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LETTER TO THE EDITOR

On the statistical mechanics of non-crossing chains: part 3

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Abstract. I have shown in a previous paper that the generating function for self-avoiding walks with end-to-end displacement specified can be converted into a Mayer-like cluster series by simply taking the reciprocal of the generating function. In a previous letter the results of doing this for the plane square lattice were reported for terms up to z^{16}. The cluster series terms are much less numerous and numerically much smaller than those of the 'raw' self-avoiding walk series and point to the existence of a set of rapidly converging successive approximations for such problems. Guttman's conclusion that the singularity of the self-avoiding walk series may be a confluent one received support. We now report the results of extending the work on the plane square lattice up to z^{25} and the results of similar work on the simple cubic lattice up to z^{15} and discuss them briefly. Conclusions from the earlier work are confirmed.

In a recent letter, referred to as L (Temperley 1989), I reported some preliminary results of a new method of analysing data on numbers of self-avoiding walks (SAW) on lattices. I had previously shown (Temperley 1988), that if we have the generating function for self-avoiding walks with end-to-end displacements specified we can simply take its reciprocal and obtain the cluster series obtained from two-point Mayer irreducible cluster integrals or sums. The clusters are obtained by adding diagonals to open polygons of all lengths.

The expectation was that the terms of the cluster series would be less numerous and numerically much smaller than the corresponding terms of the 'raw' SAW series. In L the cluster series for the plane square lattice were reported for up to 16 steps. The above expectations were entirely confirmed, and it was also found that the magnitude of the terms fell off very rapidly indeed as the distance between the end-points of the clusters increases. Indeed, it turned out that a satisfactory first approximation to the SAW generating function is obtained by retaining just the first two cluster sub-series, $c_{0,0}(z)$ and $c_{1,0}(z)$ in table 1 of L; that is to say that we have, as a good approximation for the SAW series,

$$W(z,\theta,\phi)\approx[1-c_{0,0}(z)-c_{1,0}(z)(\cos\theta+\cos\phi)]^{-1}+\mathrm{O}(z^6) \qquad \text{(equation (2) of L)}$$

and examination of the data in L shows that introducing further sub-series only has a small effect and that such successive approximations converge very rapidly.

One point that was left doubtful in L was whether the radius of convergence of the cluster series is the same as that of the SAW series. It is known from the earlier work of Sykes and Hammersley that the radius of convergence of the 'domain' (or self-avoiding polygon) generating function is the same as that of the SAW generating

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function, so one might expect the same of the cluster series. However, the data in L seemed to point to the radius of convergence of the cluster series being definitely larger than that of the SAW series. The work now reported was undertaken in order to examine this point further and to look at the simple cubic lattice.

The data used in L were originally obtained by Watson at Kings' College, London, though they were actually communicated to the author by Guttmann. The SAW series for the plane square lattice has since been confirmed and extended to 25 terms by Guttmann. The programme for finding the reciprocal of a series the higher terms of which are long and complicated functions of $\cos\theta$ and $\cos\phi$ was written and run by G Evans of Swansea Computer Centre, who has also modified the programme to deal with three-dimensional lattices. We now report the results of extending the work of L to 25 terms and also of analysing similarly the first 15 terms of the simple cubic lattice, also obtained originally by Watson and communicated to the author by Guttmann. Guttmann has also, at my request, very kindly applied some of his powerful 'log Padé' methods of analysis to throw light on the behaviour of the cluster series. I am very grateful for this, and also for his helpful and patient discussions and correspondence on all these matters.

A formal definition of the cluster integrals (sums for a lattice model) is as follows. Consider an open polygon of l sides, corresponding to l segments of a polymer. Successive points along the chain correspond to the ends of polymer segments and the segments are constrained to lie along the lattice so that successive points are nearest neighbours on the lattice exactly one lattice distance apart. We now add diagonals to the open polygon in all possible ways, giving each diagonal a weight of -1 if its two ends are on the same lattice point and zero otherwise. The effect of introducing such cluster sums is to remove from the generating functions walks that intersect themselves at one or more points. The algorithm described above does *not* give a generating function for individual clusters formed from segments, but only a generating function for the sums of all Mayer-irreducible (multiply connected) cluster sums of size l. It is possible to evaluate any particular cluster-sum by drawing out on the lattice all possible paths of length l that are consistent with the restrictions imposed by the presence of the diagonals. A few of the early terms of the cluster series have been explicitly checked by this means, but the process quickly becomes time-consuming as l increases.

The terms of the sub-series from z^{16} to z^{25} are given in table 1. (The terms up to z^{16} are given in table 1 of L.) As in L, $c_{0,0}(z)$ corresponds to clusters whose end-points are coincident, $c_{1,0}(z)$ to clusters whose end-points are one lattice distance apart (coefficient of $\cos\theta+\cos\phi$), $c_{1,1}(x)$ to clusters whose end-points are one lattice distance apart horizontally and vertically (coefficient of $\cos\theta\cos\phi$) and so on.

Plane square lattice (data in L and table 1)

In L it was suggested that the radius of convergence of the cluster series might be slightly greater than the accepted value $(2.638\ldots)^{-1}$ for the 'raw' SAW series. This is somewhat surprising, as the domain or polygon generating function (which forms a part of the $c_{0,0}$ series) is known to have the same radius of convergence, though not the same exponent, as the SAW series. This was based on analysis of the $c_{0,0}$ and $c_{1,0}$ series up to z^{15}. Guttmann (private communication) has now analysed the longer series now available up to z^{25} and finds a radius of convergence indistinguishable from the SAW value and an effective exponent of about zero for both the $c_{0,0}$ and $c_{1,0}(z)$ series, that is to say they behave asymptotically like $\ln(1-z/z_c)$.

Table 1. Later terms in the functions $c_{i,j}(z)$ for the plane square lattice. The first column gives the first non-vanishing term in each series. The remaining columns give the terms from z^{16} onwards. (The terms up to z^{16} are given in table 1 of L.)

	z^{16}	z^{18}	z^{20}	z^{22}	z^{24}
$c_{0,0}(z)=-4z^2\ldots$	− 446 796	− 2813 012	− 17 871 476	− 114 383 324	− 736 638 908
$c_{1,1}(z)=-8z^6\ldots$	− 102 304	− 655 680	− 4 240 000	− 27 608 192	− 180 774 736
$c_{2,0}(z)=-4z^8\ldots$	− 1 220	− 83 860	− 570 844	− 3 870 300	− 26 201 300
$c_{2,2}(z)=-32z^{14}$	− 536	− 4 928	− 36 176	− 245 776	− 1 630 784
$c_{3,1}(z)=-8z^{14}$	− 176	− 1 704	− 12 464	− 83 984	− 553 648
$c_{3,3}(z)=+8z^{18}$		+8	− 48	− 3 208	− 45 696
$c_{4,0}(z)=+12z^{18}$		+12	+ 236	+ 2 104	+ 14 300
$c_{4,2}(z)=+4z^{18}$		+4	− 16	− 1 736	− 26 704
$c_{4,4}(z)=+128z^{24}$					+ 128
$c_{5,1}(z)=-8z^{20}$			− 8	− 320	− 5 136
$c_{5,3}(z)=+64z^{24}$					+ 64
$c_{5,5}(z)=?$					0
$c_{6,0}(z)=+20z^{24}$					+ 20
$c_{6,2}(z)=+4z^{24}$					+4
	z^{17}	z^{19}	z^{21}	z^{23}	z^{25}
$c_{1,0}(z)=+2z\ldots$	+ 707 418	+ 4500 366	+ 28 840 534	+ 185 970 106	+ 1205 537 498
$c_{2,1}(z)=+4z^9\ldots$	+ 8 328	+ 67 128	+ 512 508	+ 3 790 008	+ 27 461 672
$c_{3,0}(z)=+16z^{15}$	+ 276	+ 2 652	+ 22 316	+ 182 500	+ 1 460 192
$c_{3,2}(z)=+4z^{15}$	+ 12	− 484	− 6 768	− 55 388	− 365 512
$c_{4,1}(z)=-8z^{17}$	− 8	− 232	− 2 808	− 23 448	− 167 936
$c_{4,3}(z)=+28z^{21}$			+ 28	− 68	− 11 208
$c_{5,0}(z)=+16z^{21}$			+ 16	+ 372	+ 3 628
$c_{5,2}(z)=+4z^{21}$			+ 4	− 64	− 4 488
$c_{6,1}(z)=-8z^{23}$				− 8	− 424

Notation: $c_{0,0}(z)$ are the terms independent of θ and ϕ, $c_{1,0}(z)$ is the coefficient of $(\cos\theta+\cos\phi)$, $c_{2,0}(z)$ is the coefficient of $(\cos 2\theta+\cos 2\phi)$, $c_{1,1}(z)$ is the coefficient of $\cos\theta\cos\phi$, etc.

Simple cubic lattice (data in table 2)

A preliminary analysis by Guttmann (private communication) of the available terms of the $c_{0,0,0}$ and $c_{1,0,0}$ series shows the same tendency for the radius of convergence estimates from the early terms to be higher than the accepted value for the 'raw' SAW series $(4.638\,39)^{-1}$ Guttmann (1989). (They are approaching this value but are still some 10% higher.) While it is conceivable that the limiting radii of convergence may be different, the above evidence strongly suggests that they will turn out to be the same. Assuming that they are, Guttmann estimates the exponent to be 2, that is to say, both the $c_{0,0,0}$ and $c_{1,0,0}$ series behave asymptotically like $(1-z/z_c)^{-2}$.

The finding in L that the analysis of SAW data can be simplified by taking the reciprocal of the generating function seems to be entirely confirmed. (This remains true for the simpler generating function for the total number of SAWs of given length obtained by putting $\theta=\phi=\psi=0$ for which the coefficients of each power of z are just numbers and it is a simple matter to find the reciprocal by computer.) In particular, Guttmann's suggestion (1987) that the SAW generating function has a confluent singularity seems to have been confirmed and this explains the difficulty in analysing 'raw' SAW data experienced by him and other workers.

Table 2. Terms up to z^{15} in the function $c_{i,j,k}(z)$ for the simple cubic lattice.

$c_{0,0,0}(z) =$	$-6z^2$	$-\ 30z^4$	$-\ 366z^6$	$-\ 5022z^8$	$-\ 76\,062z^{10}$	$-\ 1230\,462z^{12}$	$-\ 20\,787\,102z^{14}$	
$c_{1,1,0}(z) =$		0	$-\ 8z^6$	$-\ 96z^8$	$-\ 1\,032z^{10}$	$-\ 9\,840z^{12}$	$-\ 69\,512z^{14}$	
$c_{2,0,0}(z) =$			0	$-\ 8z^8$	$-\ 232z^{10}$	$-\ 3\,888z^{12}$	$-\ 58\,176z^{14}$	
$c_{2,2,0}(z) =$						0	$-\ 128z^{14}$	
$c_{3,1,0}(z) =$						0	$+\ 8z^{14}$	
$c_{1,0,0}(z) =$	$2z$	$+\ 2z^3$	$+\ 26z^5$	$+\ 394z^7$	$+\ 5778z^9$	$+\ 90\,714z^{11}$	$+\ 1490\,378z^{13}$	$+\ 25\,345\,514z^{15}$
$c_{1,1,1}(z) =$				0	$-\ 48z^9$	$-\ 576z^{11}$	$+\ 5\,424z^{13}$	$+\ 388\,992z^{15}$
$c_{2,1,0}(z) =$				0	$+\ 4z^9$	$+\ 60z^{11}$	$+\ 1\,904z^{13}$	$+\ 65\,712z^{15}$
$c_{2,2,1}(z) =$							0	$-\ 240z^{15}$
$c_{3,0,0}(z) =$							0	$+\ 800z^{15}$
$c_{3,1,1}(z) =$							0	$+\ 80z^{15}$
$c_{3,2,0}(z) =$							0	$+\ 4z^{15}$

Notation is an obvious extension of that in table 1, e.g. $c_{2,1,0}(z)$ is the coefficient of $(\cos 2\theta \cos \phi + \cos 2\phi \cos \theta + \cos \theta \cos 2\psi + \cos 2\theta \cos \psi + \cos 2\phi \cos \psi + \cos 2\psi \cos \phi)$.

Particularly striking is the rapid decrease in the magnitudes of the cluster series terms as the end to end spacing increases. Also interesting is the uniformity in signs in the cluster subseries, which persists out to z^{16} for the plane square lattice and z^8 for the simple cubic lattice. Departures only occur for some of the series corresponding to large end to end separations, whose terms are small in any case.

The conclusion in L that renormalization group and self-consistent field-type calculations should give reliable results receives further support.

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Note added in proof. These results and those reported in L strongly suggest that, despite the failure of many attempts to find them, analytic solutions to some of these SAW problems may exist.

References

Guttmann A J 1987 *J. Phys. A: Math. Gen.* **20** 1839
—— 1989 *J. Phys. A: Math. Gen.* **22** 2807
Temperley H N V 1988 *Discrete Appl. Math.* **19** 367
—— 1989 *J. Phys. A: Math. Gen.* **22** L843