NUMERICAL STUDY OF A CONJECTURE IN THE SELF-AVOIDING RANDOM WALK PROBLEM

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Abstract

It has been conjectured that the sum of the critical attritions μ and ν of a self-avoiding random walk on a triangular and a honeycomb lattice respectively should be precisely six. Estimates of the critical attrition obtained from the analysis of exact series expansions support this conjecture. Assuming the conjecture, estimates of the two critical attritions are made and found to be in good agreement with those obtained by other methods. The exact inequality $\nu^2 \geqslant \mu^2/(1+\mu)$ is proved, and it is shown that an analogous inequality applies to a pair of three-dimensional lattices.

I. INTRODUCTION

In recent years, the problem of self-avoiding random walks on a lattice has been the subject of much discussion (see Oguchi 1951; Fisher and Sykes 1959; Sykes 1961; Domb 1969). The problem is of interest not only as a model of a long chain polymer but also because of its connection with other mathematical models. Of particular interest is the correspondence between the self-avoiding random walk problem and the Ising model of ferromagnetism. The connection between these two problems was first noticed by Oguchi (1951) and was discussed in more detail by Fisher and Sykes (1959) and recently by Domb (1969).

In the Ising problem, a number of exact analytical results are available for the two-dimensional system (Newell and Montroll 1953; Fisher 1967). In particular, the critical point is known exactly for the common two-dimensional lattices. For the random walk problem in two-dimensions, no exact knowledge of the critical attrition is available. Some progress has been made in this direction by Hammersley (1961, 1963*a*, 1963*b*) and Kesten (1963, 1964), who have obtained rigorous upper and lower bounds on various quantities of interest, as well as certain asymptotic expressions. In general, however, the bounds are too weak to be of much use in numerical calculations.

In this paper we investigate a long standing conjecture due to one of us (M.F.S.)‡ that, if μ denotes the critical attrition of the self-avoiding walk on a triangular lattice and ν the corresponding attrition on a honeycomb lattice then

$$\mu+\nu = 6. \tag{1}$$

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‡ This conjecture was first reported by Guttmann *et al.* (1968).

This conjecture was originally based on the numerical estimates of μ and ν. For the Ising model on this pair of lattices we have

$$\mu_{\mathrm{I}} - \nu_{\mathrm{I}} = 2, \tag{2}$$

where $\mu_{\mathrm{I}} = 1/\tanh(J/kT_{\mathrm{c}})$ is the critical point of the Ising model on a triangular lattice and ν_{I} is the corresponding critical point on the honeycomb lattice. In passing, we mention an analogous result in the percolation (bond) problem (Sykes and Essam 1964), namely,

$$p_{\mathrm{c}}^{\mathrm{T}} + p_{\mathrm{c}}^{\mathrm{H}} = 1, \tag{3}$$

where $p_{\mathrm{c}}^{\mathrm{T}}$ and $p_{\mathrm{c}}^{\mathrm{H}}$ denote the critical percolation probabilities on the triangular and honeycomb lattices respectively.

Numerical estimates of μ and ν based on the analysis of the series expansion of the chain generating function

$$C(x) = \sum_{n=0}^{\infty} c_n x^n,$$

where c_n is the number of n-step self-avoiding random walks, are given by Martin *et al.* (1967) and Guttmann *et al.* (1968) as $\mu = 4{\cdot}1515$ and $\nu = 1{\cdot}8480$. Since these analyses of the honeycomb series we have generated 10 additional terms. The first 34 coefficients in the chain generating function are found to be

$$\begin{aligned} C_{\mathrm{H}}(x) = {} & 1 + 3x + 6x^2 + 12x^3 + 24x^4 + 48x^5 + 90x^6 + 174x^7 + 336x^8 \\ & + 648x^9 + 1218x^{10} + 2328x^{11} + 4416x^{12} + 8388x^{13} + 15\,780x^{14} \\ & + 29\,892x^{15} + 56\,268x^{16} + 106\,200x^{17} + 199\,350x^{18} \\ & + 375\,504x^{19} + 704\,304x^{20} + 1\,323\,996x^{21} + 2\,479\,692x^{22} \\ & + 4\,654\,464x^{23} + 8\,710\,212x^{24} + 16\,328\,220x^{25} + 30\,526\,374x^{26} \\ & + 57\,161\,568x^{27} + 106\,794\,084x^{28} + 199\,788\,408x^{29} \\ & + 372\,996\,450x^{30} + 697\,217\,994x^{31} + 1\,300\,954\,248x^{32} \\ & + 2\,430\,053\,136x^{33} + 4\,531\,816\,950x^{34} + \ldots . \end{aligned} \tag{4}$$

At first sight one might expect that a very accurate estimate of ν could be obtained from such a long series. Unfortunately this does not seem to be the case because of the difficulties endemic in the extrapolation of series associated with extremely loose-packed lattices (see Guttmann *et al.* 1968). Nevertheless, employing the usual techniques of series analysis (for a review, see Gaunt and Guttmann 1973) we estimate that

$$\nu = 1{\cdot}8481 \pm 0{\cdot}0010, \tag{5}$$

while a re-examination of the triangular lattice series by Sykes *et al.* (1972) suggests that

$$\mu = 4{\cdot}1517 \pm 0{\cdot}0010. \tag{6}$$

As usual, the quoted errors are in no sense rigorous but rather represent a subjective assessment of the rate of convergence of the numerical data. Combining these estimates, we obtain

$$\mu+\nu = 5\cdot 9998 \pm 0\cdot 0020, \tag{7}$$

so that numerically the conjecture is well supported.

In the next section we show how estimates of μ and ν can be obtained from a series derived by assuming that $\mu+\nu = 6$. Good numerical agreement is found between the estimates obtained in this way and those quoted above.

II. Numerical Study of Conjecture

It is well known that there exists a correspondence between the magnetic susceptibility of the Ising model and the chain generating function of the random walk problem (Oguchi 1951; Fisher and Sykes 1959; Domb 1969). For the Ising problem, Fisher (1959) has developed a magnetic moment transformation that relates the susceptibilities χ_T and χ_H of the triangular and honeycomb lattices respectively. Then

$$\chi_T(v) = \tfrac{1}{2}\{\chi_H(w)+\chi_H(-w)\}, \tag{8}$$

where

$$w^2 = h(v) = v(1+v)/(1+v^3) = v+v^2-v^4-v^5+v^7+\dots. \tag{9}$$

For the random walk problem, we denote the chain generating function on the triangular and honeycomb lattices by C_T and C_H respectively and write as a formal analogy

$$C_T(x) = \tfrac{1}{2}\{C_H(w^*)+C_H(-w^*)\}, \tag{10}$$

where

$$w^{*2} = f(x). \tag{11}$$

This formal procedure defines the function $f(x)$. Although this function is of course not known exactly, the first 17 terms of its series expansion may be obtained by combining equations (10) and (11) with the known series expansions for C_T and C_H. In this way we obtain

$$\begin{aligned} f(x) = {} & x+x^2-2x^4-x^5+3x^6+4x^7+12x^8+57x^9+127x^{10}+253x^{11} \\ & +907x^{12}+4224x^{13}+14\,162x^{14}+43\,817x^{15}+148\,625x^{16} \\ & +535\,910x^{17}+\dots. \end{aligned} \tag{12}$$

Our first hope was that a study of the series (12) would reveal some regular behaviour and that the function f could be identified. Unfortunately we have not been successful in this approach and we have therefore adopted a numerical procedure, which is first applied here to the Ising problem. The values of the attritions μ_I and ν_I are related through equation (9) by

$$\nu_I^{-2} = h(\mu_I^{-1}), \tag{13}$$

which on eliminating v_{I} with the help of equation (2) leads to

$$v^2 - (1-2v)^2 h(v) = 0, \tag{14}$$

when $v = \mu_{\mathrm{I}}^{-1}$. It is possible for (14), as an equation in v, to have solutions other than $v = \mu_{\mathrm{I}}^{-1}$. Of course $h(v)$ is known explicitly but, if we assume it is unknown so that we have only the first few terms of its series expansion, we can obtain successive estimates of μ_{I}^{-1} by truncating the series expansion after n terms and solving the resultant $(n+1)$th degree polynomial given by equation (14). From a theorem of Hurwitz (Titchmarsh 1932), it follows that μ_{I}^{-1} is a limit point of the zeros of these

TABLE 1

ISING MODEL AND RANDOM WALK PROBLEM ON TRIANGULAR LATTICE

Truncation point n	Estimate of Ising critical point μ_{I}^{-1}	Estimates of critical attrition* Walk generating function μ_n	ρ_n	Polygon generating function μ_n	ρ_n
1	0·250 000 000 000				
2	0·269 594 436 405	4·166 860			
3	0·269 594 436 405	4·166 860	4·166 860		
4	0·268 270 383 636	4·150 254	4·101 221	4·166 860	
5	0·267 917 772 988	4·148 194	4·139 971	4·166 860	4·166 860
6	0·267 917 772 988	4·149 685	4·157 159	4·158 665	4·117 686
7	0·267 943 027 119	4·150 162	4·153 029	4·154 643	4·130 517
8	0·267 949 797 178	4·150 505	4·152 919	4·153 177	4·142 910
9	0·267 949 797 178	4·150 900	4·154 048	4·152 665	4·148 567
10	0·267 949 311 052	4·151 110	4·153 008	4·152 427	4·150 288
11	0·267 949 180 797	4·151 211	4·152 222	4·152 294	4·150 965
12	0·267 949 180 797	4·151 299	4·152 258	4·152 210	4·151 287
13	0·267 949 190 149	4·151 396	4·152 569	4·152 150	4·151 425
14	0·267 949 192 655	4·151 475	4·152 501	4·152 105	4·151 520
15	0·267 949 192 655	4·151 534	4·152 357	4·152 070	4·151 589
16	0·267 949 192 475	4·151 583	4·152 302	4·152 044	4·151 651
17	0·267 949 192 427	4·151 624	4·152 289	4·152 024	4·151 702

* For the random walk the results are obtained on the assumption $\mu + \nu = 6$.

polynomials. Unfortunately we know of no results about the rate of approach to the limit point. Proceeding in this way we obtain the results shown in the second column of Table 1. It should be noted that, if $n \bmod(3) = 0$, the coefficients of v^n in equation (9) are zero and hence repeated roots occur in this column. Convergence appears to be extremely rapid and it can be estimated that

$$\mu_{\mathrm{I}}^{-1} = 0{\cdot}267\,949\,1924 \pm 0{\cdot}000\,000\,0001, \tag{15}$$

which in fact agrees to 10 significant figures with the known exact result of $2-\sqrt{3}$.

Having tested the method for the Ising problem we now apply it to the random walk problem. From equation (13) we obtain

$$x^2 - (6x-1)^2 f(x) = 0. \tag{16}$$

This equation has a solution $x = \mu^{-1}$, if and only if the conjecture $\mu+\nu = 6$ is correct. As before we obtain successive estimates of μ^{-1} by truncating the series expansion (12) of f after n terms. Unlike the Ising problem we find a root of equation (16) on the positive real axis closer to the origin than the physical root. This is a spurious root in that it is a solution of equation (16) but not equation (13). We therefore do not display the numerical estimates for this root in Table 1. The successive estimates μ_n of the physical root are given in the third column of the table. They are monotonically increasing. Extrapolating against n^{-1} by forming the sequence $\rho_n = n\mu_n-(n-1)\mu_{n-1}$ we obtain the estimates given in the fourth column of the table. While this sequence is not as smooth as μ_n, the last five entries are monotonically decreasing. Assuming these monotonicities persist would imply

$$4\cdot 151\,62 < \mu < 4\cdot 152\,29. \tag{17}$$

To obtain independent bounds on μ, we consider the polygon generating function

$$P(x) = \sum_{n=0}^{\infty} p_n x^n,$$

where p_n is the number of self-avoiding polygons. For the hypercubic lattice, Kesten (1963) has proved that

$$\lim_{n\to\infty} \frac{c_{n+2}}{c_n} = \lim_{n\to\infty} \frac{p_{n+2}}{p_n} = \beta^2, \tag{18}$$

where β is the critical attrition for the hypercubic lattice. Although unproved, condition (18) is almost certainly true for the honeycomb lattice with ν replacing β. For the triangular lattice the result

$$\lim_{n\to\infty} \frac{p_{n+1}}{p_n} = \lim_{n\to\infty} \frac{c_{n+1}}{c_n} = \mu \tag{19}$$

is almost certainly true. The second equality has been proved by Kesten (1963). We shall assume without further discussion the correctness of equations (18) and (19) when applied to the present problem, so that $\mu+\nu = 6$ will be correct for $P(x)$ if it is correct for $C(x)$. The estimates of μ and ν obtained from the polygon generating function are usually far less smooth than those obtained from the chain generating function (Martin *et al.* 1967) and so cannot be used directly to give useful comment on the conjecture. However, if we proceed as for the chain generating function and assume the conjecture we get rather better behaved estimates of μ and ν.

The polygon generating function $P_{\mathrm{T}}(x)$ has been given by Martin *et al.* (1967) through x^{17}. For the honeycomb lattice we find

$$\begin{aligned} P_{\mathrm{H}}(x) = {} & x^6 + 3x^{10} + 2x^{12} + 12x^{14} + 18x^{16} + 65x^{18} + 138x^{20} + 432x^{22} \\ & + 1074x^{24} + 3231x^{26} + 8718x^{28} + 25\,999x^{30} + 73\,650x^{32} \\ & + 220\,215x^{34} + \dots . \end{aligned} \tag{20}$$

We now write

$$P_{\mathrm{T}}^{*}(x) = P_{\mathrm{T}}(x) - x^3 \tag{21}$$

and

$$P_{\mathrm{T}}^{*}(x) = \tfrac{1}{2}\{P_{\mathrm{H}}(w) + P_{\mathrm{H}}(-w)\}. \tag{22}$$

The function g is then defined by

$$g(x) = w^2. \tag{23}$$

The first 15 terms of the power series expansion of g can be obtained as for the chain generating function and are

$$g(x) = x + x^2 - x^4 - 2x^5 - 3x^6 - 4\tfrac{1}{3}x^7 - 8\tfrac{1}{3}x^8 - 19\tfrac{1}{3}x^9 - 50\tfrac{2}{3}x^{10}$$
$$- 151\tfrac{1}{3}x^{11} - 468x^{12} - 1481\tfrac{4}{9}x^{13} - 4700\tfrac{4}{9}x^{14} - 14970\tfrac{4}{9}x^{15} - \dots \tag{24}$$

Proceeding as before, if $\mu + \nu = 6$ then the equation

$$x^2 - (6x-1)^2 g(x) = 0 \tag{25}$$

has a solution $x = \mu^{-1}$. We substitute the power series for g, truncated at the nth term, to obtain successive approximations. We find two limit points on the real positive x axis, one of which may be discarded as spurious. Estimates of the physical root are shown in the fifth column and the corresponding extrapolants ρ_n in the sixth column of Table 1. Both sequences appear to be comparable in smoothness with the corresponding sequences for the self-avoiding walks. Assuming the established monotonicities persist would imply

$$4\cdot 151\,70 < \mu < 4\cdot 152\,02. \tag{26}$$

These limits are slightly closer and quite consistent with those of (17). The inequality (26) gives an estimate of

$$\mu = 4\cdot 1519 \pm 0\cdot 0002, \tag{27}$$

which is in good agreement with the direct estimate (6). It is of course quite possible that the observed monotonicities do not persist and thus there is no reason to suppose that (27) is a better estimate. However, we conclude that the data are consistent with the hypothesis $\mu + \nu = 6$ within narrow limits and further that this assumption enables consistent estimates for the attritions to be obtained from the polygons.

We have repeated the above calculations for a range of values of the parameter ε defined by

$$\mu + \nu = 6 + \varepsilon. \tag{28}$$

In the range $|\varepsilon| < 10^{-3}$ the results may be summarized as

$$\mu = 4\cdot 1519 + 0\cdot 8\,\varepsilon \pm 0\cdot 0002 \quad \text{and} \quad \nu = 1\cdot 8481 + 0\cdot 2\,\varepsilon \pm 0\cdot 0002, \tag{29}$$

so that estimates for μ are more sensitive to changes in ε than estimates for ν.

III. Geometrical Interpretation of Conjecture

We have sought a geometrical interpretation of the unidentified function f, defined by the expansion (12), along the general lines of the well-known star–triangle substitution (Domb 1960). If we write

$$w^{*2} = x(1+x) \tag{30}$$

(which incidentally corresponds to truncating expansion (12) after the quadratic term) this corresponds to replacing each two-step segment of the even walks on the honeycomb lattice either by a one-step or two-step walk on the corresponding triangular lattice, as shown in Figure 1. The first of the substitutions conserves the self-avoiding property but the second does not if the point C also lies on the original walk or becomes occupied as a result of a substitution of the second type in either of the

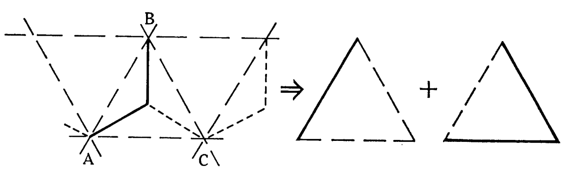

Fig. 1.—Pseudo star–triangle transformation (equation (30)), obtained by the replacement of an even walk on the honeycomb lattice by a one- or two-step walk on the derived triangular lattice.

adjacent triangles. It can be shown that if these failures are deleted the remaining walks correspond to all the walks on the triangular lattice. If there were no failures, equation (30) would relate the limits exactly. However, the failures are all positive and therefore we have the *exact inequality*

$$C_{\mathrm{T}}(x) \leqslant \tfrac{1}{2}\{C_{\mathrm{H}}(x^{\frac{1}{2}}(1+x)^{\frac{1}{2}})+C_{\mathrm{H}}(-x^{\frac{1}{2}}(1+x)^{\frac{1}{2}})\}. \tag{31}$$

The radius of convergence of the series expansion of C_{T} around the origin is $x = \mu^{-1}$ and that of C_{H} is $x^{\frac{1}{2}}(1+x)^{\frac{1}{2}} = \nu^{-1}$. Hence from inequality (31)

$$\mu^{-1} \geqslant \tfrac{1}{2}\{-1+(1+4\nu^{-2})^{\frac{1}{2}}\}, \tag{32}$$

which can be rewritten

$$\nu^2 \geqslant \mu^2/(1+\mu). \tag{33}$$

An alternative way of deriving this result is to consider the replacement of each step of a walk on the triangular lattice by an even-step walk on the corresponding honeycomb lattice. In this way one obtains

$$t_n \leqslant \sum_{i=0}^{[\frac{1}{2}n]+1} \binom{n-i}{i} h_{2(n-i)}, \tag{34}$$

where t_n and h_n are the number of n-step self-avoiding random walks on a triangular and honeycomb lattice respectively, $[x]$ denotes the largest integer not greater than x, and

$$\binom{a}{b} = \frac{a!}{(a-b)!\,b!},$$

the usual binomial coefficient. (The upper limit to the summation in inequality (34) may be replaced by ∞ since the binomial coefficient ensures that the extra terms introduced in this way make no contribution to the sum.) Multiplying both sides of (34) by x^n and summing over all integer values of n, using the observation that the sum in (34) is just the coefficient of x^n in

$$\sum_{n=0}^{\infty} h_{2n}\{x(x+1)\}^n, \tag{35}$$

gives equation (31) from which, as we have seen, inequality (33) is immediately derived. Thus inequality (33) follows from the geometrical property of the substitution and is independent of the assumptions made in previous sections.

This inequality is quite strong since on substituting the estimate $\mu = 4\cdot 1517$ we obtain $\nu \geqslant 1\cdot 8292$, the estimate $\nu = 1\cdot 8481$ being only 1% above this. Furthermore if we *assume* $\mu+\nu = 6$ we can derive the (hypothetical) inequalities

$$\mu \leqslant 4\cdot 166\,86 \qquad \text{and} \qquad \nu \leqslant 1\cdot 833\,14. \tag{36}$$

The neglected coefficients in expansion (12) correct, term by term, for the intersections generated by the quadratic substitution.

The substitution $w^{*2} = x(1+x)$, which we call the pseudo star–triangle substitution, can be applied without modification to the three-dimensional hydrogen peroxide lattice and hypertriangular lattice (Leu *et al.* 1969). The lattices of this pair are related to one another in the same way by the star–triangle substitution and so, on denoting the corresponding limits by primes, we must have

$$\nu'^2 \geqslant \mu'^2/(1+\mu'). \tag{37}$$

In this case it is to be expected that the inequality will be more closely satisfied since the hydrogen peroxide lattice is more weakly linked than the honeycomb lattice. The numerical evidence of Leu (1969) that $\mu' = 4\cdot 6181$ and $\nu' = 1\cdot 948$ shows a departure from equality of only 0·4%. The corresponding correct substitution function is found to be

$$f'(x) = x+x^2-10x^6-25x^7+15x^8+14x^9+\ldots. \tag{38}$$

By applying the pseudo star–triangle substitution to every node of the expanded honeycomb lattice we can similarly derive the walks on the Kagomé lattice. If λ denotes the attrition for the Kagomé lattice it follows by analogous arguments that

$$\nu_{\mathrm{E}}^2 \geqslant \lambda^2/(1+\lambda), \tag{39}$$

where ν_{E} is the critical attrition for the expanded honeycomb lattice.

IV. Conclusions

From the above numerical examination we conclude that the available data are consistent with the conjecture $\mu+\nu = 6$. This conjecture also enables consistent estimates for the attrition to be obtained from the polygon generating functions. We believe that the conjecture is very probably correct but we have been unable to prove it. We have established some exact inequalities in Section III but it is evident that arguments based solely on the pseudo star–triangle substitution do not suffice since they would also apply to the three-dimensional pair of lattices cited in that section. It seems likely that the well-known duality of the triangular and honeycomb pair plays a significant role.

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