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1987 J. Phys. A: Math. Gen. 20 763

(http://iopscience.iop.org/0305-4470/20/3/038)

J. Phys. A: Math. Gen. **20** (1987) 763-766. Printed in the UK

COMMENT

On the convergence of the series expansion analysis for self-avoiding walks attached to a surface

T Lookman† and K De'Bell‡

† Department of Applied Mathematics, University of Western Ontario, London, Ontario, Canada N6A 3K7

‡ Department of Physics, Dalhousie University, Halifax, Nova Scotia, Canada B3H 3J5

Received 20 May 1986

Abstract. Extensions of exact enumeration data for self-avoiding walks attached to the surfaces of face-centred cubic and triangular lattices are reported. The convergence of the estimates for the critical point p_c and exponent γ_1 obtained by the Baker-Hunter confluent singularity analysis is discussed and comparison made with estimates of p_c from the corresponding bulk series.

In a previous letter (De'Bell and Lookman 1985, hereafter referred to as I) an analysis of the generating function

$$\chi_1 = \sum_{n=0} C_n p^n \underset{p \to p_c^-}{\sim} (p_c - p)^{-\gamma_1}(1+\ldots) \tag{1}$$

for self-avoiding walks (SAW) attached to a lattice surface, based on the values of C_n for $n \leqslant 13$ in the case of the triangular lattice and $n \leqslant 9$ in the case of the face-centred cubic (FCC) lattice, was described. Here the extension of the available data by three terms ($C_{14} = 392\,228\,772$, $C_{15} = 1623\,219\,782$, $C_{16} = 6718\,815\,168$) for the triangular lattice and by one term ($C_{10} = 5899\,819\,497$) for the FCC lattice is reported.

In I the Baker-Hunter (1973) confluent singularity method was used to analyse the available terms in χ_1. This method allows an estimate of γ_1 to be obtained without interference from correction to scaling terms (contained in the ellipsis of (1)) by constructing an auxiliary function with a simple pole at $1/\gamma_1$. Weaker confluent singularities only contribute simple poles further removed from the origin. γ_1 may then be estimated by forming Padé approximants to the auxiliary function. The Baker-Hunter method requires p_c as input and since this is not known exactly in the present problems a number of trial values are used. An estimate of p_c is then obtained by looking for a range of p_c in which the Padé approximants to the auxiliary function are best converged.

The application of the Baker-Hunter method to the available coefficients for the triangular lattice in I led to the estimate $0.240\,915 \leqslant p_c \leqslant 0.240\,93$. Examination of the higher-order approximants obtained by using the values of C_{14}, C_{15} and C_{16} (above) show that they have a region of best convergence

$$p_c = 0.240\,930 \pm 0.000\,005 \qquad \text{(triangular).}$$

The corresponding estimate of γ_1 is (triangular)

$$\gamma_1 = 0.9549^{+0.0011}_{-0.0015}$$

where the error bounds in γ_1 represent only the variation in the Padé approximants for values of p_c in the range quoted above. Even at the lowest value of γ_1 allowed by these bounds, there is a slight discrepancy between this estimate and the proposed exact value (Cardy 1984, Guttmann and Torrie 1984)

$$\gamma_1 = 61/64.$$

The estimates of $1/\gamma_1$ obtained from different approximants rapidly reach the proposed exact value as p_c is decreased below 0.240 925 and only a very small change in the lower error bound on p_c is required to remove the discrepancy. The estimate of p_c given above may be compared with the value

$$p_c = 0.240\,92^{+0.000\,02}_{-0.000\,02}$$

obtained by an analysis of the corresponding bulk series (based on 18 terms) by Guttmann (1984).

In I it was reported that the Padé approximants, formed from the first ten terms of the Baker–Hunter auxiliary function, for the FCC lattice were not convergent in the range of p_c scanned. On examining the additional approximants ([4/6], [5/5], [6/4]) obtained using C_{10} (above) it was found that these do have a region of good convergence for $0.099\,80 < p_c < 0.099\,95$. Such a high value for p_c would be inconsistent with the estimate

$$p_c \approx 0.099\,634 \qquad (\text{FCC})$$

obtained by McKenzie (1979) from an analysis of the first fifteen terms in the corresponding bulk series. As a check on the consistency of the Baker–Hunter method, it was applied to the bulk series analysed by McKenzie (1979). Trial values of p_c in the range $p_c = [0.0994, 0.100]$ were used. Within this range the value of p_c given by McKenzie (1979) clearly gave the best convergence of the Padé approximants. In addition to the best overall agreement in the estimates of $1/\gamma_1$ for approximants based on ten or more terms of the series most of the higher-order approximants exhibit interfering defects (nearly coincident pole zero pairs on the real positive axis closer to the origin than $1/\gamma_1$) except in a narrow range around $p_c = 0.099\,634$. (In most cases the defects are present for $p_c \leqslant 0.0996$, $p_c \geqslant 0.099\,65$.) The disappearance of such defects appears to be a common feature of the region of best convergence (Lookman and De'Bell 1986). It is also seen in the approximants for the SAW attached to a triangular lattice surface discussed above, where the higher-order approximants are free of such defects at $p_c = 0.240\,93$ but the defects reappear for $p_c \geqslant 0.240\,935$, in most cases. The estimate of the bulk exponent γ assuming $p_c = 0.099\,634$ is

$$\gamma = 1.162 \pm 0.001$$

in excellent agreement with the value of $\gamma = 1.1615 \pm 0.0005$ obtained by McKenzie (1979) and the values $\gamma = 1.160 \pm 0.004$ from the ε expansion and 1.1615 ± 0.002 from perturbation expansion in three dimensions (Le Guillou and Zinn-Justin 1985).

The equivalence of p_c for bulk and surface walks is an exact result due to Hammersley and Whittington (1985). We therefore conclude that the apparent convergence of the [4/6], [6/4] and [5/5] approximants to the FCC surface series at $p_c \approx 0.0999$, described above, is a short series effect. Unfortunately, the approximants to the Baker–Hunter auxiliary function for the surface problem are not well converged when $p_c = 0.099\,634$ and we cannot obtain a reliable estimate of γ_1 by this method.

In I an estimate of γ_1 for the FCC lattice was obtained from a Dlog Padé approximant analysis of the available terms. The two additional points obtained by including the value of C_{10} in the analysis lie close to the pole-residue curve shown in figure 2 in I (with poles at $p_c = 0.0998$ and 0.1008). Assuming $p_c = 0.099\,634$ one obtains

$$\gamma_1 = 0.736 \pm 0.006$$

which is substantially higher than the value 0.676 ± 0.009 obtained by Guttmann and Torrie (1984).

In addition we have analysed the series χ_1 for walks attached to the surface of an FCC lattice, when the surface is a square lattice, given by Ma *et al* (1977). There is no clearly defined region of best convergence for the Padé approximants to the Baker-Hunter auxiliary function in the range $p_c = 0.0993$–0.1000. Adopting the value of p_c given by McKenzie leads to $\gamma_1 = 0.71^{+0.07}_{-0.05}$, but the error bounds are too wide to allow a meaningful comparison with the value of γ_1 obtained by Guttmann and Torrie (1984).

In conclusion, for the triangular lattice, application of the Baker-Hunter method to the series χ_1 produces an estimate of p_c which is in good agreement with the estimate obtained from the corresponding bulk series by Guttmann (1984). Our analysis is just consistent with the value of $\gamma_1 = 61/64$ proposed by Cardy (1984) if one allows a p_c just below 0.240 925, which certainly cannot be ruled out on the basis of our present analysis. However, this consistency occurs only at the extreme lower edge of the estimated error bounds for p_c. (We take the opportunity of again emphasising that our error bounds represent only the variation over the considered approximants and that judgement of the range of p_c over which the best convergence is obtained is to some extent subjective.) However, at the central estimate of p_c and throughout almost the whole error bound range there is a small inconsistency with the proposed exact result of Cardy (1984).

In the case of the FCC lattice we have analysed both the available terms for χ_1 and the previously published terms of the corresponding bulk series by the Baker-Hunter method. In the case of the bulk series the values of p_c and the bulk exponent γ are in excellent agreement with those obtained previously by other methods. This indicates that the discrepancy in the value of p_c obtained from the χ_1 series is a short series effect. An additional difficulty in the analysis of the χ_1 series for the FCC lattice is the possibility of crossover effects. If one considers the two-variable generating function

$$\chi_1(p, p) = \sum_{n, n_1} C_{n, n_1} p_1^{n_1} p^n$$

where n_1 is the number of steps in the surface, the special transition is expected to occur at $p = p_c$, $p_1 = 0.13$ (De'Bell and Essam 1980). In view of the closeness of the value of p_1 at which the special transition occurs to p_c it seems possible that the poor convergence of the $p_1 = p$ series at p_c (and high γ_1 from the Dlog Padé analysis) is connected to crossover effects.

Overall we believe that the present comment demonstrates that the Baker-Hunter method is capable of an accuracy comparable to other correction to scaling analysis.

This work is supported in part by the Natural Sciences and Engineering Research Council of Canada.

We thank J Nuttall for relevant discussions concerning the analysis of series expansions.

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