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LETTER TO THE EDITOR

Residual entropy of the square Ising antiferromagnet in the maximum critical field: the Fibonacci matrix

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Abstract. We find the analytical expression for the residual entropy of the square Ising model with nearest-neighbour antiferromagnetic coupling J, in the maximum critical field $H_c = 4J$, in terms of the Fibonacci matrix, which itself represents a self-similar, fractal object. The result coincides with the existing numerical data. By considering regular self-similar fractal objects rather than seemingly random transfer matrices, this approach opens the possibility of finding the corresponding solutions in more complicated cases, such as the antiferromagnets with longer than nearest-neighbour interactions and the three-dimensional antiferromagnets, as well as the possibility of unification of results pertinent to different lattices in two and three dimensions.

The ground-state degeneracy of highly frustrated systems has attracted considerable attention over the past decades. Almost half a century ago, in 1951, Brooks and Domb [1] estimated that the entropy per spin of an Ising system on the square lattice with antiferromagnetic nearest-neighbour (NN) interaction J, in the maximum critical field $H_c = 4J$, retains at the absolute zero temperature over 50% of its maximum value $\ln 2$. Although the numerical value for the residual entropy has subsequently been established with high precision [2, 3], the problem has to date defied exact solution. In contrast, the problem of the residual entropy of an Ising antiferromagnet on the triangular lattice was analytically solved by Wannier [4] in 1950 for the zero-field case, and by Baxter and Tsang [5, 6] in 1980 in the case of maximum critical field $H_c = 6J$. The solutions to more complicated problems, such as the antiferromagnets with longer then nearest-neighbour interactions and the three-dimensional antiferromagnets, have not yet been reported in the literature.

In this letter we revisit the problem of the square lattice residual entropy in the maximum critical field, from an analytical viewpoint. We show that the Fibonacci matrix¶ of order n represents the transfer matrix relating the possible ground states of an $n \times m$ system with those of an $n \times (m + 1)$ system. The residual entropy can thus be represented in terms of the leading eigenvalue of the infinite Fibonacci matrix, which is itself a self-similar object composed of blocks of 0's and 1's appearing on all scales, with the fractal

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¶ The Fibonacci matrix is available as a function in the 'linalg' package of the Maple V algebraic manipulation software.

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dimension $d = \ln(1+\sqrt{2})/\ln[(1+\sqrt{5})/2] = 1.8316$. Alternatively, the residual entropy of an $n \times m$ system is represented in terms of any entry of the mth power of the nth-order Fibonacci matrix, where different entries correspond to different boundary conditions. In order to test the validity of the present approach we first use a simple assumption to analytically establish the residual entropy in the thermodynamic limit to within 2% of the known numerical value. Then we perform the numerical analysis of the leading eigenvalues of the first nine Fibonacci matrices, which yields the result with nine digit precision using Maple V algebraic manipulation software with minimum computational effort.

The transfer matrix approach has already been employed in the problem of finding the residual entropy of the square Ising antiferromagnet in the maximum critical field by Metcalf and Yang [2] in 1978. They performed an extensive numerical transfer matrix study of finite systems with up to 9×15 spins, finding $\sigma = 0.4075$. It was subsequently shown [3] that finite-size scaling can be used in conjunction with the numerical transfer matrix approach to obtain a much higher precision result ($\sigma = 0.407\,495\,101\,260\,68$) on a personal computer. In what follows, we modify the numerical transfer matrix approach of Metcalf and Yang [2], to show that the transfer matrix itself is the Fibonacci matrix.

We consider the square lattice Ising model with the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle nn \rangle} S_i S_j - H_c \sum_i S_i \tag{1}$$

where $J < 0$ is the antiferromagnetic nearest-neighbour interaction parameter, $S_i = \pm 1$ is the Ising spin variable at the site i, $H_c = 4|J|$ is the external magnetic field that exactly compensates the energy increase produced by a single upward spin flip, and $\langle nn \rangle$ denotes summation over the nearest-neighbour pairs. The ground state of Hamiltonian (1) is highly degenerate, it corresponds to the Neel spin configuration, as well as to all the configurations obtained therefrom by flipping upward (in the direction of the field) an arbitrary number of non-neighbouring downward-oriented spins. Another way of expressing this condition is to say that a certain spin configuration corresponds to the ground state if it does not contain any pairs of downward-oriented neighbouring spins. This statement is strictly true only in the case of periodic boundary conditions (torus), while in the case of open boundaries it is true only for the interior spins, the boundary spins being aligned with the field. For the moment we will assume that boundary conditions are irrelevant, and we will consider all such configurations for arbitrary system size.

If we denote by $\mathcal{D}_{nm}$ the ground-state degeneracy of an $n \times m$ system, the residual entropy (the configurational zero-temperature entropy) is given by

$$\sigma = \lim_{n,m\to\infty} \frac{\ln \mathcal{D}_{nm}}{nm}. \tag{2}$$

To determine the ground-state degeneracies $\mathcal{D}_{nm}$ for arbitrary n and m, let us begin by considering the special case $m = 1$, that is, the linear chain. Possible spin configurations satisfying the condition of not having any pairs of downward-oriented neighbouring spins are shown in table 1 for $n = 1, 2, \ldots, 6$, where upward-oriented spins are depicted as 1's, and downward-oriented spins as 0's. Each column (corresponding to a given chain length n) is divided into the upper set (ending with 1's), and the lower set (ending with 0's). The upper set of any given column is obtained by rewriting the whole previous column and adding 1's at the and, while the lower set is obtained by adding 0's to the upper set of the previous column. This procedure ensures both that two neighbouring 0's will never be encountered in the spin configurations for arbitrary n, and that all such sequences are generated. It is also easily seen that the length of any given column (number of spin

Table 1. Possible configurations of a chain of length n satisfying the condition of not containing any downward oriented neighbouring spin pairs. Here, 1's and 0's are used to represent the $+1$ and -1 spins, respectively. The horizontal bars divide each column into the upper and the lower sets, ending with 1's and 0's, respectively (see the text for details on construction of the table).

$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$
1	11	111	1111	11111	111111
0	01	011	0111	01111	011111
	10	101	1011	10111	101111
		110	1101	11011	110111
		010	0101	01011	010111
			1110	11101	111011
			0110	01101	011011
			1010	10101	101011
				11110	111101
				01110	011101
				10110	101101
				11010	110101
				01010	010101
					111110
					011110
					101110
					110110
					010110
					111010
					011010
					101010

configurations) is equal to the sum of the lengths of the two previous columns, and is thus given by Fibonacci numbers f_n†.

Let us now consider adding a new chain in the configuration γ' to an $n \times m$ system ending with a chain in configuration γ. Both γ and γ' belong to the set of f_n valid chain configurations (depicted in table 1 for $n = 1, 2, \ldots, 6$). The new spin configuration will be 'valid' (in the sense of not having two neighbouring downward spins) if γ and γ' are 'compatible' (also in the sense of not having two neighbouring downward spins). The transfer matrix (or 'compatibility' matrix) F_n can thus be defined [2], such that $F_n(\gamma, \gamma') = 1$ if γ and γ' are compatible, and $F_n(\gamma, \gamma') = 0$ otherwise. Considering the fact that all the f_{n-1} 'upper' spin configurations end with 1's and all the f_{n-2} 'lower' spin configurations end with 0's, and utilizing the structure of columns in table 1, we will now demonstrate that the transfer matrix F_n has the block form

$$F_n = \begin{pmatrix} F_{n-1} & G_{n-1} \\ G_{n-1}^{\mathrm{T}} & 0 \end{pmatrix} \tag{3}$$

where G_{n-1} represents an $f_{n-1} \times f_{n-2}$ submatrix of F_{n-1}. More to the point, the block F_{n-1} in the upper left corner comes from the fact that compatibility of the configurations in the upper set is not affected by the trailing 1's, and the $f_{n-2} \times f_{n-2}$ zero matrix in the

† The usual definition of the Fibonacci sequence is $f_{n+2} = f_{n+1} + f_n$ with $f_0 = 0$ and $f_1 = 1$, so that the actual sequence is 0, 1, 1, 2, 3, 5, 8, 13, 21, ... Since the first number encountered in the chain ground-state degeneracies is 2 (associated with the chain size of $n = 1$), we modify this definition by mapping $n + 2 \to n$, so that $f_1 = 2$, $f_2 = 3$ etc. A similar definition is employed by mapping $n + 1 \to n$ in the case of associated Pell numbers, so that $q_{n+2} = 2q_{n+1} + q_n$ with $q_0 = 1$ and $q_1 = 3$.

lower right corner comes from the fact that the configurations in the lower set are always incompatible to each other because of the trailing 0's. The G_{n-1} matrix represents the compatibility matrix of configurations from the upper set with those from the lower set. The trailing 1's are compatible with the trailing 0's, and apart from the trailing spins the lower set is identical to the (upper) subset of the upper configuration set. For $n = 1$ we have

$$F_1 = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \tag{4}$$

and the higher n matrices are obtained through recursive relation (3). Equations (3) and (4) represent the definition of the Fibonacci matrices, and the first five are shown in table 2. The Fibonacci matrices themselves represent fractal objects, where in the thermodynamic limit the blocks of 0's increasing with the golden mean factor $(1+\sqrt{5})/2$ can be found on all length scales. To demonstrate this fact, in figure 1 we show the 987×987 Fibonacci matrix F_n for $n = 14$, where 1's are represented by black and 0's by white pixels.

Table 2. Fibonacci matrices F_n for $n = 1, 2, \ldots, 5$ obtained through recursive relation (3). They represent the transfer matrices between possible $n \times m$ and $n \times (m+1)$ system configurations that satisfy the condition of not having any pairs of neighbouring downward-oriented spins.

$n = 1$

$$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$$

$n = 2$

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$n = 3$

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{pmatrix}$$

$n = 4$

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \end{pmatrix}$$

$n = 5$

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The entry $F_n(i, j)$ of the transfer matrix corresponds to compatibility of the n-spin chain in the ith configuration of table 1 with the n-spin chain in the jth configuration. Similarly, applying the transfer matrix m times, the entry $F_n^m(i, j)$ of the mth power of the transfer matrix corresponds to the number of valid configurations (that is, the ground-state degeneracy) of an $n \times (m+1)$ system starting with the chain in the ith configuration of table 1, and ending with the chain in jth configuration. Since boundary conditions should

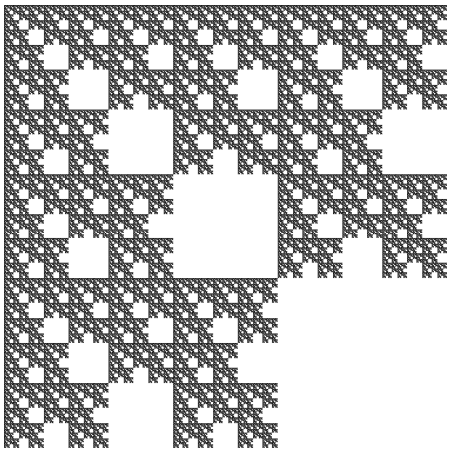

Figure 1. Graphical representation of the 987×987 Fibonacci matrix F_n for $n = 14$ (with 1's represented by black and 0's by white pixels) displaying the intrinsic fractal structure. The ratio of the sides of emergent rectangles corresponds to the golden mean ratio $(1+\sqrt{5})/2$, while the fractal dimension is given by $d = \ln(1+\sqrt{2})/\ln[(1+\sqrt{5})/2] = 1.8316$.

become negligible in the thermodynamic limit, from (2) it then follows that for arbitrary boundary spin configurations i and j the limiting value of the residual entropy is given by

$$\sigma = \lim_{n,m\to\infty} \frac{\ln F_n^m(i,j)}{nm}. \tag{5}$$

Using the spectral decomposition of F_n, we finally find

$$\sigma = \lim_{n\to\infty} \frac{\ln \lambda_n}{n} \tag{6}$$

where λ_n is the leading eigenvalue of the nth-order Fibonacci matrix.

Unfortunately, while the Fibonacci matrix is well defined for arbitrary order n, its leading eigenvalue and the elements of its arbitrary powers do not seem to be analytically tractable. In what follows we present an analytical approach, based on simple assumption of statistical independence of different spin configurations, to evaluate the residual entropy σ. Explicitly writing out the elements of the nth power of the Fibonacci matrix we have

$$F_n^m(i,j) = \sum_{k_1,\ldots,k_{m-1}=1}^{f_n} F_n(i,k_1)F_n(k_1,k_2)\ldots F_n(k_{m-1},j). \tag{7}$$

There are altogether f_n^{m-1} terms, each representing a product of m elements that can be either 0 or 1. Denoting by q_n the number of non-zero elements in the Fibonacci matrix F_n, and twice applying equation (3) to yield

$$F_n = \begin{pmatrix} F_{n-2} & G_{n-2} & F_{n-2} \\ G_{n-2} & 0 & G_{n-2} \\ F_{n-2} & G_{n-2} & 0 \end{pmatrix} \tag{8}$$

we find the recursion relation

$$q_{n+2} = 2q_{n+1} + q_n \tag{9}$$

with initial conditions $q_0 = 1$ and $q_1 = 3$, which is precisely the definition of associated Pell numbers (see earlier). We now assume that the actual values $F_n(i,j)$ (which are either

0 or 1) in (7) can be substituted with the probability q_n/f_n^2 of the element being non-zero, and obtain

$$F_n^m(i,j) \approx f_n^{m-1}\left(\frac{q_n}{f_n^2}\right)^m = \frac{1}{f_n}\left(\frac{q_n}{f_n}\right)^m. \tag{10}$$

Finally, using the known expressions for the Pell and Fibonacci numbers

$$\begin{aligned} q_n &= \frac{1}{2}[(1+\sqrt{2})^{n+1} + (1-\sqrt{2})^{n+1}] \\ f_n &= \frac{1}{\sqrt{5}}\frac{1}{2^{n+2}}[(1+\sqrt{5})^{n+2} - (1-\sqrt{5})^{n+2}] \end{aligned} \tag{11}$$

for the residual entropy in the thermodynamic limit we find

$$\sigma = \ln\left(2\frac{1+\sqrt{2}}{1+\sqrt{5}}\right) = 0.400\,16 \tag{12}$$

within 2% error of the known numerical value.

The fractal dimension of the Fibonacci matrix F_n can now be easily found. Associating mass M with q_n (number of 1's in the matrix F_n) and linear size L with f_n (number of rows/columns in F_n), from the relation

$$M = L^d \tag{13}$$

we find the fractal dimension

$$d = \lim_{n\to\infty}\frac{\ln q_n}{\ln f_n} = \frac{\ln(1+\sqrt{2})}{\ln((1+\sqrt{5})/2)} = 1.8316. \tag{14}$$

The limiting value of the residual entropy σ can be found with extremely high precision using the leading eigenvalues of the first few Fibonacci matrices. To find the eigenvalues we have used Maple V algebraic manipulation software on an Intel 33Mhz 80486DX processor with 8Mb RAM. Implementing the simple Maple script

```
with(linalg);
lambda:=vector(10,0);
for i from 1 to 9 do
  lambda[i]:=max(eigenvals(1.*fibonacci(i+1)));
od;
```

yields the first nine eigenvalues in roughly 20 min CPU time. Direct application of (6) to the obtained values reveals the existence of an $\mathcal{O}(1/n)$ correction term in the corresponding sequence of σ's, which is effectively eliminated by considering sequences $\sigma_n \equiv \ln(\lambda_n/\lambda_{n-1})$. The obtained numerical values λ_n and σ_n are shown in table 3 for $n = 1, \ldots, 9$. Note that the system size used ($n = 9$) is the same as that of [2] where convergence to only four decimal places was found, while the result obtained here agrees up to nine decimal places with the numerical value of [3]. It should be mentioned that the first entry for σ_n in table 3 is equal to our estimate (12) obtained using the assumption of statistical independence. The other entries may be regarded as successive higher-order approximations.

In summary, we find the expression for the nearest-neighbour square antiferromagnetic Ising model residual entropy in the maximum critical field, in terms of the Fibonacci matrix. It is shown that the Fibonacci matrix F_n represents the transfer matrix relating the possible ground states of an $n \times m$ system with those of an $n \times (m+1)$ system. Each element of the mth power of F_n corresponds to ground-state degeneracy of the $n \times m$ system with

Table 3. The leading eigenvalues of the first nine Fibonacci matrices with the corresponding numerical estimates for the residual entropy.

n	λ_n	$\sigma_n = \ln(\lambda_n/\lambda_{n-1})$
1	01.618 033 989	
2	02.414 213 562	0.400 161 7615
3	03.631 381 260	0.408 239 5013
4	05.457 705 396	0.407 415 3558
5	08.203 259 194	0.407 503 0940
6	12.329 882 22	0.407 494 2267
7	18.532 407 38	0.407 495 1854
8	27.855 099 10	0.407 495 0916
9	41.867 553 32	0.407 495 1023

boundary spins fixed in a particular configuration. The complicated conventional counting procedure is thus reduced to finding the properties of a quite regular, self-similar fractal object (the Fibonacci matrix). At this time we have not succeeded in finding the analytical expression for the largest eigenvalue of an infinite Fibonacci matrix, that should yield a closed form expression for the residual entropy, and thus the final solution to this 50 year old problem [1]. Instead, we first use a simple assumption of statistical independence of various spin configurations to deduce analytically the residual entropy to within 2% of the known numerical value [2, 3]. Then we use the leading eigenvalues of the first nine Fibonacci matrices to find the residual entropy (with practically no computational effort) to nine decimal places precision. Although these results are not superior to the ones obtained via a strictly numerical approach [3], the fact that they agree with the known numerical value and that they stem from consideration of a regular self-similar fractal object rather than a seemingly random transfer matrix [2], suggests that the more complicated cases, such as the three-dimensional antiferromagnet, may become tractable via a similar approach. Moreover, this approach opens the possibility of unification of results pertinent to different lattices in two and three dimensions.

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