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Applications of Canterbury approximants to power series in critical phenomena

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Abstract. The effectiveness of Chisholm's new rational approximation scheme for functions of two variables is examined for applications to problems in the field of critical phenomena. The examples chosen are double power series expansions for the high-temperature susceptibility $\chi_0(\alpha, T)$ where the additional variable α is (i) the degree of anisotropy in the anisotropic Heisenberg model, (ii) the relative strength of second-neighbour interactions in Ising model systems and (iii) the relative strength of pair and three-spin interactions in a two-dimensional pair–triplet Ising model. In case (i) additional support is obtained for the principle of universality in relation to the discontinuous increase in the value of the exponent γ at the suspected symmetry breaking point $\eta = 1$ for *all* quantal cases.

1. Introduction

The previous paper (Roberts *et al* 1975, hereafter referred to as I) has examined the performance of Canterbury approximants (CA) on a selection of known but simple two-variable functions, and has established that Chisholm's recent two-variable approximation scheme (Chisholm 1973, Chisholm and McEwan 1974, Graves-Morris *et al* 1974, Hughes-Jones 1973 preprint) could be a successful technique in determining numerical estimates of analytic features from truncated double power series. The functions that have been tested in this way are obvious generalizations of a variety of single-variable functions chosen by Hunter and Baker (1973) in a recent survey of the efficiency of the well known Padé approximant scheme, which is widely used in the field of critical phenomena to determine the location of critical points and the values of the much studied critical exponents (for reviews of critical phenomena see Fisher 1967, Gaunt and Guttmann 1974, Wood 1974). The purpose of the present publication is in part to examine Chisholm's new scheme of rational approximation in action upon a selection of problems in critical phenomena. For such applications there will invariably be a much smaller number of terms available than in the orders of the expansions which were employed in the previous paper.

In many problems in critical phenomena the original expansion of the thermodynamic potential is naturally in terms of two or more variables; examples are when the variables are thermodynamic intensities such as temperature and magnetic field, or cases where the original set of microscopic coupling constants in the Hamiltonian leads to a set of reduced temperature variables. In our present applications of Canterbury approximants we choose the following examples from the latter type of expansions.

(i) High-temperature expansions of the susceptibility χ_0 in zero field for the general spin anisotropic Heisenberg model, which were calculated recently by Wood and

Dalton (1972). These expansions are triple power series in terms of the spin variable $X = S(S+1)$, the inverse temperature T^{-1} and the longitudinal anisotropy parameter η†.

(ii) High-temperature expansions of χ_0 for Ising model lattices in which next-nearest-neighbour (NNN) interactions are included in the Hamiltonian. These are double power series in the variables J_1/kT and the relative strengths of the nearest-neighbour (NN) (J_1) and NNN (J_2) coupling constants, $\alpha = J_2/J_1$ (Dalton and Wood 1969).

(iii) High-temperature expansions of χ_0 for the two-dimensional triangular lattice triplet Ising model which is a double power series in the variables $v_2 = \tanh J_2/kT$ and $v_3 = \tanh J_3/kT$, where J_2 and J_3 are the two-spin and three-spin coupling constants (Wood and Griffiths 1972, 1973, 1974a, Griffiths and Wood 1973, Watts 1974, Baxter and Wu 1974, Baxter 1974, Baxter *et al* 1975).

All the above susceptibility functions may be expressed as a double power series in the form

$$\frac{kT}{m^2}\chi_0 = 1+\sum_{n,m} c_{n,m}z_1^n z_2^m = 1+\sum_l P_l(z_2)z_1^l \tag{1}$$

where $P_l(z_2)$ is a polynomial of degree l; hence the coefficient matrix $\mathbf{C}(c_{n,m})$ is triangular. For such 'triangular' expansions the Canterbury approximants do not exist, and it is necessary to effect some transformation of the variables, thus filling the transformed coefficient matrix. Following the procedure outlined in I we choose the origin-preserving rotation

$$\begin{aligned} z_1 &= x+y \\ z_2 &= x-y \end{aligned} \tag{2}$$

for this purpose. In the three examples above the variable z_2 corresponds to (i) η, (ii) α and (iii) $v_2/v_3 = x$ (Wood and Griffiths 1973). In the calculation of the *critical lines* $T_c(\eta)$, $T_c(\alpha)$ and $T_c(J_3/J_2)$ and the corresponding exponents $\gamma(\eta)$, $\gamma(\alpha)$ and $\gamma(J_3/J_2)$ using Canterbury approximants, we follow the procedure of I (see also Wood and Griffiths 1974b) in obtaining the CA(n,m) to the logarithmic derivatives of the susceptibility expansions.

A secondary purpose of this paper is to present an overall study of the power series in (i), which are based upon the general spin N-site lattice Hamiltonian

$$\mathscr{H}(S) = -\sum_{\mathrm{NN}}[J^{\parallel}S_i^zS_j^z+J^{\perp}(S_i^xS_j^x+S_i^yS_j^y)]-mH\sum_{i=1}^{N}S_i^z \tag{3}$$

where the initial summation is over nearest-neighbour pairs, and the measure of the longitudinal anisotropy is the parameter $\eta = J^{\perp}/J^{\parallel}$; hence the extreme points $\eta = 0$ and $\eta = 1$ correspond to the Ising model and isotropic Heisenberg models respectively. Interest in the $S = \frac{1}{2}$ case and the analogy with the quantum lattice gas (Matsubara and Matsuda 1956) was originally stimulated by Fisher (1966) who conjectured that the susceptibility exponent γ would be fixed at its suspected Ising model value $\gamma(0) = \frac{5}{4}$ (three-dimensional lattices) on the interval $0 \leqslant \eta < 1$, and change discontinuously at $\eta = 1$ to its value for the three-dimensional Heisenberg model. There is no consensus on the value of $\gamma(1)$: Ritchie and Fisher (1972) (see also Bowers and Woolf 1969) find that $\gamma = 1{\cdot}375^{+0{\cdot}02}_{-0{\cdot}01}$ represents $\gamma(1)$ for all three-dimensional lattices and spin; however, the rival claim of $\gamma = 1{\cdot}405 \pm 0{\cdot}02$ for the infinite spin case has been given by Ferrer *et al* (1971) (for a discussion of $\gamma(1)$ see Rushbrooke *et al* 1974).

† There are two printing errors in $b_6(\eta)$ of Wood and Dalton (1972). The coefficients of $p_{5a}X^4\eta^5$ and $p_{5a}X^4\eta^6$ should read −216760320, and −92897280 respectively.

Evidence for the independence of γ on the anisotropy η is important in its support of the principle of smoothness, which was stated in general terms by Griffiths (1970) and later incorporated into the more general principle of universality (Kadanoff 1973, Watson 1969a, b, Betts *et al* 1971, Ferrer and Wortis 1972). Previous studies of the extreme quantum case $S = \frac{1}{2}$ (Dalton and Wood 1967, Jou and Chen 1973) have yielded results which are consistent with such a discontinuity in γ, but the strongest evidence so far has been obtained for the classical Heisenberg model ($s = \infty$) by Jasnow and Wortis (1968), who also distinguished between the coupling constants for the x–x and y–y spin–spin terms in (3). In terms of our longitudinal parameter these authors obtained the following result to within confidence limits of 1 or 2%.

$$\begin{array}{llllllll} \eta = 0 & 0{\cdot}2 & 0{\cdot}4 & 0{\cdot}6 & 0{\cdot}8 & 0{\cdot}9 & 1{\cdot}0 \\ \gamma = 1{\cdot}23 & 1{\cdot}23 & 1{\cdot}23 & 1{\cdot}24 & 1{\cdot}19 & 1{\cdot}19 & 1{\cdot}38. \end{array} \tag{4}$$

Following the derivation of the general spin high-temperature series for this model (Wood and Dalton 1972), which have been expressed in an algebraic form valid for an arbitrary lattice structure, it is now possible to examine this model at a variety of spin values from which we have obtained good evidence for both the initial invariance of γ, and the discontinuous change at $\eta = 1$ to be valid for all the quantal cases.

2. The anisotropic Heisenberg model with general spin

Adopting the variable z_2 in (1) as the anisotropy parameter the polynomials $P_l(\eta)$ are known through to $l = 7$ for the case $s = \frac{1}{2}$ and through to $l = 6$ for the general spin case. In table 1 we compare Jou and Chen's Padé approximant (PA) analysis of the longer $s = \frac{1}{2}$ series for χ_0 with an analysis using Canterbury approximants, which of course

Table 1. A comparison of Canterbury approximants and Padé approximant results for the predictions of the critical point function $K_c(\eta)$ for the $s = \frac{1}{2}$ anisotropic Heisenberg model on the BCC (1) and FCC (1) lattices. Listed are the deviations from the overall Padé estimates in units of 10^{-3}. The values of $K_c(1)$ are taken from Baker *et al* (1967).

η	Overall estimate using PA		CA (3, 3)		CA (2, 2)		CA (2, 3)		CA (3, 2)	
	FCC (1)	BCC (1)	FCC (1)	BCC (1)	FCC (1)	BCC (1)	FCC (1)	BCC (1)	FCC (1)	BCC (1)
0	0·204	0·315	2	5	0	3	−2	−7	3	‡
0·1	0·204	0·315	2	6	1	3	−2	−6	3	
0·2	0·205	0·316	1	6	0	4	−2	−6	3	
0·3	0·206	0·318	1	6	1	4	−2	−5	4	
0·4	0·207	0·321	2	6	2	4	1	−4	—	
0·5	0·209	0·325	2	6	3	5	3	−2	3	
0·6	0·212	0·330	2	7	3	7	−1	0	4	
0·7	0·216	0·337	2	9	5	8	−6†	4	4	
0·8	0·222	0·347	1	7	6	8	−12	13	2	
0·9	0·231	0·364	0	0	7	3	−20	26	0	
1·0	0·249	0·396	−12	−18	4	−14	−39	36	−14	

† CA diverges away rapidly beyond this point.
‡ The root appears split into two branches throughout the range.

yield one complete representation of $\chi_0(K, \eta)$ and $T_c(\eta)$ $(K = J^{\parallel}/kT)$ for each approximant (see Wood and Griffiths 1974). The lattices represented in table 1 are the nearest-neighbour body-centred cubic BCC(1) and face-centred cubic FCC(1) lattices (see Dalton and Wood 1969). The confidence limits on the Padé approximant critical points $J^{\parallel}/kT_c = K_c$ are such that the results are expected to be correct to the number of figures quoted, and for each CA we list the deviation from these results in units of 10^{-3}. Quite clearly the CA listed give an excellent representation of the function $\chi_0(K, \eta)$ over the very wide interval $0 \leqslant \eta \lesssim 0{\cdot}9$ for both lattices; the representations appear to deteriorate beyond $\eta = 0{\cdot}9$. It is our experience that such a good fit with this number of terms is over a much wider range than might normally be expected for such complex functions. The corresponding comparison for the numerical estimates of the critical exponent γ is given in table 2. For these $s = \frac{1}{2}$ models the confidence limits of the overall estimates in the region $\eta \to 1$ deteriorate; however, the evidence of a discontinuous change in γ is much stronger in the overall Padé results than could be obtained from the corresponding CA; this is to be expected in view of the wide range in η needed for a good fit near $\eta = 1$.

Table 2. The unbiased estimates of $\gamma(\eta)$ obtained from the diagonal Canterbury approximants in table 1

η	Overall estimate using PA†		CA (3, 3)		CA (2, 2)	
	FCC (1)	BCC (1)	FCC (1)	BCC (1)	FCC (1)	BCC (1)
0	1·25±0·01	1·24±0·02	1·29	1·36	1·26	1·31
0·1	1·25±0·01	1·24±0·02	1·29	1·36	1·26	1·31
0·2	1·25±0·01	1·24±0·03	1·29	1·35	1·26	1·31
0·3	1·24±0·02	1·23±0·03	1·28	1·35	1·26	1·31
0·4	1·24±0·02	1·23±0·03	1·30	1·34	1·27	1·30
0·5	1·24±0·02	1·22±0·04	1·28	1·34	1·27	1·30
0·6	1·23±0·03	1·21±0·04	1·29	1·35	1·28	1·30
0·7	1·23±0·03	1·21±0·04	1·29	1·47	1·29	1·30
0·8	1·23±0·03	1·21±0·04	1·31	1·34	1·29	1·30
0·9	1·24±0·03	1·22±0·04	1·32	1·33	1·28	1·30
1·0	1·38±0·03	1·38±0·04	1·35	1·33	1·25	1·30

† These results are reported by Jou and Chen (1973); the recent estimates of $\gamma(0)$ (Domb 1974) confirm the value of $\frac{5}{4}$ (for all three-dimensional lattices) to within error bounds of 10^{-3}.

What the CA do very clearly support however is an invariance in $\gamma(\eta)$ as η increases away from the Ising model limit $\eta = 0$, thus providing additional numerical support to the principle of universality (Kadanoff 1973, Griffiths 1970, Kadanoff and Wegner 1971, Wilson 1971, Ferrer and Wortis 1972).

The generalized lattice form of the expansion of Wood and Dalton (1972) and Jou and Chen (1973) enables these series to be developed for the $s = \frac{1}{2}$ equivalent-neighbour (EN) model lattices (BCC (1, 2) etc) in which both NN and NNN interactions are equal. This effectively defines a new lattice of higher coordination number (Dalton and Wood 1969, Bowers and Woolf 1969). The CA (2, 2) and CA (3, 3) for the BCC (1, 2) and FCC (1, 2) anisotropic Heisenberg model lattices are listed in table 3. The CA behave remarkably well giving a good representation of $\chi_0(K, \eta)$ over the whole range; the confidence limit in the CA (3, 3) critical point varies from $\frac{1}{2}\%$ to 4% between the points $\eta = 0$ and $\eta = 1$ respectively, and the CA (3, 3) for the BCC (1, 2) series $(q = 14)$ is beginning to evidence a rapid change in γ near $\eta = 1$, as well as very clearly suggesting that γ is invariant to

Table 3. The unbiased estimates of the critical point $K_c(\eta)$ and susceptibility exponent γ obtained from the diagonal Canterbury approximants for the equivalent-neighbour model lattices FCC (1, 2) and BCC (1, 2); the independent estimates of $K_c(0)$ are respectively 0·1291 and 0·1720 and of $K_c(1)$, 0·1474 and 0·203

η	CA (2, 2)				CA (3, 3)			
	$K_c(\eta)$		$\gamma(\eta)$		$K_c(\eta)$		$\gamma(\eta)$	
	FCC (1, 2)	BCC (1, 2)	FCC (1, 2)	BCC (1, 2)	FCC (1, 2)	BCC (1, 2)	FCC (1, 2)	BCC (1, 2)
0	0·1286	0·1719	1·21	1·25	0·1286	0·1723	1·21	1·26
0·1	0·1286	0·1721	1·21	1·25	0·1286	0·1724	1·21	1·26
0·2	0·1288	0·1726	1·21	1·25	0·1288	0·1729	1·21	1·26
0·3	0·1291	0·1736	1·21	1·25	0·1291	0·1737	1·21	1·26
0·4	0·1296	0·1751	1·20	1·26	0·1297	0·1749	1·20	1·26
0·5	0·1304	0·1773	1·20	1·26	0·1305	0·1766	1·20	1·27
0·6	0·1315	0·1805	1·20	1·27	0·1316	0·1789	1·20	1·27
0·7	0·1329	0·1850	1·20	1·28	0·1331	0·1819	1·21	1·28
0·8	0·1346	0·1917	1·22	1·28	0·1349	0·1856	1·22	1·29
0·9	0·1366	0·2015	1·23	1·27	0·1372	0·1900	1·23	1·31
1·0	0·1390	0·2161	1·24	1·24	0·1398	0·1953	1·25	1·34

$\eta(\neq 1)$. It is a simple matter to establish that $\lim \eta \to 0\, \mathrm{d}K_c(\eta)/\mathrm{d}\eta = 0$ for all lattices (Jou and Chen 1973); thus we see that the Canterbury approximants are also very clearly reproducing this qualitative detail in the function $K_c(\eta)$.

In tables 2 and 3 the discrepancies shown by the CA (2, 2) and CA (3, 3) in the estimates of γ between the two lattices are in our view a result of different convergence errors at these low orders, and do not represent a change in the exponent between the two lattices. The errors in a CA analysis are very likely to be dependent upon the magnitude of the singularity; this follows from the empirical relationship between the rotation of the axes and the size of the error which was discussed in I. Thus with the rotation used in tables 1 and 2 the errors for the FCC lattice should be less than those of the BCC lattice at $\eta = 0$, with the relative error decreasing towards $\eta = 1$. This appears to be the case if $\gamma = \frac{5}{4}, \eta \neq 1$. Similar effects apply to table 3, although here the error differences might be expected to be smaller; thus differences of this type might occur more frequently in using a CA analysis than one encounters in a corresponding Padé analysis.

The very good performance of the Canterbury approximants for the $s = \frac{1}{2}$ series expansions in tables 1, 2 and 3 rapidly deteriorates for the corresponding series of the higher-spin models; typically for the cases $s = 1$ and $\frac{3}{2}$ the range over which a good representation of $\chi_0(K, \eta)$ is obtained is much reduced, and individual CA often fail to approximate any physical singularities over the whole range of η. These general spin expansions contain one less term than the $s = \frac{1}{2}$ case; however, the Padé approximants appear to yield a very accurate representation of $\chi_0(K)$ at discrete intervals of η, indicating confidence limits on $K_c(\eta)$ which vary from 0·1% to 0·5% from the end-points $\eta = 0$ and $\eta = 1$ respectively. These numerical values are of little interest and are not listed here; however, the behaviour of $\gamma(\eta)$ is of interest and has not previously been examined for the general spin cases. In table 4 we record the behaviour of $\gamma(\eta)$ as given by the Padé approximants to the logarithmic derivative of χ_0 for the BCC (1) lattice (the FCC (1) results are essentially of the same behaviour). If one accepts the Ising model value of $\gamma(0) = 1·25$ then the Padé approximants [2, 3] and [3, 2] are approximating γ to

Table 4. The Padé approximant representation of the behaviour of $\gamma(\eta)$ for the cases $s = 1$ and $s = \frac{3}{2}$ on the BCC (1) lattice.

η	$s = 1$		$s = \frac{3}{2}$	
	[3, 2]	[2, 3]	[3, 2]	[2, 3]
0	1·22	1·23	1·20	1·21
0·1	1·22	1·22	1·20	1·21
0·2	1·22	1·22	1·20	1·20
0·3	1·22	1·22	1·20	1·21
0·4	1·21	1·22	1·20	1·21
0·5	1·21	1·21	1·20	1·20
0·6	1·21	1·21	1·20	1·20
0·7	1·21	1·22	1·20	1·20
0·8	1·23	1·24	1·22	1·23
0·9	1·27	1·29	1·27	1·27
1·0	1·39	1·39	1·38	1·38

within 2–4% at $\eta = 0$, and the evidence for the invariance of $\gamma(\eta)$ ($\eta \neq 1$) and the discontinuous jump at $\eta = 1$ to $\gamma(1) = 1{\cdot}38 \pm 0{\cdot}01$ is very good. Combining these results with the previous work of Jasnow and Wortis (1968) probably represents the best non-trivial example of the association between a break in the symmetry of the interaction Hamiltonian and a discontinuous change in the critical exponents, originally proposed by Griffiths (1970).

A further problem of interest concerns the critical behaviour of two-dimensional anisotropic Heisenberg models, where there is controversy over the question of the existence of a phase transition in two-dimensional isotropic Heisenberg model systems (Stanley and Kaplan 1966, Mermin and Wagner 1966, Wegner 1971, Yamaji and Kondo 1973, Kosterlitz and Thouless 1973, Kosterlitz 1974, Camp and VanDyke 1975, Bloembergen 1975). The present series expansions allow one to examine the approach of $T_c(\eta)$ to $T_c(1)$ for a two-dimensional network using both Padé and Canterbury approximants for any spin value; thus, assuming that $T_c(\eta)$ is continuous in the region $\eta \to 1$, additional information on this question can be obtained. For both the square (SQ) and triangular lattices the Padé approximants fail to give a representation of a physical singularity beyond $\eta \simeq 0{\cdot}8$ (Jou and Chen 1973) for the $s = \frac{1}{2}$ model. By comparison the Canterbury approximants yield a representation of $\chi_0(K, \eta)$ which evidences the existence of a critical point over the whole range $\eta = 0, 1$. The CA (2, 2) and CA (3, 2) estimates of $T_c(\eta)/kJ^{\parallel}$ are compared with the overall Padé approximant results of Jou and Chen in figure 1 for the triangular lattice. Similar calculations using the CA (2, 2) and CA (3, 3) for the triangular lattice with equivalent NN and NNN interactions very clearly indicate a *continuous* line of critical points which intersect the $\eta = 1$ axis; the results are

	$\eta = 0$	0·1	0·2	0·3	0·4	
CA (2, 2) K_c	= 0·2287	0·2287	0·2287	0·2288	0·2293	
CA (3, 3) K_c	= 0·2271	0·2272	0·2275	0·2281	0·2290	
	$\eta = 0{\cdot}5$	0·6	0·7	0·8	0·9	1·0
CA (2, 2) K_c	= 0·2302	0·2318	0·2341	0·2371	0·2410	0·2458
CA (3, 3) K_c	= 0·2306	0·2327	0·2357	0·2395	0·2443	0·2501

(5)

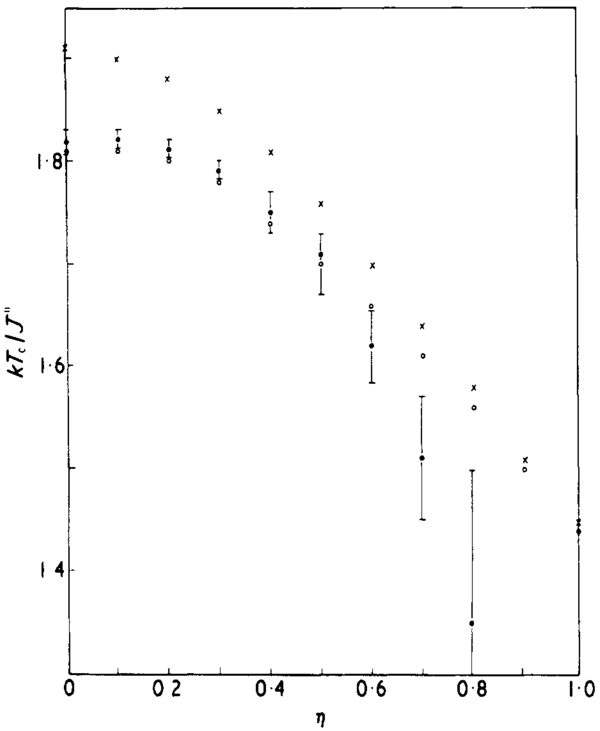

Figure 1. A comparison of the predictions for the existence of a critical point covering the interval $0 \leqslant \eta \leqslant 1$ for the two-dimensional triangular lattice obtained from Padé and Canterbury approximants. × : CA (3, 2); ○ : CA (2, 2); and ⧳ : PA results from Jou and Chen (1973).

A corresponding analysis of the general spin series using Padé approximants supports the existence of a phase transition for two-dimensional Heisenberg models; a summary of the calculations for the SQ lattice is given in table 5. The evidence for

Table 5. A two-dimensional (SQ lattice) Heisenberg model for cases $s = 1, \frac{3}{2}$ and 2. The overall Padé approximant results for the critical point $K_c(\eta)$ are listed together with an unbiased estimate of $\gamma(\eta)$ taken from the Padé approximant which yields the closest fit to $K_c(\eta)$.

η	$s = 1$		$s = \frac{3}{2}$		$s = 2$	
	$K_c(\eta)$	$\gamma(\eta)$	$K_c(\eta)$	$\gamma(\eta)$	$K_c(\eta)$	$\gamma(\eta)$
0	0·293	1·79	0·151	1·76	0·0930 ± 0·0001	1·74
0·1	0·294	1·78	0·151	1·76	0·0931 ± 0·0001	1·74
0·2	0·296	1·76	0·152	1·74	0·0936 ± 0·0001	1·72
0·3	0·299	1·71	0·154	1·70	0·0944 ± 0·0001	1·69
0·4	0·305	1·66	0·156	1·66	0·0956 ± 0·0001	1·66
0·5	0·313 ± 0·001	1·62	0·158 ± 0·001	1·61	0·0972 ± 0·0002	1·61
0·6	0·323 ± 0·001	1·60	0·165 ± 0·001	1·59	0·0990 ± 0·001	1·58
0·7	0·338 ± 0·001	1·64	0·170	1·62	0·104 ± 0·001	1·60
0·8	0·360 ± 0·001	1·76	0·180 ± 0·001	1·72	0·109 ± 0·001	1·70
0·9	0·40 ± 0·02	2·06	0·190 ± 0·01	2·01	0·117 ± 0·002	1·98
1·0	0·50 ± 0·05	3·20	0·24 ± 0·01	3·44	0·14 ± 0·02	3·51

universality in relation to $\gamma(\eta)$ is also good, with an indication of a jump in the value of γ at $\eta = 1$; the data suggest $\gamma = 3{\cdot}5 \pm 0{\cdot}5$ (assuming γ to be spin invariant). Recently Yamaji and Kondo (1973) have provided two additional terms to the susceptibility expansion of the two-dimensional isotropic models. In a Padé approximant analysis of the effect of the extra terms these authors find that many off-diagonal approximants possess no positive real singularity, and suggest that the susceptibility is finite for all temperatures. However their additional diagonal and para-diagonal approximants still yield real singularities in χ_0 which are consistent with the lower-order approximants corresponding to the order of the approximants in table 5.

3. Further applications of Chisholm approximants

Further examples of double power series in critical phenomena are the high-temperature expansions of Dalton and Wood (1969) for Ising model ($s = \frac{1}{2}$) systems which include interactions over NNN distances; thus the interaction Hamiltonian is given by

$$\mathscr{H} = -J_1 \sum_{\text{NN}} \sigma_i\sigma_j - J_2 \sum_{\text{NNN}} \sigma_k\sigma_l - mH \sum_{i=1}^{N} \sigma_i \tag{6}$$

where the relative strengths of the NN and NNN interactions can be measured by the parameter $\alpha = J_2/J_1$ (see § 1). The polynomials $P_l(\alpha)$ in (1) are known through to $l = 6$ for a variety of common lattices. On the whole a numerical analysis of the power series of the function $\chi_0(\alpha, K)$ ($K = J_1/kT$) using CA yields much inferior results to the previous expansions in § 2, and to parallel PA calculations.

The n-variable rational approximation scheme of Chisholm and McEwan (1974) possesses the important projective property that if any k-variables are set to zero, the approximants in the $N-k$ variables formed from the corresponding power series are obtained. Thus in the two-variable case the CA (n, m) to a function $F(z_1, z_2)$ reduce to the $[n, m]$ Padé approximants of $F(z_1, 0)$ and $F(0, z_2)$ when $z_2 = 0$ and $z_1 = 0$ respectively. In cases where the Padé approximants to $F(z_1, 0)$, say, yield highly convergent results (as is common in the analysis of power series in critical phenomena), there can be high expectations for the CA to $F(z_1, z_2)$ at the point $z_2 = 0$ (the results will not be identical in many cases because of the rotation operation in (2)) and therefore one might expect reliable results to extend over a range of z_2 centred on $z_2 = 0$. A good fit centred on the zero of one of the variables is indeed a characteristic feature of the majority of CA calculated by the authors and is well illustrated by the examples given in table 6 and figure 2 for the function $\chi_0(K, \alpha)$ on the BCC and FCC lattices.

In this instance the projective property of the CA can be employed to shift the centre of the range where a good fit is obtained from the point $\alpha = 0$ to $\alpha = 1$. If we rewrite (6) in the form

$$\mathscr{H} = -J_1\left(\sum_{\text{EN}} \sigma_i\sigma_j - \alpha' \sum_{\text{NNN}} \sigma_k\sigma_l\right) - mH \sum_{i=1}^{N} \sigma_i \tag{7}$$

where the initial summation is over equivalent NN and NNN interactions, thus developing the power series for $\chi_0(K, \alpha')$ ($\alpha' = 1-\alpha$), the PA and CA will coincide at the new zero $\alpha' = 0$ ($\alpha = 1$) and a good fit can be anticipated to be centred on the point $\alpha = 1$. This shift in the origin of a good fit is illustrated in figure 2 and table 6 where the CA of $\chi_0(K, \alpha')$ ($\alpha' = 1-\alpha$) are compared with the CA of $\chi_0(K, \alpha)$. In the case of the BCC lattice the

Table 6. Some Canterbury approximants relating to the functions $\chi_0(\alpha, K)$ and $\chi_0(\alpha', K)$ ($\alpha = 1-\alpha'$) for the second-neighbour Ising model on the BCC and FCC lattices ($\alpha = J_2/J_1$).

	BCC					FCC				
α	Independent estimate of $K_c(\alpha)$	CA (2, 2) to $\chi_0(K, \alpha)$		CA (2, 2) to $\chi_0(K, \alpha')$		Independent estimate of $K_c(\alpha)$	CA (3, 2) to $\chi_0(K, \alpha)$		CA (3, 2) to $\chi_0(K, \alpha')$	
		$K_c(\alpha)$	$\gamma(\alpha)$	$K_c(\alpha)$	$\gamma(\alpha)$		$K_c(\alpha)$	$\gamma(\alpha)$	$K_c(\alpha)$	$\gamma(\alpha)$
0	0·157	0·158	1·26			0·102	0·102	1·26		
0·1	0·145	0·145	1·26			0·0962	0·0962	1·25		
0·2	0·134	0·135	1·26			0·0912	0·0912	1·24		
0·3	0·125	0·128	1·27			0·0864	0·0871	1·24		
0·4	0·117	0·124†				0·0823	0·0842	1·25		
0·5	0·111					0·0786	0·0821	1·26	0·0744†	
0·6	0·104			0·133†	1·21	0·0753	0·0812†	1·27	0·0728	1·24
0·7	0·0991			0·104	1·29	0·0722			0·0709	1·20
0·8	0·0943			0·0951	1·26	0·0694			0·0686	1·20
0·9	0·0899			0·0900	1·25	0·0669			0·0669	1·21
1·0	0·0860			0·0859	1·25	0·0645			0·0640	1·20

† The approximations either fail or rapidly deteriorate beyond this point.

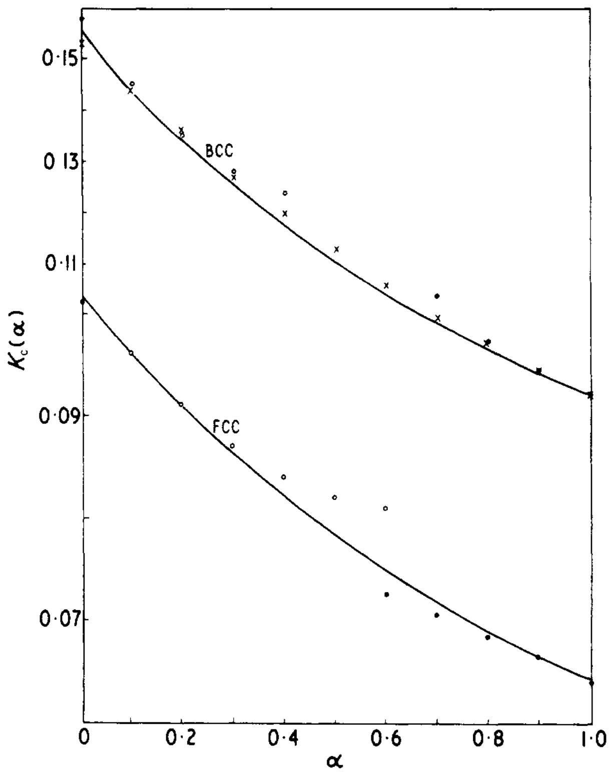

Figure 2. A comparison of the critical points $T_c(\alpha)$ obtained from the Canterbury approximants to $\chi_0(\alpha, K)$ and $\chi_0(\alpha', K)$ ($\alpha = 1-\alpha'$) and the independent estimates based upon PA methods for the second-neighbour Ising model on the BCC and FCC lattices. For the BCC lattice ○ and ● are the CA (2, 2) points to $\chi_0(\alpha, K)$ and $\chi_0(\alpha', K)$ respectively, and × is the CA (3, 2) to $\chi_0(\alpha', K)$. For the FCC lattice ○ and ● are the CA (3, 2) points to $\chi_0(\alpha, K)$ and $\chi_0(\alpha', K)$ respectively.

CA (3, 2) to $\chi_0(K, \alpha')$ yields superior results to any of the CA to the function $\chi_0(K, \alpha)$. The numerical results clearly support the invariance of γ to the value of α over the range $\alpha = 0, 1$ (Wilson 1971); the CA to $\chi_0(\alpha, K)$ also give a clear indication that $\gamma(\alpha)$ also remains constant for the initial negative values; a typical example is the CA (2, 2) for the BCC lattice where we obtain

$$\begin{array}{lllll} \alpha = & -0{\cdot}1 & -0{\cdot}2 & -0{\cdot}3 & -0{\cdot}4 \\ \gamma = & 1{\cdot}26 & 1{\cdot}26 & 1{\cdot}25 & 1{\cdot}24. \end{array} \tag{8}$$

Some recent and interesting examples of double power series have arisen from the study of Ising models which include three-spin coupling terms in the Hamiltonian function. An example of particular interest is the two-dimensional triangular lattice with an interaction Hamiltonian in the form

$$\mathscr{H} = -J_2 \sum_{\mathrm{NN}} \sigma_i\sigma_j - J_3 \sum_{\mathrm{TRI}} \sigma_i\sigma_j\sigma_k - mH \sum_{i=1}^{N} \sigma_i \tag{9}$$

(Wood and Griffiths 1972, 1973, 1974a, Griffiths and Wood 1973, Watts 1974, Baxter and Wu 1974, Baxter 1974, Baxter *et al* 1975). In the zero-field case ($H = 0$) the exact solution for the thermodynamic functions (principally the specific heat) for this model is known at the extreme points $J_3 = 0$ (the conventional Ising model) and $J_2 = 0$ (the pure triplet model, Baxter and Wu 1974). The particularly interesting feature of this model is the change in the critical exponent α (the specific heat) from a weak logarithmic form ($\alpha = 0$) when $J_3 = 0$ to a strong branch-point singularity with $\alpha = \frac{2}{3}$ at $J_2 = 0$. The recently conjectured solution for the magnetization function of the pure triplet case (Baxter *et al* 1975) yields the critical exponent $\beta = \frac{1}{12}$ (compared with $\beta = \frac{1}{8}$ for the pure pair case). Hence assuming the scaling theory to remain valid, the susceptibility exponent γ should change from the value $\frac{7}{4}$ at $J_3 = 0$ to $\frac{7}{6}$ at $J_2 = 0$. The high-temperature polynomials $P_l(\alpha)$ ($\alpha = J_3/J_2$) in (1) have been obtained for the model Hamiltonian (9) through to order $l = 6$ (Wood and Griffiths 1973). A summary of the PA analysis of this series is given in table 7 which also includes the CA (2, 2) estimates of $v_c = \tanh(J_2/kT_c)$ for comparison. Such a small number of terms for a model of this type is unlikely to yield enough members of PA and CA sequences to draw firm conclusions; it is therefore interesting to see that the qualitative behaviour of the function $v_c(\alpha)$ obtained from the CA (2, 2) is in agreement with the overall PA analysis. In this instance the two schemes PA and CA act in a manner which lends qualitative support to each other. The confidence

Table 7. A summary of the PA analysis and the CA (2, 2) of the susceptibility function $\chi_0(\alpha, v)$ ($\alpha = J_3/J_2$) for the two-dimensional pair–triplet Ising model of equation (7) ($v = \tanh J_2/kT$).

α	PA summary	CA (2, 2)	PA summary
	v_c	v_c	$\gamma(\alpha)$
0	$0{\cdot}267 \pm 0{\cdot}001$†	0·244	$1{\cdot}70 \pm 0{\cdot}05$
0·10	$0{\cdot}261 \pm 0{\cdot}001$	0·237	$1{\cdot}65 \pm 0{\cdot}1$
0·20	$0{\cdot}244 \pm 0{\cdot}001$	0·223	$1{\cdot}46 \pm 0{\cdot}03$
0·29	$0{\cdot}223 \pm 0{\cdot}003$	0·209	$1{\cdot}26 \pm 0{\cdot}1$
0·39	$0{\cdot}202 \pm 0{\cdot}004$	0·195	$1{\cdot}1 \pm 0{\cdot}1$
0·50	$0{\cdot}180 \pm 0{\cdot}006$	0·183	$1{\cdot}0 \pm 0{\cdot}15$

† The exact value at $\alpha = 0$ is $v_c = 2 - \sqrt{3} = 0{\cdot}2679\ldots$.

limits given for the PA estimates of $\gamma(\alpha)$ at fixed values of α are probably exaggerated by the small number of PA available. Even allowing for this, a rapid decline in the value of $\gamma(\alpha)$ in the region of $\alpha = \frac{1}{5}$ is perhaps suggested by these data.

4. Summary and conclusions

The effectiveness of Chisholm's new rational approximation scheme for functions of two variables has been examined for use on difficult problems which arise in the field of critical phenomena where the thermodynamic functions are naturally in terms of two or more variables. The overall prognosis for such two-variable approximants is good; they are however likely to be restricted in their application to these problems by the often much reduced number of terms available in such double power series. This is a natural consequence of the added complexity in deriving the power series originally, and it is unlikely that they will be as extensively tested and successful as have been the now widely used and related Padé approximant techniques.

Even with a restricted number of terms available in the examples included in §§ 2 and 3 we have found a case where the CA yield a good representation, and the corresponding PA method fails to obtain any physical singularity. This is the susceptibility $\chi_0(K, \eta)$ of the two-dimensional Heisenberg model lattices for the extreme quantal case $s = \frac{1}{2}$.

At the present time our experience in many CA calculations to two-variable functions $F(z_1, z_2)$ indicates that a good representative fit to $F(z_1, z_2)$ can be expected in a region centred on the zero value of either z_1 or z_2; this is particularly the case when the PA sequences to either $F(z_1, 0)$ or $F(0, z_2)$ are rapidly convergent. In cases similar to the susceptibility function $\chi_0(K, \alpha)$ of the second-neighbour Ising models (§ 3) the centre of this 'good fitting' region may be translated to an alternative value of z_2 by simply changing the origin under $z_2' = 1 - z_2$ which effectively redefines the perturbation term in the Hamiltonian (see (7)).

In many cases for these problems it is of interest to obtain the qualitative behaviour of one critical parameter under the variation of some microscopic interaction parameter. The Canterbury approximants are ideally suited for such purposes since they approximate directly such functional relationships. An example of such qualitative information is very well illustrated by the CA predictions for the behaviour of $\gamma(\eta)$ listed in table 3 for the three-dimensional anisotropic Heisenberg model lattices. The evidence for the invariance of $\gamma(\eta)$ is excellent; thus in this instance the CA have given new numerical support to the universality principle of critical phenomena.

A secondary purpose of this paper has been to present new evidence for (i) the discontinuous jump in the susceptibility exponent $\gamma(\eta)$ at the isotropic limit point $\eta = 1$ and (ii) the existence of a phase transition for the two-dimensional isotropic Heisenberg models. The recent series expansions of $\chi_0(K, \eta, S)$ obtained by Wood and Dalton (1972) for the general spin Heisenberg model have been examined, and some of the results are presented in tables 4 and 5. Both the invariance of $\gamma(\eta)$ in the range $0 \leqslant \eta < 1$ and the discontinuous jump at $\eta = 1$ are supported with surprising precision, which places the earlier evidence of Jasnow and Wortis (1968) in support of the universality postulate, obtained for the classical Heisenberg limit ($s = \infty$), as being undoubtedly valid for *all* the quantal cases. The analysis of these general spin series also lends support to the existence of a phase transition in two-dimensional Heisenberg models ($\eta = 1$) with a *continuous* line of critical points over the interval $0 \leqslant \eta \leqslant 1$; also suggested is a large increase in γ at $\eta = 1$.

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References

Baker G A, Gilbert H, Eve J and Rushbrooke G S 1967 *Phys. Rev.* **164** 1566–77
Baxter R J 1974 *Aust. J. Phys.* **27** 369–81
Baxter R J, Sykes M F and Watts M G 1975 *J. Phys.* A: *Math. Gen.* **8** 245–51
Baxter R J and Wu F Y 1974 *Aust. J. Phys.* **27** 357–67
Betts D D, Guttmann A J and Joyce G S 1971 *J. Phys.* C: *Solid St. Phys.* **4** 1994–2008
Bloembergen P 1975 *University of Amsterdam* Preprint
Bowers R G and Woolf M E 1969 *Phys. Rev.* **177** 917–32
Camp W J and VanDyke J P 1975 *J. Phys.* C: *Solid St. Phys.* **8** 336–52
Chisholm J S R 1973 *Math. Comput.* **27** 841–8
Chisholm J S R and McEwan J 1974 *Proc. R. Soc.* A **336** 421–52
Dalton N W and Wood D W 1967 *Proc. Phys. Soc.* **90** 459–74
—— 1969 *J. Math. Phys.* **10** 1271–1302
Domb C 1974 *Phase Transitions and Critical Phenomena* vol 3, eds C Domb and M S Green (New York: Academic Press) pp 357–484
Ferrer M, Moore M A and Wortis M 1971 *Phys. Rev.* B **4** 3954–63
Ferrer M and Wortis M 1972 *Phys. Rev.* B **6** 3426–44
Fisher M E 1966 *Phys. Rev. Lett.* **16** 11–4
—— 1967 *Rep. Prog. Phys.* **30** 615–730
Gaunt D S and Guttmann A J 1974 *Phase Transitions and Critical Phenomena* vol 3, eds C Domb and M S Green (New York: Academic Press) pp 181–243
Graves-Morris P, Hughes-Jones R and Makinson G 1974 *J. Inst. Math. Applic.* **13** 311–20
Griffiths R B 1970 *Phys. Rev. Lett.* **24** 1479–80
Griffiths H P and Wood D W 1973 *J. Phys.* C: *Solid St. Phys.* **6** 2533–55
Hunter D L and Baker G A 1973 *Phys. Rev.* B **7** 3346–92
Jasnow D and Wortis M 1968 *Phys. Rev.* **176** 739–50
Jou D C and Chen H H 1973 *J. Phys.* C: *Solid St. Phys.* **6** 2713–20
Kadanoff L P 1973 *Varenna Conf. on Phase Transitions* 1970 (New York: Academic Press)
Kadanoff L P and Wegner F J 1971 *Phys. Rev.* B **4** 3989–93
Kosterlitz J M 1974 *J. Phys.* C: *Solid St. Phys.* **7** 1046–60
Kosterlitz J M and Thouless D J 1973 *J. Phys.* C: *Solid St. Phys.* **6** 1181–1203
Matsubara T and Matsuda H 1956 *Prog. Theor. Phys.* **16** 569–82
Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133–6
Ritchie D S and Fisher M E 1972 *Phys. Rev.* **5** 2668–92
Roberts D, Griffiths H P and Wood D W 1975 *J. Phys.* A: *Math. Gen.* **8** 1365–72
Rushbrooke G S, Baker G A and Wood P J 1974 *Phase Transitions and Critical Phenomena* vol 3, eds C Domb and M S Green (New York: Academic Press) pp 245–355
Stanley H E and Kaplan T A 1966 *Phys. Rev. Lett.* **17** 913–5
Watson P G 1969a *J. Phys.* C: *Solid St. Phys.* **2** 1883–5
—— 1969b *J. Phys.* C: *Solid St. Phys.* **2** 2158–9
Watts M G 1974 *J. Phys.* A: *Math. Nucl. Gen.* **7** L85–8
Wegner F J 1971 *J. Math. Phys.* **14** 1715–22
Wilson K G 1971 *Phys. Rev.* B **4** 3174–205
Wood D W 1975 *Statistical Mechanics*, vol 2 (London: Chemical Society) pp 55–187
Wood D W and Dalton N W 1972 *J. Phys.* C: *Solid St. Phys.* **5** 1675–86
Wood D W and Griffiths H P 1972 *J. Phys.* C: *Solid St. Phys.* **5** L253–5
—— 1973 *J. Math. Phys.* **14** 1715–229
—— 1974a *J. Phys.* C: *Solid St. Phys.* **7** 1417–27
—— 1974b J. *Phys.* A: *Math. Nucl. Gen.* **7** L101–4
Yamaji K and Kondo J 1973 *J. Phys. Soc. Japan* **35** 25–32