

One-dimensional Ising model in an incommensurate field

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For the one-dimensional Ising model with a special incommensurate field, the ground-state magnetization as function of the field exhibits a staircase with an infinite number of almost exponentially decreasing steps. With increasing temperature, the steps get smoother and disappear successively. The specific heat resembles that of the Ising model with a constant field.

I. INTRODUCTION

In the last few years one-dimensional incommensurate systems have been studied intensively by several authors. For earlier references we refer to the review by Bak.¹

One of the most striking features of the investigated systems seems to be the existence of a devil's staircase. The first explicit expression for a complete devil's staircase was given by Aubry² for the Frenkel-Kontorova (FK) model with piecewise parabola potential. Recently, Bak and Bruinsma³ have proven rigorously that the ground-state magnetization as a function of the external field for a one-dimensional Ising model with long-range antiferromagnetic interactions exhibits a complete devil's staircase too. The equivalence of both models has been shown by Aubry.⁴

With this equivalence, the low-energy excitations of the FK model with parabola potential can be described, as shown by Aubry *et al.*,⁵ by a one-dimensional Ising model with long-range antiferromagnetic interactions and an *incommensurate* field. The low-temperature specific heat which was deduced from that (Ref. 5) for an incommensurability ratio equal to $\phi = (\sqrt{5}-1)/2$, the inverse of the golden mean, exhibits as a function of the temperature an infinite number of peaks. These were interpreted as transition points (not real phase transitions) between commensurate phases related to the continued fraction expansion of ϕ . This anomalous low-temperature behavior was already found before by Pietronero and Strässler.⁶

Two questions may arise now for one-dimensional incommensurate systems.

- (i) How generic is the existence of a devil's staircase?
- (ii) How generic is the anomalous behavior of the specific heat at low temperatures?

The following incommensurate Ising model leads to exact answers:

$$H = \sum_{i=1}^N (J\sigma_i\sigma_{i+1} - h_i\sigma_i), \quad \sigma_{N+1} = \sigma_1 \quad (1)$$

where $\sigma_i = \pm 1$, N represents the number of sites, and the magnetic field h_i at the site i is given by

$$h_i(\alpha) = h(i\phi + \alpha) \quad (2a)$$

with $h(t)$ being a periodic (period equal to 1) piecewise constant function:

$$h(t) = \begin{cases} a_0, & -\phi < t \leq -\phi^3 \\ a_1, & -\phi^3 < t \leq \phi^2 \end{cases} \quad (2b)$$

$$h(t+1) = h(t), \quad \phi = (\sqrt{5}-1)/2$$

with a_0 and a_1 representing constants. The phase α in Eq. (2a) ($0 \leq \alpha < 1$) can be chosen arbitrarily for the incommensurate case. We take $\alpha=0$. Studying the incommensurate Ising model may also be motivated by extending recent work by Derrida *et al.*,^{7,8} Williams,⁹ Doman and Williams,¹⁰ Bruinsma and Aeppli,¹¹ and Aeppli and Bruinsma¹² for the Ising model with a random field.

II. FINITE TEMPERATURE

We calculate the partition function for (1):

$$Z(\beta, N) = \text{tr} \left[\prod_{i=1}^N \underline{T}(i\phi) \right], \quad \beta = (k_B T)^{-1} \quad (3)$$

with the use of the transfer matrix

$$\underline{T}(t) = \begin{bmatrix} \exp\{-[K-H(t)]\} & \exp[K+H(t)] \\ \exp[K-H(t)] & \exp\{-[K+H(t)]\} \end{bmatrix}, \quad (4)$$

$$K = \beta J, \quad H(t) \equiv \beta h(t)$$

which is related to the one-dimensional Schrödinger equation with incommensurate potential, given by (2). This was recently studied independently by Kohmoto *et al.*¹³ and Ostlund *et al.*¹⁴ From Eq. (4), it follows that $\det \underline{T}(t)$ is independent of t . We define

$$\underline{M}^{(k)} = (\det \underline{T})^{-k/2} \prod_{i=1}^k \underline{T}(i\phi), \quad (5)$$

for which $\det \underline{M}^{(k)} = 1$. From this, it follows that $\underline{M}^{(k)}$ can be obtained recursively:

$$\underline{M}^{(k_1+k_2)}(t) = \underline{M}^{(k_1)}(t+k_2\phi) \underline{M}^{(k_2)}(t), \quad (6)$$

with $\underline{M}^{(1)}(t) = \underline{M}(t)$ and where $\underline{M}(t) = (\det \underline{T})^{-1/2} \underline{T}(t)$. Then, Eq. (2) implies

$$\underline{M}(t) = \begin{cases} \underline{M}_0, & -\phi < t \leq -\phi^3 \\ \underline{M}_1, & -\phi^3 < t \leq \phi^2 \end{cases}$$

where the matrix elements of \underline{M}_0 and \underline{M}_1 are constant.

Thus, for arbitrary t , $\underline{M}(t)$ is equal either to \underline{M}_0 or to \underline{M}_1 , which is a result quite similar to that of Ref. 13.

Therefore it follows from Ref. 13, that the recursion relation (6) for k_1 and k_2 , restricted to the Fibonacci numbers F_l , becomes

$$\underline{M}_{l+1} = \underline{M}_{l-1} \underline{M}_l, \quad l \geq 1 \quad (7)$$

where

$$\underline{M}_l = \underline{M}^{(F_l)} \quad (t=0),$$

$$\underline{M}_0 = \underline{M}(-\phi^3), \quad \underline{M}_1 = \underline{M}(0)$$

and F_l are defined by

$$F_{l+1} = F_l + F_{l-1}, \quad l \geq 1, \quad \text{with } F_0 = 1 \text{ and } F_1 = 1. \quad (8)$$

Using (7), it is easy to prove that the following identity (Ref. 13):

$$\underline{M}_{l+1} + \underline{M}_{l-2}^{-1} \equiv \underline{M}_{l-1} \underline{M}_l + \underline{M}_{l-1} \underline{M}_l^{-1} \quad (9)$$

is true.

Let $X_l = \text{tr} \underline{M}_l$ (notice that we have omitted the factor $\frac{1}{2}$, compared to Ref. 13), then taking the trace of Eq. (9) we obtain

$$X_{l+1} = X_l X_{l-1} - X_{l-2}, \quad (10)$$

where we have used $\text{tr} \underline{M}_l = \text{tr}(\underline{M}_l^{-1})$ and $\underline{M}_l + \underline{M}_l^{-1} = (\text{tr} \underline{M}_l) \underline{1}$ ($\underline{1}$ is the unit matrix) which holds for 2×2 real matrices with a determinant equal to 1. Taking the trace of Eq. (5) and $k = F_l$ we obtain for the partition function $Z_l = Z(\beta, N = F_l)$:

$$\begin{aligned} Z_l(\beta, K, H_0, H_1) &\equiv \text{tr} \left[\prod_{i=1}^{F_l} \underline{T}(i\phi) \right] \\ &= (\det \underline{T})^{F_l/2} \text{tr} \underline{M}_l \\ &= (\det \underline{T})^{F_l/2} X_l. \end{aligned} \quad (11)$$

$\det T$ follows from Eq. (4). Then, substituting X_l from Eq. (11) into Eq. (10) and using (8) we find

$$\begin{aligned} Z_{l+1} &= Z_l Z_{l-1} - [2 \sinh(2K)]^{F_l-1} Z_{l-2}, \quad l \geq 1 \\ Z_{-1} &= 2 \cosh(H_0 - H_1), \\ Z_i &= 2 \exp(-2K) \cosh H_i, \quad H_i = \beta a_i, \quad i=0,1. \end{aligned} \quad (12)$$

The asymptotic behavior of Z_l , for $l \rightarrow \infty$, is

$$Z_l \rightarrow \exp(-\beta f F_l), \quad (13)$$

where $f(\beta, K, H_0, H_1)$ is the free energy per spin.

We have not succeeded in deriving an analytical expression for f but Eq. (12) can easily be iterated on a computer. Performing only $l=30$ iterations, the partition function for $N = F_{30} \cong 1.3 \times 10^6$ spins is obtained for given K , H_0 , and H_1 . To our knowledge there is no other example apart from the exactly solvable models where this can be done with such little effort.

Because of Eq. (13) we have iterated $\ln Z_l$. This was performed for $H_0 = -H_1 = H$. $F_l^{-1} \ln Z_l$ converges rapid-

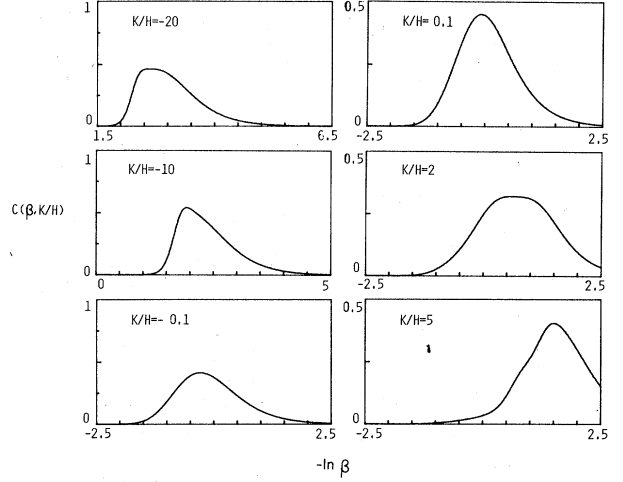


FIG. 1. Specific heat (in units of k_B) as a function of $\ln \beta$ (β in units of J^{-1}) for different K/H and $l=30$.

ly such that for $l=30$, $F_l^{-1} \ln Z_l \cong f$. From this, one easily obtains the specific heat per spin:

$$c(\beta, K, H) = -k_B \beta^2 \frac{\partial^2}{\partial \beta^2} [\beta f(\beta, K, H)] \quad (14)$$

and the magnetization (per spin) with respect to the local field direction:

$$\begin{aligned} m'(\beta, K, H) &= \lim_{l \rightarrow \infty} F_l^{-1} \sum_{i=1}^{F_l} \langle \sigma_i \rangle \text{sgn} h_i \\ &= -\frac{\partial}{\partial H} [\beta f(\beta, K, H)], \end{aligned} \quad (15)$$

which are represented in Figs. 1 and 2. Whereas the specific heat resembles that for the Ising model in a constant field, the "magnetization" exhibits a peculiar behavior which can be understood by the exact results for the ground state, which will be discussed now.

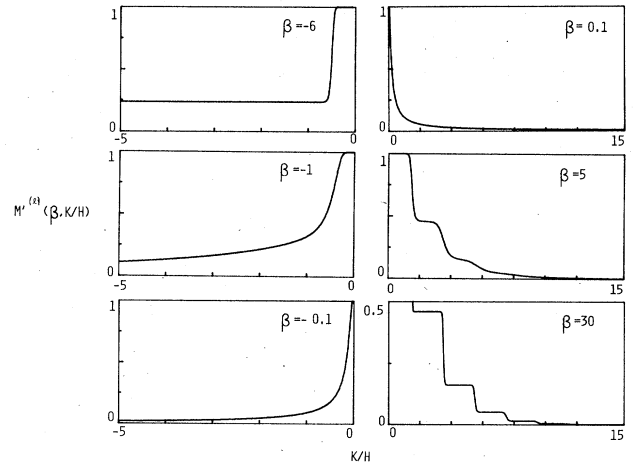


FIG. 2. Magnetization as function of K/H for different temperatures and $l=30$.

III. GROUND STATE

For this purpose, some properties of the sequence

$$\{\epsilon_i(0)\}_l = \{\text{sgn}h_i(0) \mid 1 \leq i \leq F_l\}$$

will be crucial. Because of the periodic boundary conditions [we have chosen in (1)], two sequences $\{h_i\}$ and $\{h'_i = h_{i+n}\}$ ($h_{N+1} = h_1$, n is an arbitrary integer) are physically equivalent. It is easy to prove that in that sense $\{\epsilon_i(\alpha)\}_l$ and $\{\epsilon_i(0)\}_l$ are equivalent for arbitrary phases α .

For convenience, we choose $\alpha = 2\phi - 1 = \phi^3$. The sequence $s_l = \{\epsilon_i(\phi^3)\}_l$ has the following property.

$$s_l = \{\epsilon_i(\phi^3)\}_{1 \leq i \leq F_l} = \{\epsilon_i(\phi^3)\}_{1 \leq i \leq F_{l-1}} \cup \{\epsilon_{F_{l-1}+i}(\phi^3)\}_{1 \leq i \leq F_{l-2}} = s_{l-1} \cup \{\text{sgn}h(F_{l-1}\phi + i\phi + \phi^3)\}_{1 \leq i \leq F_{l-2}}. \quad (17)$$

Using a further property of ϕ (Ref. 15),

$$F_l\phi - F_{l-1} = (-1)^l \phi^{l+1}, \quad (18)$$

one can easily prove that

$$\text{sgn}h(F_{l-1}\phi + i\phi + \phi^3) = \text{sgn}h(i\phi + \phi^3) \quad (19)$$

for $1 \leq i \leq F_{l-2}$ and $l \geq 5$. Then, we obtain, from (17),

$$\begin{aligned} s_l &= s_{l-1} \cup \{\text{sgn}h(i\phi + \phi^3)\}_{1 \leq i \leq F_{l-2}} \\ &= s_{l-1} \cup s_{l-2} \quad \text{for } l \geq 5, \end{aligned}$$

which was what we set out to prove.

(P1) implies the following properties.

(P2) In s_l the plus signs are always isolated, the minus signs are either isolated or appear in pair and the largest subsequence of s_l ($l \geq 4$) with alternating signs is s_4 .

(P3) The number of minus and plus signs in s_l is equal to F_{l-1} and F_{l-2} , respectively.

(P3) follows from (P1) and Eq. (8) by induction.

$$\cdots (-+-)(-++-)(-+-+)(-+-)(-+-+)(-+-) \cdots \quad (22)$$

which we represent as

$$\cdots F_3 F_4 F_4 F_3 F_4 \cdots, \quad (23)$$

because there are only blocks of F_3 and F_4 alternating spins. For $J < 0$ the modulated ground state (22) becomes unstable if

$$2J + a = 0$$

(we have chosen $a_0 = -a_1 = a$) because then the energy to flip the isolated up spins [because of (P2)] vanishes. Thus for the ferromagnetic case there is a transition at

$$K/H = -0.5$$

from the modulated state (22) with $m_0^{(l)} = 1$ to the ferromagnetic state with all spins down and $m^{(l)} = (F_{l-1} - F_{l-2})/F_l$ [where (P3) is used]. $m^{(l)} \rightarrow \phi^3$ for $l \rightarrow \infty$.

The antiferromagnetic case is much more interesting. Because the F_3 and F_4 blocks in (22) (displaced by

(P1) s_l is the union of s_{l-1} and s_{l-2} :

$$s_l = s_{l-1} \cup s_{l-2}, \quad l \geq 5 \quad (16)$$

with

$$s_3 = - + - ,$$

$$s_4 = - + - + - .$$

For simplicity we omit the union symbol in the explicit representation of s_l by plus and minus signs, as for s_3 and s_4 given above. We only sketch the proof of (P1), which is analogous to that of Eq. (7). Using Eq. (2) with $\alpha = \phi^3$ and Eq. (8), we obtain

Using Eq. (16) ($n-1$) times, s_l can be composed as the union of only s_{l-n+1} and s_{l-n} :

$$s_l = s_{l-n+1} \cup s_{l-n} \cup \cdots \cup s_{l-n+1}, \quad (20)$$

with $2 \leq n \leq l-3$. Representing s_{l-n+1} by a minus sign and s_{l-n} by a plus sign in Eq. (20) the obtained sequence $s_l^{(n)}$ has the following property.

(P4) $s_l^{(n)}$ is equivalent to s_n .

This again is easily proven by induction. These properties are related to the "irrational decimation" discussed by Feigenbaum and Hasslacher.¹⁶

Now let us investigate the ground-state problem of (1) for $N = F_l$. We take the phase $\alpha = \phi^3$ without restricting generality.

For $K/H = 0$, the ground-state spin configuration is

$$\sigma_i^{(0)} = \text{sgn}h_i(\phi^3). \quad (21)$$

From (P1) it follows that this has the form

(parentheses) are antiferromagnetic, they already have minimum energy. But the bonds between two adjacent blocks are frustrated. Decreasing the magnetic field, the modulated ground state becomes unstable at a critical value $(K/H)_1$ where flipping the F_3 blocks does not cost energy. Representing in (22) the F_3 block by plus signs and the F_4 blocks by minus signs, one obtains a sequence which is equivalent to s_{l-3} , because of (P4). Therefore the sequence (23) consists of only two types of "alternating" blocks [(P2)]:

$$(F_4 F_3 F_4)$$

and

$$(F_4 F_3 F_4 F_3 F_4).$$

Therefore, when the F_3 blocks flip a new ground state with only two types of antiferromagnetic blocks is obtained. These blocks consist of

$$2F_4 + F_3 = F_6$$

and

$$3F_4 + 2F_3 = F_7$$

spins and are called the F_6 and F_7 blocks, respectively. Thus, the new ground state is represented as

$$\cdots F_6 F_7 F_6 F_7 F_6 \cdots \quad (24)$$

At $(K/H)_2$, the F_6 blocks become unstable, forming larger antiferromagnetic blocks. This procedure continues until the ground state is built up of antiferromagnetic F_{3n} and F_{3n+1} blocks:

$$\cdots F_{3n} F_{3n+1} F_{3n} F_{3n+1} F_{3n} \cdots \quad (25)$$

Representing in (25) F_{3n} and F_{3n+1} by plus and minus signs, respectively, the obtained sequence is equivalent to s_{l-3n} [because of (P4)]. Therefore (25) consists of only two types of "alternating" blocks [because of (P2)]:

$$(F_{3n+1} F_{3n} F_{3n+1})$$

and

$$(F_{3n+1} F_{3n} F_{3n+1} F_{3n} F_{3n+1})$$

Thus at $(K/H)_n$ the F_{3n} blocks flip forming two types of antiferromagnetic blocks with

$$2F_{3n+1} + F_{3n} = F_{3(n+1)}$$

and

$$3F_{3n+1} + 2F_{3n} = F_{3(n+1)+1}$$

spins and are called the $F_{3(n+1)}$ and $F_{3(n+1)+1}$ blocks. $(K/H)_n$ is determined by the condition that the energy to flip an F_{3n} block just vanishes. This happens if

$$-2J + (x_n a) = 0, \quad (26)$$

where $(x_n a)$ is the field energy of an F_{3n} block. (We would like to remind the reader that we have chosen $a_0 = -a_1 = a$.) With $(y_n a)$, the field energy of the F_{3n+1} block, we obtain the recursion relations:

$$x_{n+1} = 2y_n - x_n, \quad n \geq 1$$

$$y_{n+1} = 3y_n - 2x_n, \quad n \geq 1$$

$$x_1 = 3, \quad y_1 = 5$$

from which one finds easily

$$x_n = 4n - 1, \quad n \geq 1. \quad (27)$$

Equations (26) and (27) yield finally,

$$(K/H)_n = 2n - \frac{1}{2}, \quad n \geq 1. \quad (28)$$

The ground-state magnetization $m_n^{(l)}$ for $(K/H)_n < K/H < (K/H)_{n+1}$ is just $m_{n-1}^{(l)}$ reduced by twice the magnetization of an F_{3n} block, which equals $2x_n$, times F_{l-2-3n}/F_l , the numbers of F_{3n} blocks per spin:

$$m_n^{(l)} = m_{n-1}^{(l)} - 2(4n-1)F_{l-2-3n}/F_l \quad (29)$$

for $1 \leq n \leq [(l-2)/3]$ ($[x]$ is the integer part of x). If we

use (see Ref. 15)

$$F_{l-2-3n} = (-1)^n F_{3n} F_l + (-1)^{n+1} F_{3n+1} F_{l-1}$$

and

$$\lim_{l \rightarrow \infty} F_{l-1}/F_l = \phi$$

we obtain for the infinite system from (29),

$$m_n^{(\infty)} = (1 + 4n\phi^3)\phi^{3n}, \quad n \geq 1. \quad (30)$$

IV. RESULTS AND DISCUSSION

For a special incommensurate external field the partition function can be determined recursively. Performing only $l=30$ iteration steps on a computer, we obtained the specific heat and the magnetization for a system with $N \cong 1.3 \times 10^6$ spins.

The specific heat as a function of temperature does not exhibit a number of peaks but resembles the behavior of the Ising model in a constant field. The flat region occurring for $K/H \approx 2$ and $K/H \approx -20$ may be related to the existence of two typical energy gaps in the excitation spectrum leading each to a Schottky anomaly such that superimposing both may result in such a flat behavior.

Whereas the ground-state magnetization as a function of K/H has only one transition point (no real phase transition) for $J < 0$ it exhibits for $J > 0$ and for the infinite system an ordinary staircase, i.e., first-order transitions with an infinite number of decreasing steps, according to (28) and (30). Thus, there is *no* devil's staircase. This result is quite similar to that obtained by Williams⁹ for the random-bond Ising model, but there $m_n^{(\infty)} \sim 1/n$ for $n \rightarrow \infty$ which is different from (30).

For the commensurate case, replacing ϕ by F_{l-1}/F_l only $[(l-2)/3]$ steps appear and the ground state is periodic with period F_l . This is quite similar to the Frenkel-Kontorova model.¹⁷ We would like to mention that a similar behavior has been found by Nadal *et al.*¹⁸ for $h(t) = h \cos(2\pi\phi t)$.

For increasing temperature the steps become smoother and disappear one after the other, first the smaller and finally the largest ones (Fig. 2). The "transition" points are still given by (28) for $i=1, 2, \dots, n_0$, where n_0 depends on the temperature and the "magnetization" is well approximated by (30) for not too high temperatures. The same smoothening of the steps was found by Doman and Williams¹⁰ for the random-bond Ising model.

Thus the magnetization for the incommensurate Ising model with nearest-neighbor interactions differs qualitatively from the Ising model with long-range interactions studied in Ref. 3 or equivalently the Frenkel-Kontorova model in Refs. 2 and 5, but resembles that for the random-bond Ising model studied in Refs. 9 and 10.

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