Journal of Statistical Physics, Vol. 45, Nos. 1/2, 1986

The Ising Chain with Nonconstant External Field

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Received April 1, 1986; June 19, 1986

We give an exact computation of the Ising chain with nonconstant external field in terms of certain continued fractions. We then apply our general method to a specific example.

KEY WORDS: Ising chain; continued fractions.

1. INTRODUCTION

In a previous article, Allouche and Mendès France[1] discussed the Ising chain with variable interaction and constant external field. We now study the dual situation, namely constant interaction and varying external field. In contrast to previous authors,[3,4] we do not work with a randomly distributed external field. See, however, Ref. 7.

Let there be given N sites indexed by $q = 0, 1, \ldots, N-1$. The cyclic Ising chain is described through the Hamiltonian

$$\mathscr{H}(\mu) = -J \sum_{q=0}^{N-1} \mu_q \mu_{q+1} - \sum_{q=0}^{N-1} K_q \mu_q$$

where

$$\mu = (\mu_0, \mu_1, \ldots, \mu_{N-1}) \in \{-1. +1\}^N$$

and $\mu_N = \mu_0$, where $|J|$ measures the intensity of the interaction and where K_q is the effect of the external field on the qth site. We shall compute the partition function

$$Z_N = \sum_{\mu \in \{-1, +1\}^N} \exp[-\beta \mathscr{H}(\mu)], \qquad \beta = \frac{1}{kT}$$

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0022-4715/86/1000-0089$05.00/0

and the Helmholtz free energy ψ per spin

$$-\beta\psi(\beta)=\lim_{N\to\infty}\frac{1}{N}\log Z_N$$

in terms of continued fractions.

It will be necessary to express the external field K_q as a sum of two terms

$$K_q=\frac{1}{2}(H_{q-1}+H_q),\qquad q=0,1,\ldots,N-1 \tag{1}$$

At this point, both sequences (K_q) and (H_q) should be considered as infinite periodic sequences with period N; hence $K_{q+N}=K_q$ and $H_{q+N}=H_q$. If N is odd, the representation (1) yields

$$H_q=K_q-K_{q-1}+K_{q-2}-\cdots-K_{q+2}+K_{q+1}$$

If N is even, then it is necessary that

$$\sum_{q=0}^{N-1}(-1)^q K_q=0 \tag{2}$$

One can then solve Eqs. (1) and express H_q in terms of the K_p.

From now on, we shall assume that the Hamiltonian $\mathscr{H}(\mu)$ is expressed in terms of H_q:

$$\begin{aligned}\mathscr{H}(\mu)&=-J\sum_{q=0}^{N-1}\mu_q\mu_{q+1}-\frac{1}{2}\sum_{q=0}^{N-1}(H_{q-1}+H_q)\,\mu_q\\&=-J\sum_{q=0}^{N-1}\mu_q\mu_{q+1}-\frac{1}{2}\sum_{q=0}^{N-1}(\mu_q+\mu_{q+1})\,H_q\end{aligned}$$

2. CONTINUED FRACTIONS

Let λ be a real number. Consider the finite continued fraction

$$a+\cfrac{\lambda}{a_0+\cfrac{\lambda}{a_1+\cfrac{\lambda}{a_2+\cdots+\cfrac{\lambda}{a_{N-1}}}}}$$

which we denote for short

$$[a, a_0, a_1, \ldots, a_{N-1}]_\lambda$$

N is called the "depth" of the continued fraction. The symbol

$$((a_0, a_1, \ldots, a_{N-1}))_\lambda$$

represents the denominator of the continued fraction considered as a rational fraction with respect to the N variables $a_0, a_1, \ldots, a_{N-1}$, the term of highest degree being the product $a_0 a_1 \cdots a_{N-1}$. For example,

$$((\phi))_\lambda = 1$$

$$((a_0))_\lambda = a_0$$

$$((a_0, a_1))_\lambda = a_0 a_1 + \lambda$$

For $\lambda = 0$,

$$((a_0, a_1, \ldots, a_{N-1}))_0 = a_0 a_1 \cdots a_{N-1}$$

Two other special cases should be mentioned, $\lambda = +1$ and $\lambda = -1$. The first case corresponds to the usual (regular) continued fraction, in which case we delete the subscript $+1$. In the second case $\lambda = -1$ we write

$$[a, a_0, \ldots, a_{N-1}]_{-1} = \langle a, a_0, \ldots, a_{N-1} \rangle$$

The infinite continued fraction with $\lambda = -1$,

$$\langle a, a_0, a_1, a_2, \ldots \rangle$$

converges to a real number provided $a_q \geqslant 2$.

We can now state our first result, which is probably well known, but for which we could not find any reference.

Theorem. Given the external field $H_0, H_1, \ldots, H_{N-1}$, the partition function of the cyclic chain

$$Z_N = \sum_{\mu \in \{-1,+1\}^N} \exp \beta \left[J \sum_{q=0}^{N-1} \mu_q \mu_{q+1} + \frac{1}{2} \sum_{q=0}^{N-1} (H_{q-1} + H_q)\, \mu_q \right]$$

is equal to

$$((a_0, a_1, \ldots, a_{N-1}))_\lambda + \lambda((a_1, a_2, \ldots, a_{N-2}))_\lambda$$

where

$$\lambda = -2 \sinh 2\beta J$$

and

$$a_q = \exp \beta(J + H_q) + \exp \beta(J - H_{q+1})$$

Remark. $((a_q, a_{q+1}, \ldots, a_{q+N-1}))_\lambda + \lambda((a_{q+1}, \ldots, a_{q+N-2}))_\lambda$ does not depend on q, since the Ising chain is invariant by rotation.

Corollary. Let (a_n), $n \in Z$, be a periodic sequence with period N of real numbers larger than 2. Let

$$A_q = \langle a_q, a_{q+1}, a_{q+2}, \ldots \rangle$$

be the infinite periodic continued fraction. Then

$$\sum_{\mu \in \{-1,+1\}^N} \prod_{q=0}^{N-1} A_q^{(\mu_q + \mu_{q+1})/2} = \prod_{q=0}^{N-1} a_q$$

This last statement can be thought of as an application of physics to the theory of continued fractions. In our last section, we illustrate the converse situation by showing how the precise knowledge of a certain continued fraction expansion enables us to compute explicitly the Helmholtz free energy of the so called Kmošek–Shallit Ising chain.

3. PROOF OF THEOREM

To simplify the notations, put

$$\theta = \exp \beta J, \qquad h_q = \exp \beta H_q$$

It is then well known that the partition function Z_N is the trace of the matrix product

$$\prod_{q=0}^{N-1} \begin{pmatrix} \theta h_q & \theta^{-1} \\ \theta^{-1} & \theta h_q^{-1} \end{pmatrix}$$

Lemma. Let $\lambda = \theta^{-2} - \theta^2$. If $\lambda \neq 0$, then

$$\prod_{q=0}^{N-1} \begin{pmatrix} \theta h_q & \theta^{-1} \\ \theta^{-1} & \theta h_q^{-1} \end{pmatrix} = A \left[\prod_{q=0}^{N-1} \begin{pmatrix} \theta(h_q + h_{q+1}^{-1}) & 1 \\ \lambda & 0 \end{pmatrix} \right] A^{-1}$$

where

$$A = \begin{pmatrix} \lambda & 0 \\ \lambda\theta^2 h_0^{-1} & \lambda\theta \end{pmatrix}$$

In particular

$$\operatorname{Tr} \prod_{q=0}^{N-1} \begin{pmatrix} \theta h_q & \theta^{-1} \\ \theta^{-1} & \theta h_q^{-1} \end{pmatrix} = \operatorname{Tr} \prod_{q=0}^{N-1} \begin{pmatrix} \theta(h_q + h_{q+1}^{-1}) & 1 \\ \lambda & 0 \end{pmatrix}$$

Indeed, consider the matrices

$$P_q = \begin{pmatrix} 0 & 1 \\ \lambda\theta & -\theta^2 h_q \end{pmatrix}$$

$$U_q = \begin{pmatrix} \theta(h_q + h_q^{-1}) & 1 \\ \lambda & 0 \end{pmatrix}$$

We first note that

$$\begin{pmatrix} \theta h_q & \theta^{-1} \\ \theta^{-1} & \theta h_q^{-1} \end{pmatrix} = P_q U_q P_q^{-1}$$

Hence

$$\begin{aligned} &\prod_{q=0}^{N-1} \begin{pmatrix} \theta h_q & \theta^{-1} \\ \theta^{-1} & \theta h_q^{-1} \end{pmatrix} \\ &= \prod_{q=0}^{N-1} P_q U_q P_q^{-1} \\ &= P_0 U_0 \left(\prod_{q=0}^{N-1} P_q^{-1} P_{q+1} U_{q+1} \right) (P_N U_N)^{-1} \end{aligned}$$

The proof of the lemma is then completed by observing that

$$P_q^{-1} P_{q+1} U_{q+1} = \begin{pmatrix} \theta(h_q + h_{q+1}^{-1}) & 1 \\ \lambda & 0 \end{pmatrix}$$

and

$$P_0 U_0 = P_N U_N = \begin{pmatrix} \lambda & 0 \\ \lambda\theta^2 h_0^{-1} & \lambda\theta \end{pmatrix}$$

We are now led to compute the trace of matrix products of the form

$$\prod_{q=0}^{N-1} \begin{pmatrix} a_q & 1 \\ \lambda & 0 \end{pmatrix}$$

Lemma 2:

$$\prod_{q=0}^{N-1} \begin{pmatrix} a_q & 1 \\ \lambda & 0 \end{pmatrix} = \begin{pmatrix} A_N & B_N \\ C_N & D_N \end{pmatrix}$$

where

$$A_N = ((a_0, a_1, \ldots, a_{N-1}))_\lambda$$
$$B_N = ((a_0, a_1, \ldots, a_{N-2}))_\lambda$$
$$C_N = \lambda((a_1, a_2, \ldots, a_{N-1}))_\lambda$$
$$D_N = \lambda((a_1, a_2, \ldots, a_{N-2}))_\lambda$$

The result is classical and is easily established by induction on N. As a consequence, we get the following lemma.

Lemma 3:

$$\mathrm{Tr} \prod_{q=0}^{N-1} \begin{pmatrix} a_q & 1 \\ \lambda & 0 \end{pmatrix} = ((a_0, \ldots, a_{N-1}))_\lambda + \lambda((a_1, \ldots, a_{N-2}))_\lambda$$

We now relate h_q to a_q:

$$a_q = \theta(h_q + h_{q+1}^{-1})$$

Hence

$$a_q = \exp \beta(J + H_q) + \exp \beta(J - H_{q+1})$$

Finally

$$\lambda = \theta^{-2} - \theta^2 = \exp(-2\beta J) - \exp(2\beta J)$$
$$= -2 \sinh(2\beta J)$$

Theorem 1 is then established for $\lambda \neq 0$. The case $\lambda = 0$ is obtained by continuity.

4. PROOF OF THE COROLLARY

In Theorem 1 choose $J = 0$. Then λ vanishes and we obtain the equality

$$\sum_{\mu \in \{-1,+1\}^N} \exp \beta \sum_{q=0}^{N-1} \frac{1}{2} H_q(\mu_q + \mu_{q+1})$$
$$= \prod_{q=0}^{N-1} [\exp(\beta H_q) + \exp(-\beta H_{q+1})]$$

Define

$$a_q = \exp(\beta H_q) + \exp(-\beta H_{q+1})$$

Then

$$\exp \beta H_q = a_q - \frac{1}{\exp \beta H_{q+1}} = a_q - \frac{1}{a_{q+1} - \ddots} = A_q$$

Hence

$$\sum_{\mu \in \{-1,+1\}^N} \prod_{q=0}^{N-1} A_q^{(\mu_q + \mu_{q+1})/2} = \prod_{q=0}^{N-1} a_q$$

5. THE KMOŠEK–SHALLIT ISING CHAIN

Let $g > 0$ be a real number. Kmošek[5] and Shallit[6] have discovered independently the continued fraction expansion of the number

$$F_n = \sum_{j=0}^{n} \frac{1}{g^{2^j}} = \frac{A_n}{g^{2^n}}$$

Let us describe their construction (see also Ref. 2). Consider the map Λ defined on the set of finite strings of real numbers

$$\Lambda(a_1,..., a_m) = a_1,..., a_{m-1}, a_m + 1, a_m - 1, a_{m-1},..., a_1$$

We denote its iterates by Λ^2, Λ^3,..., For example,

$$\Lambda(g-1, g+1) = g-1, g+2, g, g-1$$

$$\Lambda^2(g-1, g+1) = g-1, g+2, g, g, g-2, g, g+2, g-1$$

Kmošek and Shallit observed that the continued fraction expansion of F_n was generated by

$$F_n = [0, \Lambda^{n-1}(g-1, g+1)], \qquad n > 2$$

Strictly speaking, this expansion is a regular continued fraction if and only if $g > 2$. For reasons that will become clear later, we shall assume

$$g > 2 + [2(\sqrt{5} - 1)]^{1/2}$$

The depth of the expansion of F_n is $N = 2^n$. The partial quotients $a_0, a_1,..., a_{N-1}$ are bounded independently of N, since they are equal to one of the four positive numbers $g-2$, $g-1$, g, $g+2$.

We now turn to the Ising chain, where we fix the temperature

$$kT = \frac{2J}{\log[(\sqrt{5} - 1)/2]}$$

Since the temperature is assumed to be positive, the coupling constant J is necessarily negative.

Our model is thus antiferromagnetic. We now fix the external field by choosing

$$\beta H_q = -\log\langle b_{q-1}, b_{q-2},\dots, b_0, b_{N-1}, b_{N-2},\dots\rangle$$

where

$$b_q = a_q[(\sqrt{5}+1)/2]^{1/2}$$

and where a_q is the qth partial quotient of the regular continued fraction expansion of F_n. Notice that the periodic continued fraction

$$\langle b_{q-1}, b_{q-2},\dots, b_0, b_{N-1},\dots\rangle$$

converges, since by our choice of g,

$$b_q \geqslant (g-2)[(\sqrt{5}+1)/2]^{1/2} > 2$$

An Ising chain with this special distribution will be called the Kmošek–Shallit Ising chain. Its partition function is

$$\begin{aligned} Z_n &= ((a_0, a_1,\dots, a_{N-1})) + ((a_1,\dots, a_{N-2})) \\ &= g^{2^n} + z \end{aligned}$$

where $0 < z < g^{2^n}$. The Helmholtz free energy ψ of a large Kmošek–Shallit Ising chain is thus given by

$$-\beta\psi(\beta) = \lim_{n\to\infty} \frac{1}{2^n} \log g^{2^n} = \log g$$

We have thus established the following result.

Theorem 2. The Helmholtz free energy ψ of the antiferromagnetic Kmošek–Shallit Ising chain at temperature

$$kT = \frac{2J}{\log[(\sqrt{5}-1)/2]}$$

is

$$\psi = -\frac{2J}{\log[(\sqrt{5}-1)/2]} \log g$$

Similar results can easily be obtained from the continued fraction expansion of

$$\sum_{j=0}^{n} \pm g^{-2^j}$$

by considering the two maps Λ_+ and Λ_-:

$$\Lambda_\varepsilon(a_1,..., a_m) = a_1,..., a_{m-1}, a_m + \varepsilon, a_m - \varepsilon, a_{m-1},..., a_1$$

Many other explicit examples can be treated by our method, including the simplest of all, namely when the external field is constant. We leave this as an exercise for the reader.

ACKNOWLEDGMENT

J. P. Allouche, F. Axel, M. Kleman, J. Peyriere, and I ("the gang of five") have been meeting regularly once a month since October 1984. Our seminars take place either in Orsay or Paris and are devoted to one-dimensional physics. This article is greatly influenced by our meetings. J. P. Allouche and I studied more specifically the Ising chain. We coauthored two papers (the last of which is Ref. 1) and discussed some general ideas which were at the origin of the present article. I submitted a first draft of the paper to B. Derrida, who showed me how to improve my results. I express my warmest thanks to these five friends.

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