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1986 J. Phys. A: Math. Gen. 19 1709

(http://iopscience.iop.org/0305-4470/19/9/041)

J. Phys. A: Math. Gen. 19 (1986) 1709-1714. Printed in Great Britain

On the combinatorial solution of the Ising model

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Received 3 June 1985

Abstract. An attempt to generalise the combinatorial solution of the two-dimensional (2D) nearest-neighbour (NN) Ising model to three dimensions is reported. A generating function, which fully exposes the symmetry of the lattice, is derived for the 2D square Ising model. A 'natural' extension to the 3D simple cubic (SC) lattice is shown to be false. A certain circumstance for the 2D case leads to the conjecture that $\tanh(J/kT_c) = (\sqrt{5}-2)\cos(\pi/8)$ for the SCNN Ising model.

1. Introduction

Ising (1925) solved, for the one-dimensional case only, the model for a system of interacting spins which now bears his name. It took almost two decades until Onsager (1944) presented the first solution of the two-dimensional case (in the absence of an external magnetic field), using the theory of Lie algebras. During the years following the publication of Onsager's solution there were several claims to have solved the three-dimensional Ising model. One attempt which evoked considerable discussion was due to Maddox (1952). There was also an attempt at a three-dimensional solution by Murray (1952). (The author is grateful to the referee for pointing out the last two references.) The algebraic derivation of the two-dimensional solution has subsequently been simplified, first by Kaufman (1949) using the theory of spinor representations, and later by Schultz *et al* (1964) who reduced the 2D Ising model to a soluble problem of many fermions. It has recently been realised that the model in higher dimensions also allows a fermionic representation (Polyakov 1981, Itzykson 1982). In the mean time alternative approaches to the problem have been developed, one being to reduce the problem to one of counting polygons on a lattice (van der Waerden 1941). This is the so-called combinatorial method, and the first solution was presented by Kac and Ward (1952). The proofs necessary to make this solution rigorous were later supplied by Sherman (1960, 1963) and Burgoyne (1963). The problem of counting polygons (not directed) on the lattice is solved by counting weighted directed subgraphs and expressing the number of ordinary undirected subgraphs in terms of the directed ones. The directed subgraphs are connected, so they can be described as closed weighted walks. In this paper we derive a generating function for the two-dimensional weighted walk, and interpret what the different terms in this function mean. In a certain limit we recover an expression due to Fisher (1967). We consider possible generalisations to three dimensions and show that a 'natural' choice is false. A certain circumstance for the two-dimensional case makes us put forward the conjecture that for the simple cubic NN Ising model $\tanh(J/kT_c) = (\sqrt{5}-2)\cos(\pi/8)$.

0305-4470/86/091709+06$02.50

2. The generating function

We begin by discussing the two-dimensional walk generating function for the square net and start with the simplest case. If a step to the right is denoted by a, a step to the left by $\bar{a}$, a step upwards by b and a step downwards by $\bar{b}$, we could say that we have a four-letter alphabet. Since we are interested in walks where no about-faces are allowed, we should determine the number of words of given length in which no letter is followed by its inverse, i.e. $\bar{b}$ must not be followed by b. If we denote by $f_i(\alpha, \bar{\alpha}, \beta, \bar{\beta})$ the number of words which start with the letter i ($i = a, \bar{a}, b, \bar{b}$) and contain the letter a α times, the letter $\bar{a}$ $\bar{\alpha}$ times, the letter b β times and the letter $\bar{b}$ $\bar{\beta}$ times, the following recurrence is simply derived:

$$f_a(\alpha+1, \bar{\alpha}, \beta, \bar{\beta}) = f_a(\alpha, \bar{\alpha}, \beta, \bar{\beta}) + f_b(\alpha, \bar{\alpha}, \beta, \bar{\beta}) + f_{\bar{b}}(\alpha, \bar{\alpha}, \beta, \bar{\beta}) + \delta_{\alpha,0}\delta_{\bar{\alpha},0}\delta_{\beta,0}\delta_{\bar{\beta},0} \qquad (1)$$

where we have chosen $f_i(0, 0, 0, 0) = 0$. If we define the generating function F_i, in four variables, by

$$F_i(x, y, z, u) = \sum_{\alpha,\bar{\alpha},\beta,\bar{\beta}\geqslant 0} f_i(\alpha, \bar{\alpha}, \beta, \bar{\beta}) x^{\alpha} y^{\bar{\alpha}} z^{\beta} u^{\bar{\beta}} \qquad (i = a, \bar{a}, b, \bar{b})$$

and multiply the relation (1) by $x^{\alpha+1} y^{\bar{\alpha}} z^{\beta} u^{\bar{\beta}}$ and sum over α, $\bar{\alpha}$, β, $\bar{\beta} \geqslant 0$ and do this analogously for the three corresponding relations $f_{\bar{a}}$, f_b and $f_{\bar{b}}$, we obtain

$$\begin{aligned} F_a &= (F_b + F_{\bar{b}} + 1)x/(1-x) & F_{\bar{a}} &= (F_b + F_{\bar{b}} + 1)y/(1-y) \\ F_b &= (F_a + F_{\bar{a}} + 1)z/(1-z) & F_{\bar{b}} &= (F_a + F_{\bar{a}} + 1)u/(1-u). \end{aligned} \qquad (2)$$

If we define $F = F_a + F_{\bar{a}} + F_b + F_{\bar{b}}$, we obtain

$$F = (U + V + 2UV)/(1 - UV) \qquad (3)$$

where $U = x/(1-x) + y/(1-y)$ and $V = z/(1-z) + u/(1-u)$. This is the walk (word) generating function. We now proceed to the case where we do not allow the words to end on the inverse of the initial letter, or in terms of walks we do not allow, e.g., a walk that starts with a step to the right and ends with a step to the left. We now have to keep track of both the initial and final letters, and we get sixteen instead of four relations, of the type

$$f_{aa}(\alpha+1, \bar{\alpha}, \beta, \bar{\beta}) = f_{aa}(\alpha, \bar{\alpha}, \beta, \bar{\beta}) + f_{ba}(\alpha, \bar{\alpha}, \beta, \bar{\beta}) + f_{\bar{b}a}(\alpha, \bar{\alpha}, \beta, \bar{\beta}) + \delta_{\alpha,0}\delta_{\bar{\alpha},0}\delta_{\beta,0}\delta_{\bar{\beta},0} \qquad (4)$$

where $f_{ij}(\alpha, \bar{\alpha}, \beta, \bar{\beta})$ denotes the number of words starting with the letter i and not ending with the inverse of the letter j, and the meaning of the greek letters is as before. The function F_{aa} is defined

$$F_{aa} = \sum_{\alpha,\bar{\alpha},\beta,\bar{\beta}\geqslant 0} f_{aa}(\alpha, \bar{\alpha}, \beta, \bar{\beta}) x^{\alpha} y^{\bar{\alpha}} z^{\beta} u^{\bar{\beta}} \qquad (5)$$

and correspondingly for the other functions F_{ij}. (The fact that $f_{ij} = f_{ji}$ together with (4) means that the coefficient in front of $x^{\alpha} y^{\bar{\alpha}} z^{\beta} u^{\bar{\beta}}$ in (5) is also equal to the number of words beginning and ending with the letter a, containing the letter a $\alpha+1$ times, the letter $\bar{a}$ $\bar{\alpha}$ times, and so on.)

Multiplying (4) with $x^{\alpha+1} y^{\bar{\alpha}} z^{\beta} u^{\bar{\beta}}$ and correspondingly for the other fifteen relations and summing over α, $\bar{\alpha}$, β, $\bar{\beta} \geqslant 0$ we arrive at a system of sixteen equations of which we, for brevity, give only the first four:

$$\begin{aligned} F_{aa} &= x(F_{aa} + F_{ba} + F_{\bar{b}a} + 1) & F_{a\bar{a}} &= x(F_{a\bar{a}} + F_{b\bar{a}} + F_{\bar{b}\bar{a}}) \\ F_{ab} &= x(F_{ab} + F_{bb} + F_{\bar{b}b} + 1) & F_{a\bar{b}} &= x(F_{a\bar{b}} + F_{b\bar{b}} + F_{\bar{b}\bar{b}} + 1). \end{aligned} \qquad (6)$$

The relations F_{ij}, $i \neq a$, should be obvious by now. Solving the system of equations we obtain for $F = F_{aa} + F_{\bar{a}\bar{a}} + F_{bb} + F_{\bar{b}\bar{b}}$

$$F = \left(U + V + 2UV - 2\frac{x}{1-x}\frac{y}{1-y}V - 2\frac{z}{1-z}\frac{u}{1-u}U \right)(1-UV)^{-1}. \tag{7}$$

That is, the restriction imposed on the walk has introduced two new terms in the numerator.

Now we turn to the walk encountered in the combinatorial solution of the Ising model. This walk is weighted so that a left-turn is given the weight γ, a right-turn the weight γ^{-1}, straight ahead the weight 1 and about-face the weight 0 (as before), and where $\gamma = \exp(\mathrm{i}\pi/4)$ (Kac and Ward 1952). To impose these weights (6) has to be changed to

$$\begin{aligned} F_{aa} &= x(F_{aa} + \gamma F_{ba} + \gamma^{-1} F_{\bar{b}a} + 1) \qquad & F_{a\bar{a}} &= x(F_{a\bar{a}} + \gamma F_{b\bar{a}} + \gamma^{-1} F_{\bar{b}\bar{a}}) \\ F_{ab} &= x(F_{ab} + \gamma F_{bb} + \gamma^{-1} F_{\bar{b}b} + \gamma) \qquad & F_{a\bar{b}} &= x(F_{a\bar{b}} + \gamma F_{b\bar{b}} + \gamma^{-1} F_{\bar{b}\bar{b}} + \gamma^{-1}) \end{aligned} \tag{8}$$

and correspondingly for the other twelve relations. (The alternative interpretation of f_{ij} discussed after (5) has been used.) After some lengthy and tedious algebra we have

$$\begin{aligned} F = &\left(U + V + 2UV - 2\frac{x}{1-x}\frac{y}{1-y}V - 2\frac{z}{1-z}\frac{u}{1-u}U - 16\frac{x}{1-x}\frac{y}{1-y}\frac{z}{1-z}\frac{u}{1-u} \right) \\ &\times \left(1 - UV + 4\frac{x}{1-x}\frac{y}{1-y}\frac{z}{1-z}\frac{u}{1-u} \right)^{-1}. \end{aligned} \tag{9}$$

Before discussing the three-dimensional case we examine (9) in closer detail. The generating function diverges when the denominator is zero. For the square Ising model, with the same interaction in both directions, meaning $x = y = z = u = \tanh(J/kT)$ (each edge carries in the combinatorial formulation due to van den Waerden a factor $\tanh(J/kT)$, where J is the interaction between neighbouring spins, k the Boltzmann constant and T the temperature), we obtain $\tanh(J/kT_c) = \sqrt{2} - 1$ ($x = \sqrt{2} - 1$ is a single root of the numerator and a double root of the denominator). The generating function (9) generates all walks. For the Ising model free energy we should sum all weighted closed walks of given length. That the walk is closed means that the number of x steps equals the number of y steps, and that the number of z steps equals the number of y steps, i.e. $\alpha = \bar{\alpha}$ and $\beta = \bar{\beta}$. Further, a polygon of length l is generated by $2l$ walks, the factor 2 originating from the two different directions it can be traversed, and the factor l from the l different starting points that can be chosen on the polygon. By summing up the coefficients in front of $x^\alpha y^\alpha z^\beta u^\beta$ with $2\alpha + 2\beta = l$ and dividing by $2l$ the desired expansion is obtained. We instead proceed in a more direct way to obtain the connection to the Onsager formula. Replace in (9) a step to the right, x, by $x\mathrm{e}^{\mathrm{i}\theta}$, and a step to the left, y, by $x\mathrm{e}^{-\mathrm{i}\theta}$. Similarly in (9) a step up, z, is changed to $z\mathrm{e}^{\mathrm{i}\varphi}$ and a step down, u, is changed to $z\mathrm{e}^{-\mathrm{i}\varphi}$. Further if $x = y = z = u = t$, F can be rewritten

$$F = \frac{2t(\cos\theta + \cos\varphi) - 4t^2 - 6t^3(\cos\theta + \cos\varphi) - 4t^4}{1 - 2t(\cos\theta + \cos\varphi) + 2t^2 + 2t^3(\cos\theta + \cos\varphi) + t^4} = \frac{N}{D}. \tag{10}$$

But

$$t\,\mathrm{d}D/\mathrm{d}t = -N$$

means that

$$F = -t\,\mathrm{d}\ln D/\mathrm{d}t.$$

By integrating over θ and φ from 0 to 2π and dividing by $(2\pi)^2$ we keep only the closed walks. If F_{cl} denotes the generating function for the closed walks we obtain

$$F_{\mathrm{cl}} = -2t\, \mathrm{d}f/\mathrm{d}t$$

where

$$f = \frac{1}{8\pi^2} \int\int_0^{2\pi} \ln[1 - 2t(\cos\theta + \cos\varphi) + 2t^2 + 2t^3(\cos\theta + \cos\varphi) + t^4]\, \mathrm{d}\theta\, \mathrm{d}\varphi. \qquad (11)$$

The function f is the one usually encountered and which has the well known expansion

$$f = \sum a_n t^n$$

where $a_4 = 1$, $a_6 = 2$, $a_8 = \frac{9}{2}, \ldots$ (Domb 1974). That is

$$F_{\mathrm{cl}} = -2t\, \mathrm{d}f/\mathrm{d}t = -2 \sum n a_n t^n.$$

After having elucidated the relation between the generating function defined here and the one usually encountered, we now turn to the three-dimensional case.

The expressions corresponding to (3) and (7) can be derived in a completely analogous way. For the case where we do not allow words of our now six-letter alphabet (a, $\bar{a}$, b, $\bar{b}$, g and $\bar{g}$) ending in the inverse letter of the initial letter we obtain the generating function

$$\begin{aligned} F = \{&U + V + W + 2(UV + UW + VW) + 3UVW \\ &-2[\hat{x}\hat{y}(V + W) + \hat{z}\hat{u}(U + W) + \hat{s}\hat{t}(U + V)] - 4(\hat{x}\hat{y}VW + \hat{z}\hat{u}UW + \hat{s}\hat{t}UV)\} \\ &\times [1 - (UV + UW + VW) - 2UVW]^{-1} \end{aligned} \qquad (12)$$

where $W = s/(1-s) + t/(1-t)$ and s corresponds to (say) a step into the plane and t to a step out of the plane. If the last two parentheses in the numerator of (12) are put equal to zero, we obtain the generating function for walks with no restrictions on the last step, i.e. the expression corresponding to (3) for the two-dimensional case. These last two expressions have been derived in a different way by Fisher (1967). (Note that we have defined the generating functions so that the number of walks with no steps is zero; Fisher has defined this number to be 1.) From the sequence of generating functions (3), (7), (9) and (12) one might hope to obtain a hint of what the generating function for the three-dimensional Ising model free energy looks like. A comparison between (7) and (9) suggests that it should look like (12) with 'loop' terms added in both numerator and denominator. (By 'loop' terms we mean terms containing all variables.) Further, it should contain three two-dimensional Ising free energy generating functions, i.e. if we turn off the interaction along any direction we should recover a two-dimensional generating function. We have set up one 'natural' general such expression, to be specified below, with some of the coefficients undetermined. This ansatz has been expanded in a power series. By performing the same partial sum of closed walks as described for the two-dimensional case, we can compare this expansion with the known enumeration (Domb 1974). In this way we obtain a system of equations for the undetermined coefficients in the ansatz. The ansatz set up was the following:

$$F = \left(\sum_{i=1}^{8} N_i\right)\left(\sum_{i=1}^{5} D_i\right)^{-1}$$

where $N_1 = U + V + W$, $N_2 = 2(UV + UW + VW)$, $N_3 = 3UVW$, $N_4 = -2[\hat{x}\hat{y}(V + W) + \hat{z}\hat{u}(U + W) + \hat{s}\hat{t}(U + V)]$, $N_5 = -16[\hat{x}\hat{y}\hat{z}\hat{u} + \hat{x}\hat{y}\hat{s}\hat{t} + \hat{z}\hat{u}\hat{s}\hat{t}]$, $N_6 = -4[\hat{x}\hat{y}VW + \hat{z}\hat{u}UW + \hat{s}\hat{t}UV]$, $N_7 = -A[\hat{x}\hat{y}\hat{z}\hat{u}W + \hat{x}\hat{y}\hat{s}\hat{t}V + \hat{z}\hat{u}\hat{s}\hat{t}U]$, $N_8 = -B\hat{x}\hat{y}\hat{z}\hat{u}\hat{s}\hat{t}$, $D_1 = 1 - (UV + UW +$

$VW)-2UVW$, $D_2=4[\hat{x}\hat{y}\hat{z}\hat{u}+\hat{x}\hat{y}\hat{s}\hat{t}+\hat{z}\hat{u}\hat{s}\hat{t}]$, $D_3=E[\hat{x}\hat{y}VW+\hat{z}\hat{u}UW+\hat{s}\hat{t}UV]$, $D_4=F[\hat{x}\hat{y}\hat{z}\hat{u}W+\hat{x}\hat{y}\hat{s}\hat{t}V+\hat{z}\hat{u}\hat{s}\hat{t}U]$, $D_5=C\hat{x}\hat{y}\hat{z}\hat{u}\hat{s}\hat{t}$ and $\hat{x}$ means $x/(1-x)$, etc. The ansatz contains the parameters A, B, C, E and F. We obtain five equations from the known numbers of polygons of length six, eight, ten, twelve and fourteen. Unfortunately no integer solutions were found. The ansatz goes beyond just adding another angle in the argument of the logarithm in the function f of the two-dimensional solution (11). Before discussing more general forms of ansätze we would like to report on an observation.

The system of weights, 1, 0, γ and γ^{-1}, has the consequence that when counting, e.g., walks beginning and ending with a step to the right, one obtains the same number of walks of given length as if, instead of introducing these weights, all steps to the left had been forbidden. This is so because if one iterates the 4×4 matrix of which $(1\ 0\ \gamma\ \gamma^{-1})$ is the first row, the second element in the first row is zero in each order, which is easily proven. That is, there are equally many walks, beginning and ending with a step to the right and containing backsteps, with a plus sign as with a minus sign. If one forbids backsteps for the 3D case, one obtains a recurrence relation with the largest characteristic value $\sqrt{5}+2$. (Note that we are counting all walks now and not only closed walks, but as we saw before both F and F_{cl} have the same radius of convergence.) However for the 3D case we do not expect this cancellation for walks containing backsteps; rather, there should be more such walks with a plus sign than with a minus sign, since the extra dimension gives the walks many more chances to avoid themselves. (A walk beginning and ending, e.g., with a step to the right and which intersects itself an odd number of times has a minus sign.) If we undercount in this way, we overcount by counting all walks not turning back with a plus sign, even those walks which intersect themselves in a plane perpendicular to the direction of the first step. However, even if we cannot calculate these two effects, we believe that their ratio, being a topological effect of the lattice, for large walks should converge to some 'simple' number. If we divide the best estimates of $\tanh(J/kT_c)$ by $\sqrt{5}-2$ (the radius of convergence of the generating function forbidding backsteps in 3D being the inverse of the characteristic value given above) we obtain an estimate of this 'simple' number. It turns out that the estimates of $\tanh(J/kT_c)$ are very close to $(\sqrt{5}-2)\cos(\pi/8)$, in fact so close that we conjecture that the relation $\tanh(J/kT_c)=(\sqrt{5}-2)\cos(\pi/8)$ is true. The relation gives $J/kT_c=0.221\,658\,63\ldots$, and recent series expansion estimates give 0.221 655(10) (Zinn-Justin 1981), 0.221 66(1) (Gaunt 1982) and 0.221 655(5) (Adler 1983). Further Monte Carlo renormalisation group calculations give 0.221 654(6) (Pawley *et al* 1984), and the estimate from the Monte Carlo Processor (MCP) at Santa Barbara is 0.221 650(5) (Pearson 1984, Barber *et al* 1983). Thus, the value obtained from the conjectured relation is within the margin of error of all the estimates except that of the MCP.

3. Summary

We have, for the 2D square lattice, derived three different walk generating functions, the second and third by imposing conditions on the first type of walk. The third case discussed corresponds to the 2D Ising model free energy. For the 3D simple cubic lattice the corresponding first two walk generating functions have been obtained, and for the last case, the 3D SC Ising model free energy, an ansatz based upon symmetry arguments and upon analogies with the 2D case is suggested. The ansatz is proven to be false. We believe, however, that the true generating function may be written in a form similar to the ansatz tested here, although the numerator and denominator may be of a degree higher than six in the reduced variables (the variables with circumflexes). Further, a consequence of the system of weights introduced in the combinatorial solution of the 2D Ising model leads us to conjecture that $\tanh(J/kT_c) = (\sqrt{5}-2)\cos(\pi/8)$ for the 3D simple cubic Ising model, a value in good agreement with the best estimates available. It is certainly intriguing that the conjecture contains the factor $\cos(\pi/8)$, since the factor $e^{\pm i\pi/4}$ is used in the combinatorial solution of the 2D square Ising model, the critical temperature of which obeys the relation $\tanh(J/kT_c) = 2\cos(\pi/4)-1$.

Acknowledgments

A discussion on generating functions with Dr B Lindström is gratefully acknowledged. Further, I am indebted to Dr J Åman, against whose general series expansion program I could test mine in low orders. This work was supported by the Swedish Natural Science Research Council.

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