Journal of Statistical Physics, Vol. 48, Nos. 3/4, 1987

One-Dimensional Inhomogeneous Ising Model: A New Approach

C. F. Tejero[1]

Received April 17, 1987

We present a new method for the study of a one-dimensional inhomogeneous Ising chain with nonconstant nearest neighbor interactions. The external field required to produce a given magnetization profile is derived exactly. Some properties of the pair direct correlation function are derived. Our findings generalize previous results of Percus.

KEY WORDS: Ising model; correlation function; one-dimensional; inhomogeneous.

1. INTRODUCTION

Increasing attention has been paid to the study of one-dimensional inhomogeneous Ising models in recent years. An exactly solvable one-dimensional model of an interface between coexisting phases was analyzed recently by Robert and Widom.[1] The model consisted of a one-dimensional Ising chain with constant nearest neighbor interactions in an external field that changed sign in the middle of the chain. Later, Robert and Viswanathan[2] calculated an exact expression of the pair distribution function of the above field-induced interface for finite and infinite chains. The pair direct correlation function was then obtained from a remarkable work of Percus,[3] who expressed this function in terms of the magnetization profile.

In another group of studies, exactly solvable one-dimensional inhomogeneous Ising models, i.e., inhomogeneous models for which the free energy can be exactly evaluated, have also been widely discussed recently. Allouche and Mendès-France[4] studied the Ising chain with

[1] Departamento de Fisica Aplicada (Termologia), Facultad de Fisica, Universidad Complutense, Madrid 28040, Spain.

0022-4715/87/0800-0531$05.00/0

variable interaction and constant external field at zero temperature. Mendès-France[5] gave an exact computation of the Ising chain with nonconstant external field in terms of certain continued fractions. Derrida *et al.*[6] analyzed an Ising chain in a variable external field. Using a result of Weyl,[7] they founded exact solutions from which they built the model. However, they claimed that the relationship between their point of view and that of Percus appeared to be too complicated to allow a direct comparison between both methods.

In this paper we present a new and exact method for the study of a one-dimensional Ising chain with nonconstant interactions in an inhomogeneous external field. Our findings generalize previous results of Percus. Some specific applications of our method to field-induced interfaces and exactly solvable models will be reported elsewhere.

2. THE METHOD

We consider a one-dimensional Ising chain of N spins with nonconstant nearest neighbor interactions in an inhomogeneous external field. The equilibrium statistical mechanics of the chain is determined by the partition function

$$Z_N(b_1,..., b_N; K_1,..., K_{N-1}) = \sum_{\{s_n\}} \exp\left(\sum_{n=1}^{N} b_n s_n + \sum_{n=1}^{N-1} K_n s_n s_{n+1}\right) \tag{1}$$

where b_n and K_n are dimensionless variables denoting, respectively, the external field acting on the nth spin and the interaction constant that couples s_n to s_{n+1}. As usual, the spin variables s_n assume either of the values ± 1.

As distinguished from Percus,[3] who decomposed (1) into right and left fragments, and Derrida *et al.*,[6] who used transfer matrix techniques to derive a recurrence relation for the ratios $Z_n(+)/Z_n(-)$, these being partition functions as defined in (1) with the extra conditions $s_n = \pm 1$, we shall transform (1) in a different fashion.

First, carry out in (1) the sum over the spin variable s_N to obtain

$$\sum_{s_N} \exp(b_N s_N + K_{N-1} s_{N-1} s_N) = 2\cosh(b_N + K_{N-1} s_{N-1})$$

where, in order to avoid cumbersome formulas, we detached the terms s_N in (1). We now introduce the following notation:

$$2\cosh(b_N + K_{N-1} s_{N-1}) = f_N(b_N, K_{N-1}) \exp(b^*_{N-1} s_{N-1}) \tag{2}$$

This relation defines $f_N(b_N, K_{N-1})$ and b^*_{N-1}, their analytical expressions being readily found by solving the algebraic equations obtained by setting $s_{N-1} = \pm 1$ in (2). It follows at once that

$$f_N(b_N, K_{N-1}) = 2\cosh^{1/2}(b_N + K_{N-1})\cosh^{1/2}(b_N - K_{N-1}) \tag{3a}$$

$$\exp(2b^*_{N-1}) = \cosh(b_N + K_{N-1})/\cosh(b_N - K_{N-1}) \tag{3b}$$

Equations (1) and (2) yield the identity

$$\begin{aligned} &Z_N(b_1,..., b_N; K_1,..., K_{N-1}) \\ &\quad = f_N(b_N, K_{N-1})\, Z_{N-1}(b_1,..., b_{N-1} + b^*_{N-1}; K_1,..., K_{N-2}) \end{aligned} \tag{4}$$

where the notation of (1) has been used. We note that Z_{N-1} is the partition function of an Ising chain of $N-1$ spins with the same dimensionless variables b_n and K_n ($n = 1,..., N-2$) appearing in (1) but with b_{N-1} replaced by $b_{N-1} + b^*_{N-1}$.

The outlined procedure is then continued by summing over the spin variable s_{N-1} in Z_{N-1} and arranging the sum as in (2) to obtain the next identity

$$\begin{aligned} &Z_{N-1}(b_1,..., b_{N-1} + b^*_{N-1}; K_1,..., K_{N-2}) \\ &\quad = f_{N-1}(b_{N-1} + b^*_{N-1}, K_{N-2})\, Z_{N-2}(b_1,..., b_{N-2} + b^*_{N-2}; K_1,..., K_{N-3}) \end{aligned}$$

where f_{N-1} and b^*_{N-2} depend on $b_{N-1} + b^*_{N-1}$ and K_{N-2} in the same way as f_N and b^*_{N-1} depend on b_N and K_{N-1} [see (3a), (3b)].

The method is now straightforward. We proceed exactly as above, summing *consecutively* over $s_{N-2}, s_{N-3},...,$ and s_1, each time repeating the same steps leading from (1) to (4). We thus get the following exact result for the partition function:

$$Z_N = \prod_{n=1}^{N} f_n(b_n + b^*_n, K_{n-1}) \tag{5}$$

where

$$\begin{aligned} &f_n(b_n + b^*_n, K_{n-1}) \\ &\quad = 2\cosh^{1/2}(b_n + b^*_n + K_{n-1})\cosh^{1/2}(b_n + b^*_n - K_{n-1}) \end{aligned} \tag{6}$$

and

$$K_0 = 0; \qquad b^*_N = 0 \tag{7}$$

The field variables b_n^* appearing in (6) can be shown to satisfy the recurrence relation

$$\exp(2b_n^*) = \cosh(b_{n+1} + b_{n+1}^* + K_n)/\cosh(b_{n+1} + b_{n+1}^* - K_n) \tag{8a}$$

or

$$\tanh b_n^* = \tanh(b_{n+1} + b_{n+1}^*) \tanh K_n \tag{8b}$$

from which we readily obtain that

$$\partial b_n^* / \partial b_m = 0, \qquad m \leqslant n \tag{9a}$$

$$\partial b_n^* / \partial b_m = \prod_{p=n+1}^{m} (x_p^+ - x_p^-), \qquad m > n \tag{9b}$$

with $x_n^\pm$ defined as

$$x_n^\pm = \frac{1}{2} \tanh(b_n + b_n^* \pm K_{n-1}) \tag{10}$$

Their physical meaning will become clear later.

3. A PHYSICAL INTERPRETATION

The representation developed in Section 2 is, of course, entirely equivalent to the representation of Derrida *et al.* because both representations correspond to exact transformations of (1). Indeed, from (5), (6), and (10) it is an easy matter to derive that

$$\log Z_N = N \log 2 - \frac{1}{4} \sum_{n=1}^{N} \log(1 - 4x_n^{+2})(1 - 4x_n^{-2}) \tag{11}$$

which expresses $\log Z_N$ as a function of the $2N-1$ independent variables $x_n^\pm$ instead of the original ones b_n and K_n (notice that $x_1^+ = x_1^-$ because $K_0 = 0$). A similar formula was used by Derrida *et al.* [see their equation (3a), p. 441] to compute exactly the free energy per spin for some specific models. But while they run into difficulties in giving a physical meaning to the ratios $Z_n(+)/Z_n(-)$, there is a fairly clear equation that relates $x_n^\pm$ to more physical quantities than the field variables b_n^*. We proceed as follows.

Consider the magnetization or average spin value $\langle s_n \rangle$ of the nth spin $\langle s_n \rangle = \partial \log Z_N / \partial b_n$. Using (5), (6), (9), and (10) and after a few calculations, we get

$$\langle s_n \rangle = (x_n^+ + x_n^-) + \sum_{m=1}^{n-1} (x_m^+ + x_m^-) \prod_{p=m+1}^{n} (x_p^+ - x_p^-) \tag{12a}$$

or

$$\langle s_n \rangle = (x_n^+ + x_n^-) + \langle s_{n-1} \rangle (x_n^+ - x_n^-) \tag{12b}$$

Differentiating (12b) with respect to b_{n-1} and taking into account (9a), one finds

$$\langle \Delta s_n \Delta s_{n-1} \rangle = (x_n^+ - x_n^-) \langle (\Delta s_{n-1})^2 \rangle \tag{13}$$

where we introduced the nearest neighbor correlation $\langle \Delta s_n \Delta s_{n-1} \rangle = \partial \langle s_n \rangle / \partial b_{n-1}$ with $\Delta s_n = s_n - \langle s_n \rangle$. Solving (12b) and (13) for $x_n^\pm$, it is easy to see that

$$x_n^\pm = \frac{1}{2} \left(\langle s_n \rangle \pm \frac{\langle \Delta s_n \Delta s_{n-1} \rangle}{1 \pm \langle s_{n-1} \rangle} \right) \tag{14}$$

which establishes our claim.

Before ending this section, let us apply these exact results to two simple examples. First, consider an ideal chain, i.e., $K_n = 0$, for all n. Formula (8) yields $b_n^* = 0$ for all n, while (10) leads to $x_n^+ = x_n^- = (\tanh b_n)/2$; so, using (12b) and (13), we get $\langle s_n \rangle = \tanh b_n$ and $\langle \Delta s_n \Delta s_{n-1} \rangle = 0$. Next, consider the case $b_n = 0$ for all n. Again (8) yields $b_n^* = 0$ for all n, and (10) shows that $x_n^+ = -x_n^- = (\tanh K_{n-1})/2$. Then (12b) and (13) lead to $\langle s_n \rangle = 0$ and $\langle \Delta s_n \Delta s_{n-1} \rangle = \tanh K_{n-1}$. Except for these simple cases, the exact solution becomes difficult because the field variables b_n^* are highly nonlinear in the original variables b_n and K_n.

4. THE INVERSE PROBLEM

In this section we are concerned with the so-called inverse problem, which was first solved by Percus for an Ising chain with constant interaction. In the inverse problem we obtain the external field required to evoke a given magnetization profile, that is, we express the sequence b_n as a function of the average spin values $\langle s_n \rangle$ and of the coupling constants K_n. Once this is done, direct correlation functions[3] are simply obtained as derivatives of the external field with respect to the magnetization at various spatial points.

Before proceeding to this task, we derive some preliminary results, which will be required subsequently.

As

$$\tanh(x - y) = (\tanh x - \tanh y)/(1 - \tanh x \tanh y)$$

we get from (10)

$$2x_n^- = \frac{2x_n^+ - \tanh(2K_{n-1})}{1 - 2x_n^+ \tanh(2K_{n-1})} \tag{15}$$

Combining (15) and (12b), one has

$$2\langle s_n \rangle = 2x_n^+(1 + \langle s_{n-1} \rangle) + \frac{2x_n^+ - \tanh(2K_{n-1})}{1 - 2x_n^+ \tanh(2K_{n-1})} (1 - \langle s_{n-1} \rangle) \tag{16}$$

the correct root of this second-degree equation being found as follows. Let $\langle s_n \rangle = 0$ for all n in (16). Then we find

$$x_n^+ = \frac{1}{2} \frac{1 \pm [1 - \tanh^2(2K_{n-1})]^{1/2}}{\tanh(2K_{n-1})} = \begin{cases} (2 \tanh K_{n-1})^{-1} & \text{(a)} \\ (\tanh K_{n-1})/2 & \text{(b)} \end{cases}$$

Substitution of these roots in (10) leads to the following consistency relations: (a) $\tanh^2 K_{n-1} = 1$; (b) $\tanh^2 K_{n-1} = 1$ or $\tanh(b_n + b_n^*) = 0$. But while the condition $\tanh^2 K_{n-1} = 1$ is untenable on physical grounds, $\tanh(b_n + b_n^*) = 0$ yields $b_n = 0$ and $b_n^* = 0$ for all n as the unique solution. This is just the second example reported in Section 3.

Summarizing, we find from (16) the solution

$$x_n^+ = \frac{1 + \langle s_n \rangle \tanh(2K_{n-1}) - \Delta_n^{1/2}}{2(1 + \langle s_{n-1} \rangle) \tanh(2K_{n-1})} \tag{17}$$

where we have defined

$$\begin{aligned} \Delta_n = 1 &+ (\langle s_n \rangle^2 + \langle s_{n-1} \rangle^2 - 1) \tanh^2(2K_{n-1}) \\ &- 2\langle s_n \rangle \langle s_{n-1} \rangle \tanh(2K_{n-1}) \end{aligned} \tag{18}$$

Once we obtain (17) and (18) we are ready to solve the inverse problem. Going back to (10), it is easily seen that

$$b_n + b_n^* + K_{n-1} = \frac{1}{2} \log \frac{1 + 2x_n^+}{1 - 2x_n^+} \tag{19}$$

and from the recurrence relation (8) we get

$$b_n^* = \frac{1}{4} \log \frac{1 - 4x_{n+1}^{-2}}{1 - 4x_{n+1}^{+2}} \tag{20}$$

where we have used the identity $\cosh x = (1 - \tanh^2 x)^{-1/2}$. Combining (15), (19), and (20), one has

$$b_n = \frac{1}{2}\log\frac{1+2x_n^+}{1-2x_n^+} - K_{n-1} + \frac{1}{4}\log\frac{[1-2x_{n+1}^+\tanh(2K_n)]^2}{1-\tanh^2(2K_n)} \tag{21}$$

The set of equations (21), (17), and (18) establishes the solution of the inverse problem. As observed, b_n depends on the average spin values $\langle s_{n-1}\rangle$, $\langle s_n\rangle$, and $\langle s_{n+1}\rangle$ and on the coupling constants K_{n-1} and K_n. We also note that (21) is valid provided that edge effects are neglected, i.e., in the thermodynamic limit. Otherwise, for a finite chain we have

$$b_1 = \frac{1}{2}\log\frac{1+\langle s_1\rangle}{1-\langle s_1\rangle} + \frac{1}{4}\log\frac{[1-2x_2^+\tanh(2K_1)]^2}{1-\tanh^2(2K_1)}$$

and

$$b_N = \frac{1}{2}\log\frac{1+2x_N^+}{1-2x_N^+} - K_{N-1}$$

with x_2^+ and x_N^+ determined by (17) and (18).

5. PAIR DIRECT CORRELATION FUNCTION

After solving the inverse problem, direct correlation functions are obtained systematically by simple differentiation. Let us limit briefly our considerations to the pair direct correlation function $C(n, m)$ defined as

$$C(n, m) = \partial b_n/\partial\langle s_m\rangle \tag{22}$$

From (17), $x_n^+ = x_n^+(\langle s_n\rangle, \langle s_{n-1}\rangle, K_{n-1})$, so, from (22) and (21), we have

$$C(n, n) = \frac{2}{1-4x_n^{+2}}\frac{\partial x_n^+}{\partial\langle s_n\rangle} - \frac{\tanh(2K_n)}{1-2x_{n+1}^+\tanh(2K_n)}\frac{\partial x_{n+1}^+}{\partial\langle s_n\rangle} \tag{23a}$$

$$C(n, n-1) = \frac{2}{1-4x_n^{+2}}\frac{\partial x_n^+}{\partial\langle s_{n-1}\rangle} \tag{23b}$$

$$C(n, n+1) = -\frac{\tanh(2K_n)}{1-2x_{n+1}^+\tanh(2K_n)}\frac{\partial x_{n+1}^+}{\partial\langle s_{n+1}\rangle} \tag{23c}$$

and

$$C(n, m) = 0 \qquad (|n-m| > 1) \tag{23d}$$

Therefore, $C(n, m)$ has exactly the range of the interactions. Moreover, using (17) and (18) and after a few calculations, one finds

$$C(n, n-1) = -\frac{\tanh(2K_{n-1})}{2\Delta_n^{1/2}}; \qquad C(n, n+1) = -\frac{\tanh(2K_n)}{2\Delta_{n+1}^{1/2}}$$

Hence $C(n, n+1) = C(n+1, n)$, i.e., $C(n, n+1)$ is symmetric under permutation of indices and negative or positive as $K_n > 0$ or $K_n < 0$, respectively. These findings generalize previous results of Percus.

NOTE ADDED

While these results were being prepared for publication a work by Borzi *et al.*[8] appeared containing the same finding as Eq. (23d).

ACKNOWLEDGMENT

This work was supported financially by the CAICYT (Spain) no. PB85-0024.

REFERENCES

1. M. Robert and B. Widom, *J. Stat. Phys.* **37**:419 (1984).
2. M. Robert and R. Viswanathan, *J. Chem. Phys.* **86**:4657 (1987).
3. J. K. Percus, *J. Stat. Phys.* **16**:299 (1977); *J. Math. Phys.* **23**:1162 (1982).
4. J. P. Allouche and M. Mendès-France, *J. Stat. Phys.* **42**:809 (1986).
5. M. Mendès-France, *J. Stat. Phys.* **45**:89 (1986).
6. B. Derrida, M. Mendès-France, and J. Peyrière, *J. Stat. Phys.* **45**:439 (1986).
7. G. Rauzy, *Propietés statistiques des suites arithmétiques* (Press Universitaires de France, 1976).
8. C. Borzi, G. Ord, and J. K. Percus, *J. Stat. Phys.* **46**:51 (1987).