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Lattice trails: I. Exact results†

A J Guttmann

Department of Mathematics, Statistics and Computer Science, The University of Newcastle, New South Wales 2308, Australia

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Abstract. We consider the problem of lattice trails, introduced by Malakis. We prove the existence of a finite connective constant, and establish a result for the growth of n-step trails t_n analogous to the best known result for self-avoiding walks, $t_n = \lambda^n \exp(O(\sqrt{n}))$. For the honeycomb ($d = 2$) and Lave's lattice ($d = 3$) we establish a counting theorem, from which we can deduce the exact value of the connective constant λ for the honeycomb lattice, $\lambda^2 = 2+\sqrt{2}$. Further, it follows that the trail problem is in the same universality class as the self-avoiding walk problem for those lattices. An exact amplitude relation between trails and self-avoiding walks, and between dumb-bells and trails and self-avoiding walks is established.

The non-existence of a counting theorem for arbitrary lattices is established. An inequality for the triangular lattice connective constant is proved. A high-density expansion for λ for the d-dimensional hybercubic lattice is also obtained. We argue that, contrary to recent suggestions, the model is in the *same* universality class as the self-avoiding walk model.

1. Introduction

In 1975 Malakis introduced the problem of lattice trails, (discussed in more detail in Malakis 1976) which is one of many interesting generalisations of the traditional self-avoiding walk (SAW) problem. A *trail* on a lattice is a connected path such that no bond may be traversed more than once. The SAW problem may be defined by changing 'bond' to 'site' in the above definition. This observation immediately suggests that a suitable bond to site transformation would map the trails problem into the SAW problem, and indeed, as Malakis pointed out, there exists a homomorphism between trails on a lattice L and self-avoiding walks on the covering lattice L'. This would suggest that the two problems belong to the same universality class, but this conclusion is by no means inevitable as the covering lattice‡ of a regular lattice is not regular§, and it is not certain that SAW's on non-regular lattices belong to the same universality class as their regular lattice-based counterparts.

† A preliminary account of this work was presented at the 15th Statphys. Conference, University of Edinburgh, July 1983.

‡ We define *covering lattice* as follows: (i) to every bond of lattice L there corresponds a vertex of the covering lattice L^c and (ii) two vertices of L^c are connected by a bond if the corresponding bonds of L meet at a vertex (in L).

§ A *regular lattice* is defined as one constructed by covering the plane with identical tiles. Thus for example, the covering lattice of the square lattice is not regular, as it is tiled with two distinctly shaped tiles.

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Recently Zhou and Li (1984) have raised the possibility that the trails problem belongs to a different universality class from that of the SAW problem, basing their suggestion both on series analysis and on position-space RG arguments.

In this paper we produce a range of exact results that argue to the contrary. In a subsequent paper we intend to present exact enumeration data that also support the conclusions of this paper.

2. Existence of a connective constant

We can follow the argument of Hammersley (1957) to prove the existence of a connective constant for trails. If $t_n(c_n)$ denotes the number of n-step trails (SAW's) on a particular lattice, the submultiplicative property $t_{n+m} \leqslant t_n t_m$ is obvious, from which follows the result that $-\infty \leqslant \inf_{n>0} \ln(t_n)/n = \lim_{n\to\infty} \ln(t_n)/n < \infty$. Writing $n = mp + q$ and applying the submultiplicative inequality above repeatedly gives $t_n \leqslant (t_m)^p t_q$, from which we can prove $\lim_{n\to\infty} \sup \ln(t_n)/n \leqslant \ln(\lambda)$, from which follows the result $\lim_{n\to\infty} \ln(t_n)/n = \ln(\lambda)$ and further, that $\ln(\lambda) \leqslant \ln(t_n)/n$. If μ denotes the corresponding connective constant for SAW's, the fact that $c_n \leqslant t_n$ implies that $\mu \leqslant \lambda$ for any given lattice. Further, it is clear that $\lambda \leqslant \sigma = q - 1$ where q is the lattice coordination number.

Further, the proof of Hammersley and Welsh (1962) that $c_n = \mu^n \exp(O(\sqrt{n}))$ may be repeated *mutatis mutandis* for trails, giving the equivalent result $t_n = \lambda^n \exp(O(\sqrt{n}))$. In both cases these rigorous results fall short of the generally accepted behaviour in which the correction term $O(\sqrt{n})$ is replaced by $O(\ln n)$. In § 3 we show that for one regular lattice, the honeycomb lattice, $\mu = \lambda = (2+\sqrt{2})^{1/2}$.

3. Counting theorems

One of the most useful exact results for the SAW problem is the counting theorem due to Sykes (1961), who showed that the number of SAW's could be related to the number of polygons, dumb-bells and theta-graphs (where we denote these by p_n, d_n and θ_n respectively, with the subscript n referring to the number of steps). Sykes proved the result

$$c_n - 2\sigma c_{n-1} + \sigma^2 c_{n-2} = 2(n-1)p_{n-1} - 2np_n + 8d_n + 8e_n + 12\theta_n \tag{3.1}$$

where $\sigma = q - 1$ and q is the lattice coordination number. This theorem has proved most useful in extending the enumerations of $\{c_n\}$ by counting the far less numerous graphs p_n, d_n and e_n. Guttmann and Whittington (1978) and Hammersley (1961) have shown that the classes of graph appearing on the RHS of (3.1) all have the same connective constant as do the SAW's, and Guttmann and Whittington also showed that the critical exponent for the dumb-bell generating function was the same as that for the chain generating function, while exponents of other generating functions for graphs appearing on the RHS of (3.1) were less than the corresponding dumb-bell exponent. Thus the RHS of (3.1) is dominated by the contribution of dumb-bells.

We have followed Sykes' procedure for the trails problem, and find, *for lattices with coordination number 3*, i.e. the (regular) two-dimensional honeycomb lattice and the (non-regular) three-dimensional Lave's lattice, the following counting theorem holds:

$$t_n - 4t_{n-1} + 4t_{n-2} = -2(n-1)p_{n-1} + 32d_{n-2} + 48\theta_{n-2}. \tag{3.2}$$

The absence of figure-eights is due to the lattice topology. The proof parallels that of Sykes (1961). From the existence of these results we can immediately derive four important conclusions:

(i) The connective constant λ is equal to its counterpart μ for trails. For the honeycomb lattice Nienhuis (1982, 1984) has shown (non-rigorously, but almost certainly correctly) that $\mu=(2+\sqrt{2})^{1/2}$. For Lave's lattice Leu (1969) estimated $\mu=1.956$.

(ii) Since the dumb-bell term on the RHS of (3.2) dominates this expression, as it does for the SAW problem, it follows that the critical exponent for honeycomb lattice trails is the same as that for honeycomb lattice SAW's. Nienhuis has shown (again non-rigorously) this exponent to be $\gamma=43/32$. That is, we can write the asymptotic relations $c_n \sim C\mu^n n^{\gamma-1}$, $t_n \sim T\lambda^n n^{\gamma-1}$ with $\mu=\lambda$.

(iii) Comparison of (3.1) and (3.2) gives the amplitude relations $T\mu^2=4C$, where T and C are defined above. Thus for the honeycomb lattice we have the exact amplitude relation $T=4C/(2+\sqrt{2})$, and a similar approximate relation for Lave's lattice.

(iv) Equation (3.1) gives an exact relation between the dumb-bell amplitude D, defined through $d_n \sim D\mu^n n^{\gamma-1}$, and the walk amplitude C, which is

$$D=\tfrac{1}{8}C(1-2\sigma/\mu+\sigma^2/\mu^2). \tag{3.3}$$

This holds for any lattice for which Sykes' chain counting theorem applies, unlike the first three results.

Note that combining (3.1) and (3.2) yields, for the honeycomb lattice, the simple result $t_{2n}=4c_{2n-2}$ and $t_{2n-1}=4c_{2n-3}-4(n-1)p_{2n-2}$,

Turning now to the problem of finding a chain generating function for an arbitrary lattice, we find the following results:

$$\begin{aligned}
t_0&=1\\
t_1&=\sigma+1\\
t_2&=\sigma(\sigma+1)\\
t_3&=\sigma^2(\sigma+1)\\
t_4&=\sigma^3(\sigma+1)-6p_3\\
t_5&=\sigma^4(\sigma+1)-6p_3(3\sigma-2)-8p_4\\
t_6&=\sigma^5(\sigma+1)-6p_3(5\sigma^2-4\sigma)-8p_4(3\sigma-2)-10p_5\\
t_7&=\sigma^6(\sigma+1)-6p_3(7\sigma^3-6\sigma^2)-8p_4(5\sigma^2-4\sigma)-10p_5(3\sigma-2)-12p_6-48p_{5a}-24p_{6c}\\
t_8&=\sigma^7(\sigma+1)-6p_3(9\sigma^4-8\sigma^3)-8p_4(7\sigma^3-6\sigma^2)-10p_5(5\sigma^2-4\sigma)-12p_6(3\sigma-2)-14p_7\\
&\qquad+96\sigma p_{5a}+48(p_{6a}+p_{6b})+(128-72\sigma)p_{6c}-28p_{7e}-84p_{7g}.
\end{aligned} \tag{3.4}$$

These may be combined to give

$$\begin{aligned}
&t_n-2\sigma t_{n-1}+\sigma^2 t_{n-2}=-2(n-1)p_{n-1}-2(n-2)(\sigma-2)p_{n-2} \qquad n\leqslant 6\\
&t_7-2\sigma t_6+\sigma^2 t_5=-12p_6-10(\sigma-2)p_5+48p_{5a}-24p_{6c}\\
&t_8-2\sigma t_7+\sigma^2 t_6=-14p_7-12(\sigma-2)p_6+48(p_{6a}+p_{6b})+(128-24\sigma)p_{6c}-28p_{7e}-84p_{7g}.
\end{aligned} \tag{3.5}$$

For loose-packed lattices only, we find the additional results

$$\begin{aligned} t_9-2\sigma t_8+\sigma^2 t_7 &= -16p_8+48p_{7a}-32p_{8h}-96p_{8r} \\ t_{10}-2\sigma t_9+\sigma^2 t_8 &= -16(\sigma-2)p_8+48p_{8c}+(144-32\sigma)p_{8h}. \end{aligned} \tag{3.6}$$

These results were derived following the method of Sykes (1961) in his derivation of the SAW chain counting theorem. The terms on the RHS refer to specific graphs tabulated in Domb (1960), who also gives their count for various lattices.

From (3.5) and (3.6) we see a fundamental difference in structure between these results for lattice trails and the corresponding results for SAW's. For SAW's, only four types of graph enter the RHS of the chain counting theorem. For trails, it appears that the number of graph types grows without limit with increasing n. We have been unable to derive, or even conjecture, the general form of the RHS, and hence we have no trail counting theorem for general lattices.

This observation that the number of types of graph steadily increases is of considerable significance however, for the following reason: each graph type entering to date can be shown to have the same connective constant as that of SAW's. Hence if the RHS of the trail counting theorem contained a finite number of graph types (as it does for the honeycomb and Lave's lattice) it would follow that the two problems had the same connective constants. As we shall subsequently prove that this is not generally the case, it follows that in general, the number of graph types on the RHS of the trail counting theorem *should* increase without bound.

This then raises the possibility that the trail and SAW problem might belong to different universality classes for those lattices for which no counting theorem exists, while belonging to the same universality class in those cases (lattices of coordination number 3) for which a counting theorem can be found. The following argument suggests that this is not true in general. As pointed out by Malakis (1976) there is a 1 : 1 mapping from the set of n-step trails on the L lattice onto the set of $(n-1)$-step SAW's on the Manhattan lattice. Recent studies (Guttmann 1983) provide strong evidence that the SAW problem on the Manhattan lattice is in the same universality class as the SAW problem on the square lattice. This provides strong evidence that the trails problem on the L lattice is also in the same universality class. The counting theorem for trails on the L lattice is of the same form as for the square lattice, that is, with a steadily increasing number of graph types on the RHS. Thus we conclude that this feature is not sufficient to change the universality class.

In § 4 we show that the two problems have different connective constants on the triangular lattice.

4. Triangular lattice

For the SAW problem, Guttmann and Sykes (1973) proved the following inequality between the connective constants on the honeycomb lattice (μ_{H}) and triangular lattice (μ_{T}):

$$\mu_{\mathrm{H}}^2 \geq \mu_{\mathrm{T}}^2/(1+\mu_{\mathrm{T}}). \tag{4.1}$$

This result came from the geometrical construction in which each two-step segment of the even-length walks on the honeycomb lattice is replaced by the corresponding one or two-step walk in the surrounding triangular lattice, as derived from the startriangle transformation. This substitution led to certain forbidden paths on the triangular lattice, from which the inequality follows.

Sykes has pointed out that for the trails problem on this pair of lattices, the opposite situation applies. That is, all derived paths on the triangular lattice are allowed, but certain trails on the triangular lattice are not derivable from the honeycomb lattice in this way. This observation then leads to the inequality

$$\lambda_{\mathrm{H}}^2 \leqslant \lambda_{\mathrm{T}}^2/(1+\lambda_{\mathrm{T}}). \tag{4.2}$$

Using the result proved in the previous section, that $\lambda_{\mathrm{H}} = \mu_{\mathrm{H}}$, the two equations above allow us to conclude that $\lambda_{\mathrm{T}} \geqslant \mu_{\mathrm{T}}$. If equality holds, then from Nienhuis' result $\mu_{\mathrm{H}}^2 = 2+\sqrt{2}$, we could conclude $\lambda_{\mathrm{T}} = \mu_{\mathrm{T}} = \frac{1}{2}[2+\sqrt{2}+(14+8\sqrt{2})^{1/2}] = 4.2227\ldots$. Given that the most recent estimate of μ_{T} is 4.15075 ± 0.0003 (Guttmann 1984) it appears safe to conclude that equality does not hold, and hence that $\lambda_{\mathrm{T}} > 4.227\ldots > \mu_{\mathrm{T}}$.

5. Hypercubic lattices

Following a suggestion by D S Gaunt, we have derived a 'high-density' expansion for the connective constant λ on a general d-dimensional hypercubic lattice, following the method of Fisher and Gaunt (1964). Writing equations (3.5) and (3.6) in the form $t_n - 2\sigma t_{n-1} + \sigma^2 t_{n-2} = d_n$, we express d_n in terms of σ ($\sigma = 2d-1$ for hypercubic lattices) using the lattice constants given by Fisher and Gaunt. The only lattice constant we need which was not given explicitly by them is that of the figure-eight, p_{8h}, for which we have (Sykes, private communication)

$$p_{8h} = 2\binom{d}{2} + 2\binom{d}{3} + 48\binom{d}{4}. \tag{5.1}$$

From (3.5), (3.6), (5.1) and the constants given by Fisher and Sykes we find:

$$\begin{aligned}
d_n &= 0, \qquad n \leqslant 4 \\
d_5/q\sigma^4 &= -\sigma^{-3} + \sigma^{-4} \\
d_6/q\sigma^5 &= -\sigma^{-3} + 3\sigma^{-4} - 2\sigma^{-5} \\
d_7/q\sigma^6 &= -4\sigma^{-4} + 13\sigma^{-5} - 9\sigma^{-6} \\
d_8/q\sigma^7 &= -4\sigma^{-4} + 21\sigma^{-5} - 35\sigma^{-6} + \mathrm{O}(\sigma^{-7}) \\
d_9/q\sigma^8 &= -31\sigma^{-5} + 213\sigma^{-6} + \mathrm{O}(\sigma^{-7}) \\
d_{10}/q\sigma^9 &= -31\sigma^{-5} + 67\sigma^{-6} + \mathrm{O}(\sigma^{-7}) \\
d_{11}/q\sigma^{10} &= \mathrm{O}(\sigma^{-6}) \\
d_{12}/q\sigma^{11} &= \mathrm{O}(\sigma^{-6}).
\end{aligned} \tag{5.2}$$

From (5.2) we can obtain

$$\ln(t_n(d)/q) = (n-1)\ln\sigma - (2n-9)\sigma^{-3} - (4n-33)\sigma^{-4} - (30n-312)\sigma^{-5} + \mathrm{O}(\sigma^{-6}). \tag{5.3}$$

Dividing by n and taking the limit $n \to \infty$ then gives the result

$$\lambda(d) = \sigma[1 - 2\sigma^{-3} - 4\sigma^{-4} - 30\sigma^{-5} + \mathrm{O}(\sigma^{-6})] \tag{5.4}$$

which should be compared to the corresponding result for SAW's namely:

$$\mu(d)=\sigma[1-\sigma^{-2}-2\sigma^{-3}-11\sigma^{-4}-62\sigma^{-5}+O(\sigma^{-6})]. \tag{5.5}$$

It appears from these expansions that, for $d \geqslant 2$, $\lambda(d)>\mu(d)$. However, the nature of these expansions is not well understood, though it is believed that they are asymptotic. Accordingly, it is probably only completely safe to conclude that $\lambda(d)>\mu(d)$ for *some* dimensionality. Assuming that these *are* asymptotic expansions, then stopping at the smallest term, we find $\lambda(2)\approx 2.630$ and $\lambda(3)\approx 4.888$.

6. Conclusions

The above study of the problem of lattice trails provides considerable evidence to suggest that the problem is in the same universality class as the self-avoiding walk problem. This is explicitly shown for one two-dimensional and one three-dimensional lattice. The remaining possibility, that the trails problem is in a different universality class for *some* lattices, is shown to be unlikely.

For the honeycomb lattice, exact values for the connective constant, critical exponent and critical amplitude (in terms of that for the SAW problem) are found.

For the triangular lattice, a connective constant inequality is found, from which it is argued that the connective constant is different from that of the SAW problem.

For the d-dimensional hyperbubic lattice a high-density expansion is obtained, which also implies a difference between the connective constant for the trails problem and the SAW problem for these lattices.

In a subsequent paper we intend to provide numerical evidence in support of these conclusions, as well as estimates of the various critical parameters.

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