On the statistical mechanics of noncrossing chains. II

1989 J. Phys. A: Math. Gen. 22 L843

(http://iopscience.iop.org/0305-4470/22/17/007)

J. Phys. A: Math. Gen. 22 (1989) L843–L847. Printed in the UK

LETTER TO THE EDITOR

On the statistical mechanics of non-crossing chains: part 2

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Received 23 November 1988, in final form 13 June 1989

Abstract. We report the results of taking the reciprocal of generating function for self-avoiding walks on the plane square lattice with end-to-end distance specified. In a previous paper it was shown that this produces the generating function for irreducible two-point Mayer clusters. This function is found to be far simpler than the original generating function. It is found that a renormalisation or self-consistent field calculation should give very good results and that further small corrections, due to the existence of 'traps', can also be computed. It is further found that the generating function has an unphysical singularity very near to the physical singularity and that this accounts for difficulties of series analysis that have been experienced, for example, by Guttmann.

In an old paper (Temperley (1957), referred to as I) I pointed out that the problem of enumerating self-avoiding walks on a lattice is strikingly similar to the lattice gas problem treated by the Mayer method. However, the combinatorics of the walk problem are much simpler than those of the imperfect gas problem in two respects. We need only consider cluster integrals (or sums) whose graphs are formed by adding diagonals to open or closed polygons. And if we have the generating function for clusters that are Mayer irreducible (i.e. have graphs that are multiply connected) we need only take its reciprocal to obtain the generating function for self-avoiding walks. In a later paper (Temperley (1988), referred to as II) I showed further that the same reciprocal relation holds for the generating functions of walks whose end-to-end displacement is specified and of two-point Mayer-type cluster integrals similarly weighted according to the displacements of their end points. For various reasons it was expected that the cluster generating function would be simpler than the original walk generating function.

In this paper we report on the plane square lattice, using data for walks of up to 20 steps kindly supplied by Guttmann (private communication). A program for finding the reciprocal of the three-variable generating function was written by D Evans of Swansea Computer Centre. We find indeed that the cluster generating function is far simpler than the walk generating function and the results suggest that a new and rapidly convergent system of successive approximations should exist for any lattice. This also gives an explanation of the difficulties experienced by Guttmann and others, (see, for example, Guttmann 1987), in analysing the 'raw' data. The generating functions have two real positive singularities that are very close, but definitely not coincident and we shall obtain an interpretation of these.

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For the linear lattice the results are almost trivial. The walk generating function is (II, equation (23)):

$$\begin{aligned} w(z) &= 1 + 2z\cos\theta + 2z^2\cos 2\theta + 2z^3\cos 3\theta + \ldots \\ &= (1 - C(z))^{-1} \\ &= \left(1 - \frac{2z\cos\theta}{1-z^2} + \frac{2z^2}{1-z^2}\right)^{-1} \end{aligned} \tag{1}$$

and we have pointed out in II that there are two different types of cluster integral: those that have a diagonal joining the two end points (which are thus forced to be coincident), the generating function for the sums of which we denote by $K(z)$, and those for which this diagonal is absent, the generating function for the sums of which we denote by $L(z, \theta)$. In these the power of z is the number of links in a cluster and the power of $e^{i\theta}$ is the distance between the end points. For the plane square lattice, we obtain for $C(z)$ in an obvious notation

$$\begin{aligned} c(z) = c_{0,0}(z) + (\cos\theta + \cos\phi)c_{1,0}(z) + \cos\theta\cos\phi c_{1,1}(z) + c_{2,0}(z)(\cos 2\theta + \cos 2\phi) \\ + c_{2,1}(z)(\cos 2\theta\cos\phi + \cos\theta\cos 2\phi) + \ldots \end{aligned}$$

the individual functions being given up to z^{16} in table 1.

It will be seen that these terms are numerically much smaller and far less numerous than those of the original generating function. Paper II gives reasons for expecting this.

Table 1. Expansions up to z^{16} of the functions $c_{i,j}(z)$.

$c_{0,0}(z) =$	$-4z^2$	$-12z^4$	$-60z^6$	$-332z^8$	$-1948z^{10}$	$-11\,708z^{12}$	$-71\,788z^{14}$	$-446\,796z^{16} - \ldots$
$c_{1,1}(z) =$			$-8z^6$	$-64z^8$	$-424z^{10}$	$-2\,608z^{12}$	$-16\,184z^{14}$	$-102\,304z^{16} - \ldots$
$c_{2,0}(z) =$				$-4z^8$	$-36z^{10}$	$-256z^{12}$	$-1\,268z^{14}$	$-1\,220z^{16} - \ldots$
$c_{2,2}(z) =$							$-32z^{14}$	$-536z^{16} - \ldots$
$c_{3,1}(z) =$								$-176z^{16} - \ldots$
$c_{1,0}(z) =$	$2z$	$+2z^3$	$+14z^5$	$+78z^7$	$+482z^9$	$+2926z^{11}$	$+18\,006z^{13}$	$+112\,198z^{15} + \ldots$
$c_{1,1}(z) =$					$4z^9$	$+20z^{11}$	$+120z^{13}$	$+960z^{15} + \ldots$
$c_{30}(z) =$								$16z^{15} + \ldots$
$c_{3,2}(z) =$								$4z^{15} + \ldots$

We conclude that a satisfactory first approximation to the walk generating function is obtained by neglecting everything except $c_{0,0}$ and $c_{1,0}$, thus obtaining

$$w(z, \theta, \phi) \approx [1 - c_{0,0}(z) - (\cos\theta + \cos\phi)c_{1,0}(z)]^{-1} + O(z^6) \tag{2}$$

and we can interpret $c_{0,0}$ and $c_{1,0}$ as taking account of the removal, as each step is added, of walks that intersect themselves. Thus 'self-consistent field' treatments such as that of Edwards (1986 and many earlier papers) are likely to give reasonable results. Examination of these two series show that their radius of convergence is about $(2.54)^{-1}$; quite definitely *greater* than the accepted value $(2.638)^{-1}$ for the radius of convergence of the walk generating function (Guttmann 1987).

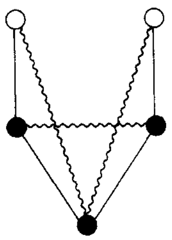
We can make several deductions from (2) and from the higher approximations obtained by introducing $c_{1,1}$, $c_{2,0}$ etc. First, the walks never return to the origin, so the constant term in $w(z, \theta, \phi)$ is exactly 1. That is to say

$$\frac{1}{4\pi^2}\int_0^{2\pi}\int w(z, \theta, \phi)\, d\theta\, d\phi = \frac{1}{4\pi^2}\int_0^{2\pi}\int (1-c(z, \theta, \phi))^{-1}\, d\theta\, d\phi = 1. \tag{3}$$

Secondly, the number of simply closed domains or polygons is clearly equal to the number of walks that end one step away from the origin. That is, the generating function is obtained by multiplying $w(z, \theta, \phi)$ by $2z(\cos\theta + \cos\phi)$ and integrating:

$$zw_{1,0}(z) = K(z) = \frac{1}{4\pi^2}\int_0^{2\pi}\int \frac{2z(\cos\theta+\cos\phi)\, d\theta\, d\phi}{1-c(z, \theta, \phi)}. \tag{4}$$

The generating function for the number of domains is clearly given by $K(z)$ because this is the generating function for closed polygons with all possible diagonals added, thus removing those with self-intersection. (This was not explicitly pointed out in II.) Note that $K(z)$ is *not* equal to $c_{0,0}(z)$ because $c_{0,0}(z)$ also includes terms of $L(z)$ for which the two end points coincide. Already, for the z^4 term we have the integral



which has the value -4. We can deduce other relations for the numbers of walks with any given end-to-end distance. Thus, for walks that end one x and one y step from the origin, we have, for the generating function,

$$w_{1,1}(z) = \frac{1}{4\pi^2}\int_0^{2\pi}\int \frac{4\cos\theta\cos\phi\, d\theta\, d\phi}{1-c(z, \theta, \phi)}. \tag{5}$$

Finally, if we do not specify the end points of the walks, we have

$$w(z, 0, 0) = (1-c(z, 0, 0))^{-1}. \tag{6}$$

Relations (3)-(6) are exact. It is of interest to examine their consequences if we insert the first approximation (2). Inspection of the remaining subseries in table 1 suggests that inserting the series $c_{1,1}(z)$ to get a second approximation should give very reliable results, the effect of the remaining subseries being minute.

Consider, first of all, the consequences of (6). The various terms of $c(z, 0, 0)$ up to z^{27} have been obtained by Privman (private communication) by taking the reciprocal of the one-variable generating function. The result is a well behaved z series with regularly alternating terms whose magnitudes are much less than those of the original series. The radii of convergence of the positive and negative subseries are still about $(2.54)^{-1}$ i.e. definitely greater than $z_c = (2.638)^{-1}$. Thus the denominator of (2) becomes zero at $z = z_c$ as a result of two large terms cancelling out. This is a perfectly possible but rather unexpected situation. Reference to equation (1) shows that the situation in one dimension is quite similar, the walk generating function diverges at $z = \frac{1}{2}$, the cluster generating function not until $z=1$. There is, moreover, a curious 'booby trap' for series analysts. If we compare the magnitudes of the terms of $c_{0,0}(z)$ and $2c_{1,0}(z)$ it is easy to mistake their sum for a single series with a singularity at $z=-(2.54)^{-1}$ and with *no* singularity on the positive real axis!

To examine the situation more closely consider the effect of using (2) in (3) and (4). Multiplying (4) by $c_{1,0}(z)/2z$ and subtracting from (3), we conclude that

$$K(z)\approx -\frac{2zc_{0,0}(z)}{c_{1,0}(z)}=4z^2+8z^4+24z^6+\ldots \tag{7}$$

which is exact up to terms in z^6, and a good approximation for higher terms.

Using (2), integral (3) becomes a complete elliptic integral with parameter

$$k=\frac{-2c_{0,0}(z)}{1-c_{0,1}(z)} \tag{8}$$

and, if k is nearly unity, then (3) gives us

$$1\approx\frac{1}{c_{0,0}(z)}\ln(4/(1-k^2)^{1/2}). \tag{9}$$

Equation (8) may be regarded as an implicit equaltion for z_c and (9) then gives us a relation between the functions $c_{0,0}(z)$ and $c_{1,0}(z)$. They are not very helpful in determining critical exponents. z_c may be regarded as known from earlier work and (8) and (9) are certainly consistent with z_c being slightly *less* than the radius of convergence of the functions $c_{0,0}(z)$ and $c_{1,0}(z)$. In principle we could have obtained these two functions by iteration. Given a few powers of z, we can determine all the terms of the walk generating function by equations like (5) and (7) and then, by finding its reciprocal, determine more terms of $c_{0,0}$ and $c_{1,0}$ and so on. Inspection of the values in table 1 shows that it may be necessary to include $c_{1,1}(z)$ in the scheme of iteration, but that inclusion of other functions in table 1 is unlikely to make much difference.

The existence of the higher-order corrections to expression (2) may perhaps be traced to the formation of 'traps' by some of the longer walks which prevent them from returning to the origin without self-intersection. One form of 'trap' is a spiral self-avoiding walk, the numbers of which have been shown by various workers to be related to the number of partitions of N which is proportional only to $A^{N^{1/2}}$, so the conclusion that their effect on the generating function is small is reasonable. These corrections can, in principle, be computed by the iteration process just described.

Our work entirely confirms the impression that analysis of walk data is simplified by converting the walk generating function to a cluster generating function by taking its reciprocal. The very rapid fall off in the magnitudes of the functions in table 1 as the distance between the end points of the clusters increases might have been anticipated from the work on the Gaussian model in II, which shows the two-point cluster integrals falling off exponentially as the end-to-end distance increases.

If the true situation is that the generating function has an unphysical real positive singularity slightly beyond the true singularity then the difficulties found by Guttmann (1987) and others in analysing the data are completely explained. According to Guttmann (1987) this is the very situation that makes '*D* log Padé' analysis ineffective. It also explains why an analysis in terms of confluent singularities seems to be 'nearly right'. Equation (1) shows that exactly this situation occurs in one dimension. The original generating function has its singularity at $z=\frac{1}{2}$ and its reciprocal has an unphysical singularity at $z=1$.

I thank Professor Guttmann and Professor Privman for making their data available and Mr D Evans for writing the program. I thank Professor Sir Sam Edwards for helpful correspondence. I also thank the Leverhulme Foundation for an Emeritus Fellowship.

Note added in proof. The coefficients of z^{17}–z^{20} inclusive are available for the plane square lattices. The uniformity of signs shown in table 1 is beginning to break down, but the conclusions are not affected. Similar information for the plane triangular and simple cubic lattices should be available soon.

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