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Application of the method of Padé approximants to the excluded volume problem

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Abstract. Padé approximants have been applied to the analysis of the chain generating functions of all the common two- and three-dimensional lattices. Estimates for the critical attrition, μ, are in very close agreement with those obtained using the ratio method. The index, g, is estimated as $0{\cdot}330 \pm 0{\cdot}003$ for the triangular lattice and $0{\cdot}1663 \pm 0{\cdot}0003$ for the face-centred-cubic. These estimates are consistent with the hypothesis that $g = \frac{1}{3}$ exactly in two dimensions and $g = \frac{1}{6}$ exactly in three dimensions. These values have been used to form estimates for the critical amplitudes, A. The Padé approximants provide further evidence for the existence of an 'antiferromagnetic singularity' in the chain generating functions of the loose-packed lattices.

1. Introduction

Since its introduction into physics by Baker and Gammel (1961) and Baker *et al* (1961), the method of Padé approximants has been successfully applied to many of the series expansions that arise in studies of the Ising and Heisenberg models of ferromagnetism and more general models in the theory of critical phenomena. There exists an extensive literature and we refer to the reviews by Baker (1965, 1970) and to the article by Gaunt and Guttmann (1974). However, no systematic investigation appears to be available for the excluded volume problem; this is surprising since the series available are very similar in many respects to those obtained for the Ising model. In this paper we repair the omission and present a summary of the conclusions we have drawn from such a study.

Self-avoiding walks on lattices were originally studied as a model of a long polymer in solution (Orr 1947, Domb 1969) and more recently have also been applied in the theory of cooperative phenomena (Domb 1969, 1970). For instance, in the self-avoiding walk approximation to the Ising model the chain generating function, $C(x)$, is used as a first approximation to the high-temperature susceptibility, $\chi(v)$, (Domb 1970). For this reason techniques, based on the ratio method, which were originally employed for the analysis of high-temperature Ising series (Sykes *et al* 1972a) have also been successfully applied to self-avoiding walks (Sykes *et al* 1972b). To date almost all analyses of excluded volume series have used ratio method techniques.

In this paper the Padé method is applied to the chain generating function

$$C(x) = 1 + \sum_{n=1}^{\infty} c_n x^n \qquad (1)$$

for each of the common two- and three-dimensional lattices. These are all regular series in which the physical singularity is dominant and have been extensively analysed by means of the ratio method (Sykes *et al* 1972b). The coefficients, c_n, are known to be very well fitted by the asymptotic form

$$c_n \sim \mu^n n^g, \qquad \text{large } n \tag{2}$$

so that the chain generating function is usually assumed to be of the form (Martin *et al* 1967)

$$C(x) \sim A(1-\mu x)^{-1-g} \tag{3}$$

and Padé approximants have here been used to estimate A, μ and g. The estimates for μ are found to be very close to the best available from the ratio method and those for g are consistent with the currently accepted values of $g = \frac{1}{3}$ and $g = \frac{1}{6}$ in two and three dimensions respectively.

The coefficients, c_n, for the close-packed lattices, are taken from Martin *et al* (1967) through $n = 12$ for the face-centred-cubic and $n = 17$ for the triangular. For the diamond lattice the data of Sykes (1973 private communication) through $n = 22$ were used. For the remaining loose-packed lattices $C(x)$ was obtained through $n = 34, 24, 19$ and 15 for the honeycomb, square, simple-cubic, and body-centred cubic lattices respectively from Sykes *et al* (1972b).

2. The dominant singularity

Following the usual procedure diagonal and para-diagonal Padé approximants were formed to the series D log $C(x)$. We are mainly interested in the closest singularity to the origin on the positive real axis since this must lie at $x = 1/\mu$, where μ is the critical attrition (cf equation (3)), and should have residue $-(1+g)$. Sequences of estimates for $1/\mu$ are given in table 1 for the square lattice and in table 2 for the face-centred-cubic lattice. These two lattices are representative of a loose-packed and a close-packed lattice respectively. In tables 1 and 2 those Padé approximants containing 'spurious' poles inside the circle of convergence are marked with a dagger. Such spurious poles possess a very small residue, usually 10^{-3} or less and are 'cancelled' by a coincident zero in the numerator (Gaunt and Guttmann 1974).

Table 1. Square lattice, D log Padé analysis of position of dominant singularity.

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
7	0·378821	0·378849	0·378855
8	0·378857	0·378847†	0·378985
9	0·378797†	0·378974	0·378984†
10	0·379174	0·379025†	0·379011
11	0·379001	0·379006	0·379009†
12	0·378986†	—	—

† Denotes presence of spurious poles inside circle of convergence.

Table 2. Face-centred-cubic lattice, D log Padé analysis of position of dominant singularity.

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
1	0·100000	0·101010	0·100202
2	0·100560	0·099691	0·099317
3	0·099404	0·099536	0·099751
4	0·100144	0·099631	0·099652
5	0·099655	0·099651	0·099654†
6	0·099648	—	—

† Denotes presence of spurious poles inside circle of convergence.

From tables 1 and 2 and corresponding tables for the other lattices the unbiased estimates for μ in table 3 were obtained. For comparison purposes table 3 also contains the latest published estimates for μ obtained using the ratio method. The source of these estimates is as follows: the honeycomb estimate was obtained by Guttmann and Sykes (1973), the diamond by Essam and Sykes (1963) and the remainder by Sykes *et al* (1972b). In each case the series analysed were the same length as those used in the present paper except for the diamond lattice for which Essam and Sykes used 17 terms while we here use 23. It should also be noted that their last term, c_{16}, contained a slight error. The two sets of estimates in table 3 agree well to within the quoted errors, and in two cases, the square and body-centred-cubic lattices, they are in precise agreement.

Table 3. Comparison of estimates obtained for μ from Padé approximants with most recently published estimates by ratio method.

Lattice	Estimate for μ		
	Unbiassed (Padé)	Biassed (Padé)	Most recently published (ratio)
H	1·8478 ± 0·0002	1·8479 ± 0·0002	1·8481 ± 0·001
T	2·6385 ± 0·0003	2·6387 ± 0·0001	2·6385 ± 0·0001
SQ	4·1520 ± 0·001	4·1516 ± 0·0005	4·1517 ± 0·0001
D	2·8792 ± 0·0005	2·8785 ± 0·002	2·878 ± 0·002
SC	4·6838 ± 0·001	4·6834 ± 0·001	4·6835 ± 0·0005
BCC	6·5295 ± 0·002	6·5295 ± 0·002	6·5295 ± 0·0005
FCC	10·035 ± 0·005	10·0346 ± 0·001	10·0355 ± 0·001

To obtain estimates for the index, g, Padé approximants were formed to

$$(\mu^{-1}-x)\mathrm{D}\log C(x)$$

and evaluated at $x = \mu^{-1}$. The estimates for g so obtained are given in table 4. For the triangular and face-centred-cubic lattices these values suggest $g = \frac{1}{3}$ and $g = \frac{1}{6}$. The accuracy of the estimation is not so high for lattices of lower coordination, and the apparent slight dependence of g upon coordination seen in table 4 may well be due to over optimism in forming the error limits.

Using the results in table 4 and previously published estimates for g (Martin *et al* 1967) it seems reasonable to assume that it is given exactly by $g = \frac{1}{3}$ in two dimensions and

Table 4. Estimates for g from $(\mu^{-1}-x)\mathrm{D}\log C(x)$ Padé approximants.

Lattice	g Using unbiassed μ	g Using biassed μ
H	0.342 ± 0.005	0.339 ± 0.005
SQ	0.335 ± 0.005	0.333 ± 0.005
T	0.330 ± 0.003	0.332 ± 0.003
D	0.157 ± 0.003	0.163 ± 0.003
SC	0.1622 ± 0.001	0.1650 ± 0.001
BCC	0.1650 ± 0.001	0.1650 ± 0.001
FCC	0.1663 ± 0.0003	0.1667 ± 0.0003

by $g = \frac{1}{6}$ in three dimensions. We will now use these values to form new, biassed, estimates for μ. If $C(x)$ is indeed given by equation (3) then forming $C(x)^{1/1+g}$ should convert the branch-point singularity to a simple pole. Padé approximants were formed to the series for $C(x)^{1/1+g}$ and the biassed estimates for μ are shown in table 3 for comparison with the unbiassed estimates. The change in μ is very small, although the estimated accuracy is higher than before.

As a consistency check the biassed estimates for μ were used to re-estimate g. These biassed estimates for g, shown in table 4, are considerably closer to the simple fractions $\frac{1}{3}$ and $\frac{1}{6}$.

We can use the new estimates for μ as a check on the conjecture $\mu_{\mathrm{T}}+\mu_{\mathrm{H}} = 6$ (Guttmann and Sykes 1973). Summing the estimates for the honeycomb and triangular lattices we obtain

$$\mu_{\mathrm{T}}+\mu_{\mathrm{H}} = \begin{cases} 5.9998 \pm 0.0012 & \text{using unbiassed estimates} \\ 5.9995 \pm 0.0007 & \text{using biassed estimates} \end{cases}$$

which give good agreement.

The critical amplitudes, A, were estimated by forming Padé approximants to the series for $(\mu^{-1}-x)C(x)^{1/1+g}$. On evaluation at $x = \mu^{-1}$ these give $\mu^{-1}A^{1/1+g}$. The biassed estimates for μ were used and the simple fractions $\frac{1}{3}$ and $\frac{1}{6}$ for g. The estimates for A are given in table 5.

Table 5. Estimates for critical amplitues from $(\mu^{-1}-x)C(x)^{1/1+g}$ Padé approximants.

Lattice	A
H	1.0667 ± 0.002
SQ	1.0893 ± 0.001
T	1.0931 ± 0.002
D	1.1182 ± 0.003
SC	1.0840 ± 0.002
BCC	1.0493 ± 0.002
FCC	1.0463 ± 0.001

3. Other singularities

For the loose-packed lattices we now look for evidence of the 'antiferromagnetic singularity' (Sykes *et al* 1972b, Watts 1974). Accordingly, we study the closest singularity to the origin on the negative real axis in the D log $C(x)$ Padé approximants. Table 6 gives details for the square lattice. The Padé approximants have placed a pole with a positive residue just outside $x = -1/\mu(1/\mu + 0{\cdot}37898 \pm 0{\cdot}00001)$. This is the manner in which the Padé approximants would be expected to simulate a finite cusp in $C(x)$ at $x = -1/\mu$ (see Gaunt and Guttmann (1974) who discuss this point in some detail with reference to the high-temperature Ising model susceptibility). A similar behaviour is seen for the other loose-packed lattices and we conclude that the data are consistent with the presence of a singularity in $C(x)$ of the form $(1+\mu x)^{\lambda}$, $\lambda > 0$.

No strong evidence was found for the presence of singularities at $x = \pm i/\mu$ for the honeycomb or diamond lattices. This is in contrast to the Ising model susceptibility, $\chi(v)$, where the Padé method indicates singularities at $\pm i v_c$.

Table 6. Square lattice, D log Padé analysis of position (and residue) of closest singularity on negative real axis.

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
7	−0·3812(0·337)	−0·3819(0·345)	−0·3817(0·343)
8	−0·3818(0·343)	−0·3818(0·344)†	−0·3821(0·348)
9	−0·3832(0·370)†	−0·3821(0·348)	−0·3821(0·348)†
10	−0·3821(0·347)	−0·3822(0·349)†	−0·3820(0·347)
11	−0·3814(0·334)	−0·3818(0·344)	−0·3821(0·348)†
12	−0·3817(0·340)†	—	—

† Denotes presence of spurious poles inside circle of convergence.

4. Summary and conclusions

The data of table 4 are consistent with the current hypothesis that $g = \frac{1}{3}$ exactly in two dimensions and $g = \frac{1}{6}$ exactly in three dimensions. Using these values the biassed estimates for μ of table 3 were formed, which are in excellent agreement with those obtained by use of the ratio method. These biassed estimates for μ and the above simple fractions for g were used in forming estimates for the critical amplitudes (table 5).

The Padé approximants provide more evidence for the existence of an 'antiferromagnetic singularity' on the loose-packed lattices, but supply no evidence of singularities at $\pm i/\mu$ for the honeycomb and diamond lattices.

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