

$$\sigma_0(\gamma)=\frac{1}{2}\left[1+(-1)^{\gamma}\left(\operatorname{th}\frac{\beta g}{4}\right)^{\gamma}\right]. \tag{4.6}$$

We now proceed to consider the case $J \neq 0$. Then $r \neq 0$ and it is necessary to solve the complete system of equations (4.2). In the case N → ∞ it can be shown that the correlation functions retain as before their multiplicative form (4.5) and at the same time we obtain for $\sigma(\gamma)$ an equation of the form

$$\sigma(\gamma)+s(\sigma(\gamma-1)+\sigma(\gamma+1))=[1+\exp(\beta\varepsilon)]^{-1}+r\sigma(\gamma-1)\sigma(2), \tag{4.7}$$

where $\sigma(\gamma)$ must satisfy the following boundary conditions: $\sigma(0) = 1$, $\sigma(\gamma)|_{\gamma\to\infty} = \text{const} < \infty$. The solution of (4.7) should be sought in the form

$$\sigma(\gamma)=hx^{\gamma}+\varkappa.$$

Then for h, x, κ we obtain the system of equations

$$\begin{gathered} h+\varkappa=1, \quad x+s(x^2+1)=r(hx^2+\varkappa), \\ \varkappa(1+2s)-r\varkappa(hx^2+\varkappa)=[1+\exp(\beta\varepsilon)]^{-1}. \end{gathered} \tag{4.8}$$

We go over to the new variables $\kappa = \frac{1}{2}(1 + R)$ and $h = \frac{1}{2}(1 - R)$ and we carry out a fractional-linear transformation of the form

$$\left(R-\operatorname{th}\frac{\beta J}{2}\right)\Big/\left(R+\operatorname{th}\frac{\beta J}{2}\right)=x. \tag{4.9}$$

Then the first equation of the system (4.8) can be rewritten in the form

$$\frac{R-\operatorname{th}(\beta J/2)}{R+\operatorname{th}(\beta J/2)}+\left[s-\frac{r}{2}(1-R)\right]\left(\frac{R-\operatorname{th}(\beta J/2)}{R+\operatorname{th}(\beta J/2)}\right)^2 +\left[s-\frac{r}{2}(1+R)\right]=0. \tag{4.10}$$

After some straightforward transformations we find that with respect to R this is a degenerate quadratic equation which is easily solved:

$$R^2=\operatorname{sh}^2\frac{\beta J}{2}\Big/\left[\operatorname{sh}^2\frac{\beta J}{2}+\exp(\beta g)\right]. \tag{4.11}$$

In solving (4.10) we used the definitions of the functions s and r (cf., (4.3)). By a direct substitution we verify that the second equation of the system (4.8) is satisfied identically, and the following expressions hold

$$x=\frac{\operatorname{ch}(\beta J/2)-\sqrt{\operatorname{sh}^2(\beta J/2)+\exp(\beta g)}}{\operatorname{ch}(\beta J/2)+\sqrt{\operatorname{sh}^2(\beta J/2)+\exp(\beta g)}},$$

$$R=\frac{\operatorname{sh}(\beta J/2)}{\sqrt{\operatorname{sh}^2(\beta J/2)+\exp(\beta g)}}. \tag{4.12}$$

Thus, the function $\sigma(\gamma)$ is completely determined, and then, according to (4.5), we have an expression for all the correlation functions for the system for $J \neq 0$ and N → ∞.

5. THE THERMODYNAMIC CHARACTERISTICS OF THE SYSTEM

According to formulas (2.6) in order to determine all the thermodynamic properties of the system it is sufficient to know d_m^{2t}. According to (2.4), in the case of the one-dimensional Ising model we have

$$d_0^2=1+W(2)-2\bar{n}, \quad d_1^2=2(\bar{n}-W(2)), \quad d_2^2=W(2), \tag{5.1}$$

i.e., we see that all the thermodynamic characteristics of the system are determined by the single correlation function W(2).

We now calculate the average occupation numbers. Utilizing the explicit form of d_m^2, after some straightforward transformations we obtain from (2.6) that

$$\bar{n}=\frac{1}{(1+2s)[1+\exp(\beta\varepsilon)]}+\frac{r}{1+2s}W(2), \tag{5.2}$$

where r and s are functions which have been defined earlier (cf., (4.3)). Comparing this expression with the second expression of the system (4.8) and taking into account the fact that $W(2) = \bar{n}(hx^2 + \kappa)$ we find that $\bar{n} = \kappa = \frac{1}{2}(1 + R)$. Further, defining the magnetization per unit spin by the expression

$$\frac{2}{N}\sum_{i=1}^{N}\langle S_i^z\rangle,$$

we easily verify, utilizing (1.3), that the previously defined quantity R is the magnetization of the system. In view of its importance we once again reproduce it explicitly

$$R=\frac{\operatorname{sh}(\beta J/2)}{\sqrt{\operatorname{sh}^2(\beta J/2)+\exp(\beta g)}} \tag{5.3}$$

Thus we see that when the external field is switched off (J = 0) the magnetization of the system vanishes, i.e., the one-dimensional Ising lattice does not exhibit any spontaneous magnetization.

Further, it is of interest to calculate the thermodynamic potential, which in this case is simply the free energy. Utilizing formulas (2.6) and (5.1) we find after straightforward transformations

$$\frac{F-F_0}{N}=\frac{g}{4}-\int_0^g dg_1\left(\frac{1+W(2)-2\bar{n}}{1+\exp(\beta\varepsilon)}+\frac{\bar{n}-W(2)}{1+\exp[\beta(\varepsilon+g_1)]}\right). \tag{5.4}$$

Now substituting the explicit expressions for the average occupation numbers $\bar{n} = \frac{1}{2}(1 + R)$ where R is given in (5.3) and the expression for the two-particle correlation function

$$W(2)=\frac{\left[\operatorname{sh}\frac{\beta J}{2}+\sqrt{\operatorname{sh}^2\frac{\beta J}{2}+\exp(\beta g)}\right][\exp(\beta J)+\exp(\beta g)]}{2\sqrt{\operatorname{sh}^2\frac{\beta J}{2}+\exp(\beta g)}\left[\operatorname{ch}\frac{\beta J}{2}+\sqrt{\operatorname{sh}^2\frac{\beta J}{2}+\exp(\beta g)}\right]^2}, \tag{5.5}$$

after straightforward calculations expression (5.4) transforms into the form

$$\frac{F-F_0}{N}= =\frac{g}{4}-\int_0^g\frac{dg_1\exp(\beta g_1)}{2\sqrt{\operatorname{sh}^2(\beta J/2)+\exp(\beta g_1)}\,[\operatorname{ch}(\beta J/2)+\sqrt{\operatorname{sh}^2(\beta J/2)+\exp(\beta g_1)}]}. \tag{5.6}$$

The integral (5.6) and F_0 (the free energy for g = 0) are evaluated in an elementary manner and we finally obtain the well known result:

$$\frac{F}{N}=\frac{g}{4}-\frac{1}{\beta}\ln\left[\operatorname{ch}\frac{\beta J}{2}+\sqrt{\operatorname{sh}^2\frac{\beta J}{2}+\exp(\beta g)}\right]. \tag{5.7}$$

APPENDIX

An interesting illustration of the effectiveness of the relations for the correlation functions (5.6) obtained above is provided by the fact that with their aid it turns out to be possible, in particular, to obtain directly the differential equation for the partition function. Thus, for example, in the case of the one-dimensional Ising model in an external field in order to obtain this equation it is necessary to make use of the expression for the average occupation numbers (cf., (5.2)) and the expression for the nearest two-particle correlation function, which is easily obtained directly from equation (4.2) and has the form

$$W(1) = \bar{n}[1 + \exp(-\beta J)]^{-1} + (r - s) W(2). \qquad (\mathrm{A.1})$$

Further, using the definition of the partition function we find that the following formulas hold:

$$\bar{n} = \frac{\partial}{\partial(\beta J)}\left(\frac{\ln Z}{N}\right) + \frac{1}{2},$$

$$W(1) = -\frac{\partial}{\partial(\beta g)}\left(\frac{\ln Z}{N}\right) + \frac{\partial}{\partial(\beta J)}\left(\frac{\ln Z}{N}\right) + \frac{1}{4}. \qquad (\mathrm{A.2})$$

Now, eliminating between equations (5.2) and (A.1) the two-particle correlation function W(2) and utilizing formulas (A.2) we obtain the equation

$$\operatorname{cth}\frac{\beta J}{2}\frac{\partial}{\partial(\beta J)}\left(\frac{\ln Z}{N}\right) + [1 - \exp(-\beta g)]\frac{\partial}{\partial(\beta g)}\left(\frac{\ln Z}{N}\right) = \frac{1}{4}[1 + \exp(-\beta g)]. \qquad (\mathrm{A.3})$$

Thus, the partition function for the one-dimensional Ising model regarded as a function of two variables satisfies a quasilinear first order partial differential equation. The equation so obtained enables us to recover the form of the partition function from a known value at the boundary when the external field or the interaction are switched off. Thus, in particular, on the basis of the expression corresponding to a switched-off external field, i.e.,

$$\left(\frac{\ln Z}{N}\right)_{\beta J=0} = -\frac{\beta g}{4} + \ln\left[1 + \exp\left(\frac{\beta g}{2}\right)\right], \qquad (\mathrm{A.4})$$

one can easily obtain from equation (A.3) the following well-known form for the partition function in an external field:

$$\frac{\ln Z}{N} = -\frac{\beta g}{4} + \ln\left[\operatorname{ch}\frac{\beta J}{2} + \sqrt{\operatorname{sh}^2\frac{\beta J}{2} + \exp(\beta g)}\right]. \qquad (\mathrm{A.5})$$

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