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LETTER TO THE EDITOR

Self-avoiding walks on the hyper face-centred cubic lattice in four dimensions

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Abstract. The star graph expansion method for calculating high temperature susceptibility series for the Ising model has been extended to the polymer problem. The generating function for self-avoiding walks on the four-dimensional face-centred cubic lattice has been calculated to ninth order. The series coefficients are analysed for singularities of the form $t^{-1}|\ln t|^p$, predicted by renormalisation group calculations. Good convergence is obtained for values of p in the vicinity of $p=\frac{1}{4}$, (the renormalisation group prediction) and we estimate $p = 0{\cdot}24 \pm 0{\cdot}03$. The critical point (connective constant for the polymer problem) is found to be $22{\cdot}072 \pm 0{\cdot}004$.

The existence of star graph expansions for the free energy and high temperature zero field susceptibility of the classical n-vector model is well known. (Domb 1972, 1974 and references therein.) For the $n = 1$ case (the Ising model), this method has been used to calculate high temperature susceptibility series (χ_0) to very high order (McKenzie 1975, Gaunt and Sykes 1979). It has been pointed out by de Gennes (1972), that $n = 0$ corresponds to the excluded volume problem, where the susceptibility becomes the generating function $C(x)$ for random self-avoiding walks on a lattice. It was shown empirically by Domb (1974) that the coefficients in the $C(x)^{-1}$ expansion could be expressed in terms of star lattice constants. We have used this method to calculate $C(x)$ on the four dimensional hyper face-centred cubic (HFCC) lattice to ninth order. All terms in the expansion are new and this is the first non-trivial application of the star graph expansion method to the $n=0$ case. It should be stressed, however, that this is only a preliminary study and the procedure can be used to derive long series for all lattices.

The HFCC lattice was chosen for this study because of its close packed structure. Self-avoiding walks on the loose packed four dimensional simple hypercubic lattice have been studied by Fisher and Gaunt (1964) and Guttmann (1978). The series there were found to exhibit odd-even oscillations which made extrapolation difficult. We find, on the contrary, that even with a relatively short series on the HFCC, we are able to obtain good convergence. We have analysed the series coefficients assuming the asymptotic form predicted by renormalisation group theory (Brézin *et al* 1976) and field theoretical calculations (Larkin and Khmel'nitskii 1969), namely,

$$C(x) \sim t^{-\gamma}|\ln t|^p \tag{1}$$

where $t = (x_c - x)/x_c$ and $\gamma = 1$.

We estimate $p = 0{\cdot}24 \pm 0{\cdot}03$, which is in excellent agreement with the RG prediction of $\frac{1}{4}$, and more precise than that of Guttmann (1978).

Derivation of series

The existence of a star graph expansion for the self-avoiding walk generating function, $C(x)$, enables us to write

$$C(x)^{-1}=\sum_{s}(s:\mathscr{L})\,W_s(x)\,. \tag{2}$$

The sum runs over all star graphs s which can be embedded on the lattice $\mathscr{L}$. $(s:\mathscr{L})$ denotes the weak lattice constant of s on the lattice. $W_s(x)$ is a function of x which can be expanded as a power series:

$$W_s(x)=\sum_{l\geq k} h_l\,x^l \tag{3}$$

where k is the number of edges of s.

The calculation of $W_s(x)$ is very similar to that for the Ising problem. The pair correlations between spins at the vertices of the star cluster s are expressed in terms of the number of self-avoiding walks between pairs of sites of s. The partial susceptibility graphs for the Ising problem are thus replaced by self-avoiding walks. The enumeration of the number of such walks on a graph is readily performed on the computer. The inversion of the partial susceptibility matrix to obtain $C(x)^{-1}$ of the star cluster s and subsequent application of (2) to the star graph s to obtain $W_s(x)$ are also performed on the computer. Finally, we derive, for the HFCC lattice,

$$C(x)=1+24x+552x^2+12\,504x^3+281\,112x^4+6\,293\,064x^5+140\,500\,200x^6$$
$$+3131\,047\,176x^7+69\,681\,616\,392x^8+1549\,185\,178\,536x^9+\ldots. \tag{4}$$

A check on our lattice constant data $(s:\mathscr{L})$ was obtained by using them to calculate the $n=1$ (Ising) susceptibility series to ninth order. Our results are in agreement with those of Moore (1970). We were also able to check the weights series $W_s(x)$ by using them to compute $C(x)$ for the FCC lattice in three dimensions. Again we obtained agreement with earlier calculations (Martin *et al* 1967). We are thus confident that the coefficients in (4) are correct.

Series analysis

We have used the method of Guttmann (1978) to analyse the coefficients in (4), assuming the asymptotic form (1). We start with a straightforward ratio analysis to obtain an approximate estimate of the critical point (or the connective constant for the polymer problem). We obtain

$$\mu_c=22{\cdot}080\pm0{\cdot}005=x_c^{-1}\,. \tag{5}$$

We now transform to a new variable y, given by

$$y=\frac{2x}{1+x/x_c}\,. \tag{6}$$

The reasons underlying such transformations have been extensively discussed elsewhere (Gaunt and Guttmann 1974 and references therein). Defining the transformed series by

$$C(y)=\sum_{n\geqslant 0} a_n y^n, \tag{7}$$

and

$$y^{-p*}(1-y)^{-1}[\ln(1/(1-y))]^{p*}=\sum_{n\geqslant 0} b_n y^n, \tag{8}$$

we form the ratios

$$R_n=(a_n/a_{n-1})/(b_n/b_{n-1}). \tag{9}$$

The sequence R_n should approach y_c^{-1} with zero slope as $n\to\infty$, for $p^*=p$.

We find that for values of p^* in the vicinity of $\frac{1}{4}$, the R_n's do extrapolate smoothly to the critical point. In table 1 we present the sequences R_n and their linear and quadratic extrapolants for values of $p^*=0{\cdot}21$, $0{\cdot}24$ and $0{\cdot}27$. We make the estimate

$$p=0{\cdot}24\pm0{\cdot}03 \qquad y_c=22{\cdot}076\pm0{\cdot}004. \tag{10}$$

Transforming back to the variable x, we obtain

$$x_c^{-1}=22{\cdot}072\pm0{\cdot}004.$$

We conclude therefore, that self-avoiding walks on the HFCC lattice behave consistently with renormalisation group predictions. The degree of convergence obtained with such a short series suggests that longer series on this lattice might be worth investigating. Work is in progress along these lines.

Table 1. Analysis of transformed self-avoiding walks series on the HFCC lattice

p	n	R_n	Linear extrapolants	Quadratic extrapolants	$n(x_cR_n-1)$ exponent	Linear extrapolants
	4	21·9734	22·3032	22·1724	−0·01932	0·01101
	5	22·0238	22·2257	22·1094	−0·01272	0·01367
0·21	6	22·0496	22·1785	22·0842	−0·00826	0·01405
	7	22·0638	22·1491	22·0754	−0·00513	0·01363
	8	22·0721	22·1301	22·0733	−0·00286	0·01302
	9	22·0772	22·1176	22·0737	−0·00116	0·01245
	4	21·9141	22·3166	22·1832	−0·03006	0·00209
	5	21·9786	22·2365	22·1162	−0·02297	0·00537
0·24	6	22·0133	22·1873	22·0890	−0·01811	0·00618
	7	22·0338	22·1563	22·0789	−0·01466	0·00609
	8	22·0466	22·1363	22·0761	−0.01211	0.00573
	9	22·0551	22·1229	22·0760	−0·01017	0·00536
	4	21·8548	22·3293	22·1942	−0·04081	−0·00693
	5	21·9332	22·2469	22·1232	−0·03325	−0·00302
0·27	6	21·9770	22·1959	22·0939	−0·02800	−0·00176
	7	22·0036	22·1635	22·0826	−0·02422	−0·00153
	8	22·0210	22·1424	22·0789	−0·02139	−0·00162
	9	22·0329	22·1281	22·0783	−0·01921	−0·00177

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