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LETTER TO THE EDITOR

Self-avoiding walks on the face-centred cubic lattice

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Abstract. The generating function $C(x)$ for the number of self-avoiding walks on the face-centred cubic lattice is extended by two terms to order 14. The series coefficients are analysed for a singularity of the form $A_1t^{-\gamma}+A_2t^{-\gamma+1}+Bt^{-\gamma+\Delta_1}$ with $t=1-\mu x$, where μ is the connective constant. Two cases of interest are studied, (*a*) $\gamma=1\frac{1}{6}$, $B=0$ as conjectured in earlier work on series expansions and (*b*) $\gamma=1{\cdot}1615$, $\Delta_1=0{\cdot}465$ as predicted by renormalisation group (RG) calculations. It is found that the series coefficients are better fitted to the RG predictions (*b*).

Self-avoiding walks (SAWs) on lattices have been extensively studied as a model of a polymer in solution (for a recent review see McKenzie 1976). It has been shown by a number of authors (de Gennes 1972, Domb 1972, Bowers and McKerrel 1973) that the SAW problem corresponds to the $n=0$ limit of the classical n-vector model. The analogy is also discussed by Domb (1974, 1976) in connection with the existence of a star graph expansion for the high-temperature zero-field susceptibility χ_0 of the n-vector model, and hence for the generating function $C(x)$ for the number of self-avoiding walks on a lattice.

Earlier work by Martin *et al* (1967), Sykes *et al* (1972) and Watts (1975) on the asymptotic behaviour of self-avoiding walks was based on the assumption that, near the critical point, $C(x)$ exhibits a singularity of the form

$$C(x)\simeq A(1-\mu x)^{-\gamma}, \tag{1}$$

where μ is the effective coordination number or the connective constant of the lattice. It is analogous to the reciprocal of the critical value v_c of the high-temperature expansion variable $v(=\tanh J/kT)$ for the Ising model. The exponent γ which corresponds to the susceptibility exponent was conjectured to be

$$\gamma=1\tfrac{1}{6} \tag{2}$$

in three dimensions. Sykes *et al* (1972) also made the more general assumption

$$C(x)\simeq A(x)(1-\mu x)^{-\gamma}+\psi(x), \tag{3}$$

where $A(x)$ and $\psi(x)$ are regular in the disc $|x|\leqslant 1/\mu$, and found that their estimates for μ and γ remained practically unchanged.

More recently, the renormalisation group approach has been applied to the excluded volume problem, and calculations by Le Guillou and Zinn-Justin (1977) and Baker *et al* (1978) predict that near the critical point

$$C(x)\simeq A(x)(1-\mu x)^{-\gamma}+B(1-\mu x)^{-\gamma+\Delta_1}. \tag{4}$$

Le Guillou and Zinn-Justin (1977) make the estimate

$$\gamma = 1{\cdot}1615 \pm 0{\cdot}0011, \qquad \Delta_1 = 0{\cdot}465 \pm 0{\cdot}010, \tag{5}$$

while Baker *et al* (1978), using a slightly modified calculation, quote

$$\gamma = 1{\cdot}161 \pm 0{\cdot}003, \qquad \Delta_1 = 0{\cdot}467 \pm 0{\cdot}005. \tag{6}$$

It is clear that the RG predictions, (4) to (6), differ from those of exact enumeration work, (2) and (3), on two points. RG theory predicts the existence of a confluent additive correction term with exponent $-\gamma + \Delta_1$ which is not present in earlier treatments. Also, RG estimates for γ are appreciably lower than $1\frac{1}{6}$. (The estimates (5) and (6), though not identical, are mutually consistent.)

In an attempt to resolve the discrepancy between the two approaches, we study the effect of including the confluent correction term $(1-\mu x)^{-\gamma+\Delta_1}$ in the analysis of $C(x)$. A similar analysis for the Ising problem ($n = 1$) by McKenzie (1979a) suggests that there is some justification for including the correction term at least on the face-centred cubic (FCC) lattice.

We have extended the $C(x)$ series on the FCC lattice by two terms to order x^{14}, to obtain

$$C(x) = \sum_{n\geq 0} a_n x^n = 1 + 12x + \ldots + 18\,208\,650\,297\,396 x^{13} + 184\,907\,370\,618\,612 x^{14} + \ldots . \tag{7}$$

The earlier coefficients to order x^{12} are given by Martin *et al* (1967).

The new coefficients were derived using the star graph expansion for $1/C(x)$ (Domb 1976, McKenzie 1979b). The number of contributing graphs at this order is about 8500, and the computations were performed on the CDC 7600 computer at the University of London. In the process of calculating a_{13} and a_{14}, we also obtained a check on the coefficients to a_{12} (Martin *et al* 1967).

We now analyse the series (7), assuming the asymptotic form (4). The method of analysis parallels that of Camp and Van Dyke (1975) and McKenzie (1979a). Expanding $A(x)$ in a Taylor series about $x = 1/\mu$, and retaining terms to first order in $(1-\mu x)$, we obtain

$$C(x) \sim A_1(1-\mu x)^{-\gamma} + A_2(1-\mu x)^{-\gamma+1} + B(1-\mu x)^{-\gamma+\Delta_1}. \tag{8}$$

The ratios $R_n (= a_n/a_{n-1})$ should behave, in the limit $n \to \infty$, as follows:

$$R_n = \mu\left(1 + \frac{r-1}{n} + \frac{b}{n^{1+\Delta_1}} + \frac{a}{n^2}\right). \tag{9}$$

The amplitudes a and b are very simply related to A_2/A_1 and B/A_1 respectively.

It would be interesting to use the ratios R_n to obtain completely unbiased estimates for γ, Δ_1, a, b and μ. But in practice, a five-parameter fit proves almost meaningless for a series of this length. Since we are mainly interested in deciding between two different sets of predictions for γ and Δ_1, we adopt the procedure of fixing γ and Δ_1 and solving for μ, a and b by using successive triplets of R_n. If the exponents are chosen correctly, successive estimates of μ (and a and b) should converge rapidly to a limiting value when plotted against n. In figure 1 we present the results for μ for various choices of γ and Δ_1.

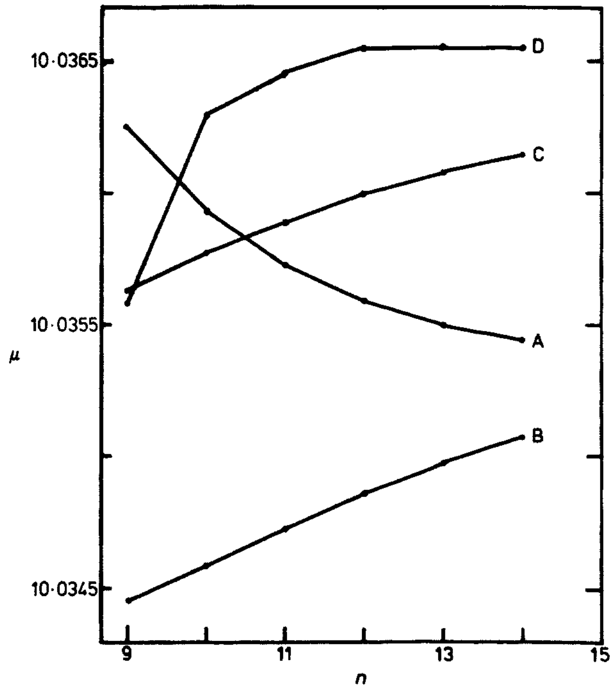

Figure 1. FCC lattice. Estimates of μ obtained by solving (9) for the cases: A, $a = b = 0$, $\gamma = 1\frac{1}{6}$; B, $b = 0$, $\gamma = 1\frac{1}{6}$; C, $a = 0$, $\gamma = 1{\cdot}1615$, $\Delta_1 = 0{\cdot}465$; D, $\gamma = 1{\cdot}1615$, $\Delta_1 = 0{\cdot}465$.

Curve A represents the situation when both a and b are set equal to zero and γ is fixed at $1\frac{1}{6}$. This corresponds to the simple algebraic singularity (1). We find that the estimates for μ are decreasing quite rapidly. Curve B represents the case where $b = 0$ and $\gamma = 1\frac{1}{6}$. This corresponds to a singularity of the form (3), where the first analytic correction term, $(1-\mu x)^{-\gamma+1}$, is included. There is little improvement to the fit. Curve D is obtained when $\gamma = 1{\cdot}1615$ and $\Delta_1 = 0{\cdot}465$, the values predicted by Le Guillou and Zinn-Justin (1977). The successive estimates of μ converge quite rapidly to a limit of about 10·036 55. The last three values of μ remain almost stationary. We also found that small changes to $\Delta_1(\pm 0{\cdot}005)$ make little difference to the fit. By trying several values of γ around 1·1615, it was found that $\gamma = 1{\cdot}1615 \pm 0{\cdot}0005$ gives the best results. We also consider the case (C) of $\gamma = 1{\cdot}1615$, $\Delta_1 = 0{\cdot}465$, $a = 0$. Again, the successive estimates of μ do not converge as rapidly as in D, suggesting that the inclusion of the term in $(1-\mu x)^{-\gamma+1}$ is necessary.

The analysis presented here does suggest that, at least to order x^{14}, the series coefficients of $C(x)$ are best fitted to the form (8), with values of γ and Δ_1 as predicted by RG calculations. Admittedly, this does not prove conclusively that the RG estimates for γ and Δ_1 are the correct ones. It is never possible to establish asymptotic behaviour from a series with a finite number of terms. Also, this investigation has been confined to one lattice. The analysis of loose-packed lattices by this method proves extremely difficult owing to the presence of a non-confluent 'antiferromagnetic-type' singularity. However, it is generally accepted (Sykes *et al* 1967, Watts 1975) that the FCC lattice provides the best converged series for most thermodynamic properties and yields the most reliable estimates for critical exponents.

We conclude therefore that the behaviour of the self-avoiding walks series on the FCC lattice is consistent with RG predictions and lends support to the RG estimates for the dominant and subdominant critical exponents.

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