Pramāṇa, Vol. 22, No. 5, May 1984, pp. 407–419. © Printed in India.

Perturbation expansions and series acceleration procedures: Part-II. Extrapolation techniques

M V SANGARANARAYANAN and S K RANGARAJAN

Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560 012, India

Abstract. Three new procedures for the extrapolation of series coefficients from a given power series expansion are proposed. They are based on (i) a novel resummation identity, (ii) parametrised Euler transformation (PET) and (iii) a modified PET. Several examples taken from the Ising model series expansions, ferrimagnetic systems, etc., are illustrated. Apart from these applications, the higher order virial coefficients for hard spheres and hard discs have also been evaluated using the new techniques and these are compared with the estimates obtained by other methods. A satisfactory agreement is revealed between the two.

Keywords. Ising models; parametrised Euler transformation; virial coefficients; hard spheres; hard discs.

1. Introduction

The problem of extrapolation of power series arises in varied contexts. We may cite as examples perturbation expansions associated with several statistical mechanical models in the context of phase transitions and critical phenomena (Gaunt and Guttman 1974). There are several problems in fluid mechanics (van Dyke 1975) and other areas of model analysis where one resorts to extrapolation techniques when the series appears to converge slowly or when one wants to extend its domain of applicability. This is particularly reflected in the evaluation of higher order virial coefficients of hard spheres and discs wherein the computed values of pressure from the partial virial series are not in agreement with those anticipated from the molecular dynamics calculations (Alder and Wainright 1960). Further, the exact evaluation of the higher order virial coefficients involves enormous computational difficulty, for example, to estimate the eighth virial coefficient in hard spheres, more than 600 cluster integrals are to be calculated and this is a prohibitive task. Similarly in the context of phase transitions, the various thermodynamic functions (like magnetisation or susceptibility) are reported as perturbation expansions in the appropriate field variables. Here again, a knowledge of the coefficients of higher powers of the field parameters is rendered difficult due to the labour involved in the enumeration (and contribution) of graphs. Needless to emphasize that, in the absence of exact solutions (even for idealised models) these coefficients assume a greater significance as these are our only aids to obtain information about possible singular/critical properties.

Earlier approaches to this problem of extrapolation of a partial power series made use of Darboux theorem (Darboux 1878) or curve fitting methods. In recent terms, extensive applications of the so-called Padé approximations (Baker and Graves-Morris 1981), have demonstrated the usefulness of this approach. Stated briefly, the Padé approximant (PA) is a particular class of rational polynomial approximation to a given function which is incompletely specified (*eg*., partial power series). Several generalisations of PA, especially the so-called d log Padé approximants have been quite valuable in providing estimates of the critical parameters for model systems (Hunter and Baker 1973; Baker and Hunter 1973). For multivariable power series, the partial differential approximant (PDA) has been introduced (Chisholm 1973; Roberts *et al* 1975; Stilck and Salinas 1981; Fisher and Styer 1982) for approximating functions of two or more variables. Apart from these rigorous analyses, empirical/intuitive approaches have also been employed (Carnahan and Starling 1969; Baram and Luban 1978) especially in liquid state physics.

2. Novel extrapolation procedures

In this paper, we present three methods hitherto unused in the context of extrapolation of coefficients of a given power series. These are (i) A novel resummation identity based on the expansion of Bessel functions (Sangaranarayanan and Rangarajan 1983a); (ii) parametrised Euler transformation (PET) (Bhattacharyya 1982), and (iii) a modified version of PET.

First, we apply the above methods to a few Ising model series expansions for which the coefficients are known, so as to facilitate a comparison and later to other problems such as (i) the Ising ferrimagnets, (ii) many-fermion systems and (iii) the evaluation of virial coefficients attempting to predict the as yet unknown (exact) ones.

3. Extrapolation from the identity

Consider a series given by

$$f(\rho) = \sum_{n=0}^{\infty} f_n \rho^n. \tag{1}$$

For the series given by (1), an identity of the form

$$\sum_{n=0}^{\infty} f_n \rho^n = \sum_{n=0}^{\infty} \varepsilon_n I_n(m\rho) T_n^f(1/m), \tag{2}$$

formally holds. There is no restriction on the range of m to be used in (2) except possibly those dictated by considerations of convergence. It is easy to see that (2) is indeed formally true—as can be verified by comparing the coefficients of power of ρ on either side of (2).

In (2), $I_n(x)$ is the modified Bessel function (Abramovitz and Stegun 1964), $T_n^f(1/m)$ is a polynomial of degree n in the auxiliary variable m and whose coefficients depend on $\{f_n\}$ as indicated below and $\varepsilon_n = 1$, $n = 0$

$= 2$, otherwise.

$T_n^f(m)$ is the polynomial sequence defined by

$$T_0^f(m) = 1; \quad T_1^f(m) = f_1/m; \quad T_2^f(m) = 4f_2/m^2 - 1$$
$$T_3^f(m) = 24f_3/m^3 - 3f_1/m; \quad T_4^f(m) = 192f_4/m^4 - 16f_2/m^2 + 1, \ldots \tag{3}$$

Note the resemblance in the structure of the above polynomial sequence to the well-known Chebyshev polynomials (Abramovitz and Stegun 1964).

By assuming $F(\rho)$ to be $\exp(m\rho)$ and identifying $1/m$ with $\cos\theta$, (2) leads to the well-known expansion (Abramovitz and Stegun 1964)

$$\exp(\rho\cos\theta) = I_0(\rho) + 2\sum_{n=1}^{\infty} I_n(\rho)\cos(n\theta). \tag{4}$$

Equation (2) is only one of the many identities of the Fourier-Bessel type. Many variations of (2) also exist that provide similar expansions in terms of special functions like the Legendre and Laguerre polynomials and generalisations to several variables are also available (Rangarajan 1983) but are not reproduced here. What interests us in this context is in demonstrating the application of (2) in deducing the extrapolated coefficients of a given polynomial sequence. For example, the given sequence of coefficients $\{f_n\}$, $n = 0, 1, \ldots (N-1)$, can be extrapolated by exploiting the expansion of the Bessel function in (2) to predict estimates for f_N and f_{N+1}, say.

3.1 *Susceptibility series: simple cubic lattice*

As an illustration, consider the reduced high temperature susceptibility series for a simple cubic lattice (Domb and Sykes 1961).

$$\chi = 1 + 6z + 30z^2 + 150z^3 + 726z^4 + 3510z^5 + 16710z^6 + 79494z^7 + \ldots \tag{5}$$

where $z = \tanh(J/kT)$. From (5),

$$\chi = 1 + 6z + 30z^2 + 150z^3(1 + 4{\cdot}83471044z + 23{\cdot}016528923z^2 + 109{\cdot}4958678z^3) + \ldots \tag{6}$$

The series in the parenthesis of (6) can be written as $\sum_{n=0}^{3} f_n z^n$.

Using (2) let us rewrite the partial sequence $\{f_n\}$ as

$$\sum_{n=0}^{2} f_n z^n = \sum_{n=0}^{2} \varepsilon_n I_n(mz) T_n^f(1/m). \tag{7}$$

The right side of (7) can be expanded to obtain

$$\sum_{n=0}^{2} \varepsilon_n I_n(mz) T_n^f(1/m) = T_0^f(m) + T_1^f(m)z + (mz)^2(T_0 + T_2)/4 + (mz)^3 T_1/8 + \ldots \tag{8}$$

Let us recall that $T_n^f(m)$ is defined by (3) and is determined entirely by the given series. For convenience, we suppress the argument m and write $T_1^f(m)$ as $T_1^{(f)}$. The value of m (the 'auxilliary variable') can be fixed by noting the efficient of z^3 as $T_1 m^3/8$ in (8) and identifying this with f_3 in (6).

Since, by definition (equation (3)), $T_1 = f_1/m$, it follows that $f_1 m^2/8 = f_3$ and m can thus be estimated for this given polynomial sequence. In the susceptibility series being considered (equation (6)) m is found to be 13·46. Using this value of m and by repeated application of the identity, the coefficients of $z^n (n \geqslant 8)$ can be evaluated as illustrated below.

From (6),

$$\chi = 1 + 6z + 30z^2 + 150z^3 + 726z^4 + 3510z$$
$$(1 + 4{\cdot}760683761z + 22{\cdot}64786325z^2). \qquad (9)$$

The series in the brackets can be represented as $\sum_{n=0}^{2} f_n^* z^n$. Hence f_3^* is given by $f_3^* = f_1^* m^2/8$. The coefficient of z^8 can therefore be estimated. Table 1 shows the coefficients obtained using this method indicating satisfactory agreement with the reported (exact) ones.

3.2 *b.c.c. lattice*

Similarly, the susceptibility series for the b.c.c. lattice is extrapolated from the expansion: (Domb and Sykes 1961)

$$\chi = 1 + 8z + 56z^2 + 392z^3 + 2684z^4 + 17864z^5 + 118760z^6 + \dots \qquad (9a)$$

m for this series is 18·798 using the earlier mentioned procedure. The final coefficients of $z^n (n \geqslant 7)$ are reported in table 2 and compared with other estimates.

3.3 *Ising ferrimagnets*

We shall now illustrate the new extrapolation procedure by applying it to another recently studied Ising ferrimagnets (Bowers and Yousif 1983). In section 8 of our earlier paper (Sangaranarayanan and Rangarajan 1984, hereafter referred to as Part-I), we have reported the critical parameters for this system. Here we calculate the unknown coefficients of the susceptibility series given by

$$\chi = \frac{11}{24} \sum_{n=0} a_n K^n. \qquad (10)$$

The coefficients $a_n (n \leqslant 7)$ are reported by Bowers and Yousif (1983) and we reproduce

Table 1. The estimated coefficients of z^n $(n \geqslant 8)$ in the high temperature susceptibility series for a simple cubic lattice.

n	Modified PET	From the Bessel function identity (equation 9)	From PET (equation 21)	From the series expansion (Domb and Sykes 1961)
8	377337·87 (0·57)	378422·2 (0·9)	378174·5 (0·7)	375174
9	1788160·26 (1·04)	1800256·9 (1·7)	1799078·7 (1·6)	1,769686
10	8462979·96 (1·88)	8569919·4 (3·1)	8558704·9 (3·0)	8306670

The % deviation from the series value is shown in parenthesis.

them in table 3. From equation (27) of Part-I,

$$\chi_0 \propto 0{\cdot}0299771\,\bar{K}[1+2{\cdot}255638847(\bar{K}^2)+4{\cdot}717026733(\bar{K}^2)^2 + 9{\cdot}552288158(\bar{K}^2)^3]$$

the value of m is estimated to be 5·820548569 using the identity (7) Hence, from the above equation,

$$\chi_0 \propto 0{\cdot}0299771\bar{K}+0{\cdot}067664\bar{K}^3[1+2{\cdot}091215417(\bar{K}^2) + 4{\cdot}234848221(\bar{K}^2)^2] \tag{11}$$

The coefficient of $\bar{K}^9$ is given by $f_1^* m^2 \times 0{\cdot}067664/8$ where $f_1^* = 2{\cdot}091215417$. The final values of a_{2n+1}, where $n = 3$ to 6 are reported in table 4. It is natural to expect that the accuracy of these estimates will progressively decrease as n increases, *i.e.*, a_9 is more reliable as compared to a_{11}, etc. Consider now the remaining part (even) of the series (10)

$$\chi_1 = \frac{11\times 3673}{24}[1+2{\cdot}72697(K')^2+5{\cdot}98325(K')^4 + 12{\cdot}377(K')^6+\ldots]$$

Table 2. The estimated coefficients of z^n in the susceptibility series for a b.c.c. lattice.

n	Modified PET	From the identity (Equation 9a)	From PET	Series expansion value (Domb and Sykes 1961)
7	—	788979·6 (0·006)	789515·9 (0·06)	789032
8	5233893 (0·6)	5245142·4 (0·8)	5248698·6 (0·9)	5201048
9	34676489 (1·2)	34845995 (1·7)	34893340·3 (1·8)	34268104

Values in parenthesis denote % deviation from the series expansion.

Table 3. The coefficients a_n of the ferrimagnetic susceptibility series for a simple cubic lattice (equation (10)) (Bowers and Yousif 1983).

n	a_n
0	3673
1	11018·18182
2	100161608·18163
3	248531985·45507
4	2197648117663·67529
5	5197379383038·48068
6	45463871209598494·26071
7	105248969765938227·28318

Proceeding as in the earlier case, m is found to be 6·0257. Hence, a^*_{2n} ($n = 4$ to 6) can be easily evaluated. The values of $\{a_n\} n = 8, 10, 12$ in (28) of Part-I so obtained are reported in table 4.

3.4 *Many fermion system: power series for the ground state energy*

The ground state energy $\varepsilon_0(x)$ of a many-fermion system interacting *via* a square well pair potential has been reported by Baker *et al* (1982) using the PA method. $\varepsilon_0(x)$ can be represented as a power series in x the dimensionless density

$$\varepsilon_0(x) = 1 + D_1 x + D_2 x^2 + D_3 x^3 + D_4 x^4 + \dots \quad (12)$$

the coefficients beyond D_4 being unknown. Using the known D'_ns and (2) we estimated D_5 to be 0·066566 and hence $[\varepsilon_0(x)]^{-1/2}$ with this extra coefficient. A slightly better agreement was found with the estimates predicted from the 'integral equation' method (Baker 1971) (table 5).

4. Principles of PET

While the PA and the continued fraction techniques have been extensively employed in the analysis of perturbation series in physical systems, the Euler transformation (ET)

Table 4. Extrapolated values of $\{a_n\}$ for the ferrimagnetic susceptibility series s.c. lattice (equation 10).

n	a_n from the identity	a_n from the PET
8	$9·97431 \times 10^{20}$	$9·4040406 \times 10^{20}$
9	$2·2009755 \times 10^{21}$	$2·1313536 \times 10^{21}$
10	$2·063295 \times 10^{25}$	$1·9453278 \times 10^{25}$
11	$4·4571196 \times 10^{25}$	$4·3161307 \times 10^{25}$
12	$4·5269747 \times 10^{29}$	$4·0241211 \times 10^{29}$
13	$9·3207972 \times 10^{29}$	$8·7404475 \times 10^{29}$

Table 5. Comparison of the values of $[\varepsilon_0(x)]^{-1/2}$ by various methods.

x	Integral equation method (Baker 1971)	From equation 12	Padé [1, 3] (Baker *et al* 1982)
0·25	0·94981	0·95024	0·95025
0·5	0·88124	0·88180	0·88197
0·75	0·79391	0·79160	0·79197
1·0	0·694491	0·68723	0·68686
1·5	0·49758	0·48414	0·47664
2·0	0·34211	0·33184	0·314928

(Morse and Feshbach 1953) and its parametrised version, *viz.* PET (Bhattacharyya 1982) have attracted relatively little attention in spite of their simplicity. Here we demonstrate the application of the PET to the several Ising model series expansions and then for the determination of the virial coefficients for hard spheres and hard discs.

For a slowly converging series, the ET (Knopp 1949) increases although not always, the rate of convergence. The ET consists in transforming an alternating power series $F(\rho) = \sum_{n=0}^{\infty} (-1)^n f_n \rho^n$ into another series in ρ_1 where

$$\rho_1 = (\rho/1+\rho) \tag{13}$$

and the transformed series can be written as

$$F(\rho) = (1/1+\rho) \sum_{n=0}^{\infty} D'_n f_0 \rho_1^n \tag{14}$$

where

$$D'_n f_0 = \sum_{r=0}^{n} (-1)^r \binom{n}{r} f_r, \quad D'_0 f_0 = f_0 \tag{15}$$

A generalised version of ET, namely the PET has been proposed by Bhattacharyya (1982) in the context of perturbation theory of atoms and it was shown that PET yields significantly better results than the conventional PA.

For a power series, given by (1), the PET consists in effecting a change of variable from ρ to $\bar{\rho}_1$ using a *parametrised* function such as $1+k\rho$. One can hence rewrite (1) as

$$F(\rho) = \frac{f_0}{1+k\rho} + \frac{\rho}{1+k\rho} \sum_{n=0}^{\infty} D_1 f_n \rho^n$$

and $$D_1 f_n = f_{n+1} + k f_n. \tag{16}$$

Also, $$F(\rho) = \sum_{n=0}^{r-1} f_n \rho^n + \frac{f_r \rho^r}{1+k\rho} + \frac{\rho}{1+k\rho} \sum_{n=r}^{\infty} D_1 f_n \rho^r. \tag{17}$$

Making use of a 'closure-like' assumption, we now let

$$D_1 f_n \equiv 0,$$

so that $$k = -(f_{r+1}/f_r). \tag{18}$$

Hence, (17) becomes

$$F(\rho) = \sum_{n=0}^{r-1} f_n \rho^n + \rho^r f_r \left(1 - \frac{\rho f_{r+1}}{f_r}\right)^{-1} + \frac{\rho}{1+k\rho} \sum_{n=r+1}^{\infty} D_1 f_n \rho^n \tag{19}$$

and in the asymptotic limit, the last term of (19) can be neglected so that

$$F(\rho) \simeq \sum_{n=0}^{r-1} f_n \rho^n + \rho^r f_r \left(1 - \frac{\rho f_{r+1}}{f_r}\right)^{-1}. \tag{20}$$

Equation (20) contains progressively higher orders of ρ as compared to the original series (1) and hence can be employed to estimate the unknown coefficients of any power series.

5. Applications of PET to Ising model series expansions

In §3 we considered some model series expansions and illustrated the use of the new resummation identity to obtain estimates of higher order coefficients. Here we demonstrate the use of PET for the same problem.

(i) Consider the high temperature susceptibility series for the simple cubic lattice given by (5).

Using eq. (20) it is easy to write (5) as

$$\chi = \sum_{n=0}^{5} f_n z^n + z^6 f_6 \left(1 - \frac{z f_7}{f_6}\right)^{-1}. \tag{21}$$

The coefficients of $z^n (n \geqslant 8)$ can be easily evaluated from the binomial expansion. The results are presented in table 1 and compared with the series estimates.

(ii) The same procedure is repeated for the susceptibility series of a b.c.c. lattice (equation (9a)). The evaluated coefficients using PET are represented and compared in table 2.

(iii) Earlier (§8 of Part-I) we analysed the coefficients of a three-dimensional ferrimagnet susceptibility series using the Bessel function identity. Here we report, in a similar manner, the evaluated coefficients a_n for the series given by (10). The two methods yield almost the same values for a_n's. The series (10) can be written as

$$\chi = \tfrac{11}{24} \times 3673[1 + 0{\cdot}02999771\,K' + 0{\cdot}067664(K')^3 + 0{\cdot}1415(K')^5 + 0{\cdot}286546769(K')^7]$$

Using (20), the coefficients of $(K')^9$ to $(K')^{13}$ have been estimated and the final estimates of a_n' in (10) are reported in table 4.

The same procedure when repeated for the even terms of the series (10) yields the coefficients of K^8 to K^{12} (table 4).

6. Estimation of virial coefficients

6.1 *Hard spheres*

6.1*a From the identity:* The seven term virial series for hard spheres is given by (Croxton 1975).

$$\begin{aligned}(P/\rho kT) &= 1 + b\rho + 0{\cdot}625b^2\rho^2 + 0{\cdot}2869b^3\rho^3 \\ &\quad + 0{\cdot}1103b^4\rho^4 + 0{\cdot}0386b^5\rho^5 + 0{\cdot}0127b^6\rho^6 + \ldots \\ &= 1 + b\rho + 0{\cdot}625b^2\rho^2 + 0{\cdot}2869b^3\rho^3 \\ &\quad (1 + 0{\cdot}384454513b\rho + 0{\cdot}134541652b^2\rho^2 \\ &\quad + 0{\cdot}044266294b^3\rho^3).\end{aligned} \tag{22}$$

The series in the brackets can be rewritten as,

$$1 + B_2^*\rho + B_3^*\rho^2 + B_4^*\rho^3$$

where $B_2^* = 0{\cdot}3844545b$, $B_3^* = 0{\cdot}134541165b^2$, $B_4^* = 0{\cdot}04426629b^3$. Using these values, m can be estimated as follows:

$$T_1 m^3/8 = B_4^*$$

$$B_2^* \times m^3/8m = 0{\cdot}04426629b^3 \text{ i.e., } m = 0{\cdot}9597b$$

This m value can be used to estimate B_8 as shown below. From (22),

$$P/\rho kT = 1 + b\rho + 0{\cdot}625b^2\rho^2 + 0{\cdot}2869b^3\rho^3 + 0{\cdot}1103b^4\rho^4$$
$$(1 + 0{\cdot}3499554669b\rho + 0{\cdot}115140525b^2\rho^2).$$

The coefficient of ρ^3 in the truncated series inside the parenthesis can be evaluated using (2). Hence B_8 is given by $0{\cdot}004446b^7$ and similarly B_9 to B_{11} can be estimated. The results are summarised in table 6.

6.1*b* *From* PET: The virial series can be written using PET as

$$P/\rho kT = 1 + b\rho + 0{\cdot}625b^2\rho^2 + 0{\cdot}2869b^3\rho^3 + 0{\cdot}1103b^4\rho^4$$
$$+ 0{\cdot}0386b^5\rho^5(1 - 0{\cdot}329015544b\rho)^{-1}.$$

The values of $B_n (n \geqslant 8)$ can be obtained in a straightforward manner and are shown in table 6.

6.2 *Hard discs*

The evaluation of the virial coefficients of hard discs follows essentially the same lines as those of the hard spheres. However, the uncertainties in the estimates of the lower order virial coefficients introduce significant inaccuracies in the final estimates of other virial coefficients.

6.2*a* *From the identity:* Let us write the virial series for hard discs in the form (Baram and Luban 1978)

$$P/\rho kT = 1 + b\rho + 0{\cdot}782b^2\rho^2 + 0{\cdot}5322b^3\rho^3$$
$$+ 0{\cdot}3338b^4\rho^4 + 0{\cdot}1992b^5\rho^5 + 0{\cdot}1143b^6\rho^6$$
$$+ 0{\cdot}0647b^7\rho^7 \ldots \tag{23}$$

Table 6. The estimated values of the higher order virial coefficients for hard spheres—(B_n/B_2^{n-1}) $(B_2 = 2\pi\sigma^3/3$, σ is the hard sphere diameter).

n	Modified PET	From the Bessel function identity	From PET	Kratky 1977	Carnahan and Starling 1969
7	0·013224	—	—	—	—
8	0·004457	0·004446	0·004179	0·00445	0·00427
9	0·001483	0·001463	0·001375	0·00150	0·001343
10	0·0004884	0·000514	0·000452	0·00051	0·000412
11	0·0001594	0·0001697	0·0001488	—	—

where $b = \pi\sigma^2/2$, σ being the hard disc diameter. The m value is found to be 1·61b. Using this m value and applying (2) successively the estimates of B_9 to B_{11} can be obtained and these are compared in table 7 with other reported values.

6.2*b From* PET: The application of PET to the evaluation of the virial coefficients for hard discs is more straightforward. Writing the virial series (23) as

$$1 + b\rho + 0{\cdot}782b^2\rho^2 + 0{\cdot}5322b^3\rho^3 + 0{\cdot}3338b^4\rho^4 + 0{\cdot}1992b^5\rho^5(1 - 0{\cdot}57379518b\rho)^{-1},$$

the estimates of B_8 to B_{11} can be obtained from the above expansion (table 7).

7. Modified PET

The PET method outlined in §4 can be viewed as the simplest of a hierarchy of methods of extrapolation of the coefficients of a power series $\sum a_r\rho^r$. Its prescription is

Given $\{a_r\}$, $r = 0, 1, 2, \ldots (N+1)$, extrapolate

$\{a_{N+s+1}\}$, $s = 1, 2, \ldots$ as

$a_{N+s+1} = (a_{N+1}/a_N)^s a_{N+1}$ or, equivalently,

$a_{N+s+1}/a_{N+s} = a_{N+1}/a_N$.

The intuitive justification for this is obviously the assumption of a finite radius of convergence ρ_c and consequently, for s sufficiently large, $a_{N+s}/a_{N+s+1} \to a$ constant $(= \rho_c)$. PET can be interpreted as a zeroth estimate for ρ_c as (a_N/a_{N+1}) employing the last two of the known coefficients alone.

The above interpretation suggests an immediate generalisation. If N is sufficiently large, an obvious improvement can be expected by writing

$$\frac{a_{N+s}}{a_{N+s+1}} \neq \frac{a_N}{a_{N+1}} \quad \text{but} \quad \frac{a_{N+s}}{a_{N+s+1}} = \rho_{c}, \varepsilon_N,$$

where ρ_c, ε_N is the 'ε-algorithm limit' for the sequence of ratios $\{a_{N-r}/a_{N-r+1}\}$, $r = 0, 1,$

Table 7. The extrapolated values of B_n/B_2^{n-1} for hard discs ($B_2 = \pi\sigma^2/2$, σ is the hard disc diameter).

n	From the identity (this paper)	Modified PET (this paper)	From PET (this paper)	Padé [4, 3] Kratky (1978)	Padé [3, 3] Kratky (1978)	From equation (10) of Kratky (1978)
7	—	0·1174	—	—	—	—
8	—	0·06724	0·06626	0·0647	0·0654	0·0650
9	0·03719	0·03914	0·03824	0·0359	0·0367	0·0362
10	0·02096	0·02267	0·022073	0·0196	0·0205	0·0199
11	0·01205	0·01308	0·01274	—	—	—

Table 8. Extrapolated coefficients of magnetisation series for the two-dimensional Ising model.

n	Darboux I app. Ninham (1963)	Darboux II app. Ninham (1963)	Exact	Modified PET	PET	Identity
8	16550	17020 (1·72)	17318	17409·6 (0·52)	16883·5	16314
9	84830	86620 (1·62)	88048	89385·04 (1·58)	82100	—

The % deviation from the exact value is shown in brackets.

$2, \ldots, N$. In contrast to the PET referred to above, such an estimate uses *all* or most* of the ratios. Still better can be the choice,

$$a_{N+s}/a_{N+s+1} = \rho_c, \varepsilon_N(1+X^*/N+s), \tag{24}$$

where X^* is a parameter to be estimated. At this stage, it is possible—for the sake of simplicity—to use one ratio alone, *i.e.*,

$$a_N/a_{N+1} = \rho_c, \varepsilon_N(1+X^*/N), \tag{25}$$

and deduce X^*, employing the ε-table for ρ_c.

Since ρ_c, ε_N can be evaluated using the ε-table and a_N/a_{N+1} is known from the given sequence, X^* can be obtained easily. As anticipated, this new procedure seems to be superior to the earlier ones. Several illustrations are presented below:

(i) Consider the magnetisation series for the two-dimensional Ising model given by equation (4) (Part-I).

$$M = 1 + \sum_{n=2}^{7} a_n (x^2)^n.$$

The limit a_n/a_{n+1} is 0·162161507 (ρ_c, ε_N) using EA.

$$a_6/a_7 = 0{\cdot}162161507(1+X^*/6). \text{ Hence } X^* = 1{\cdot}60873453.$$

The estimated coefficients from a_8 onwards using ρ_c, ε_N and X^* are reported in table 8.

(ii) Similarly, the susceptibility series for a s.c. lattice given by (6) is extrapolated and the coefficients of a_8, a_9, etc., regarded as unknown, are estimated (table 1). They compare well with the estimates obtained using other methods.

(iii) The extrapolated coefficients of the susceptibility series for a b.c.c. lattice given by (9a) using this method, are reported in table 2.

(iv) *Virial coefficients for hard spheres:* From equation (44) of Part-I, the limit of the sequence $\{B_{n+1}/B_n\}$ is $0{\cdot}298423784b$ and X^* is 1·036061222. Using these values, the virial coefficients B_8 to B_{11} were evaluated for hard spheres and table 6 shows the comparison with other reported estimates.

* We can choose a subset of the ratios instead of the entire one. It is preferable to have a bias towards the latter part, *i.e.*, the subset to include a_N/a_{N+1}, a_{N-1}/a_N, etc., in preference to a_0/a_1, etc.

(v) *Virial coefficients for hard discs:* Using equation (41) of Part-I, the limit of the sequence $\{B_{n+1}/B_n\}$ is estimated to be 0·55402543b and $X^* = 0{\cdot}457960569$. The extrapolated virial coefficients obtained by this procedure are reported in table 7 and a satisfactory agreement is noted.

8. Conclusion

The evaluation of the extrapolated coefficients starting from a partial, truncated power series has been studied using three procedures. (i) The first one, making use of a *novel* identity involving Bessel functions gives reliable estimates for the higher order virial coefficients for hard spheres and hard discs. The same method when applied to the known Ising model series expansions provide reasonably accurate estimates for higher order coefficients starting from the lower older ones. However, complete implication and the potentialities of this approach is yet to be explored. (ii) The well-known PET, despite its simplicity, provides a *straightforward* estimation for the higher order virial coefficients for hard spheres and hard discs, that is in good agreement with other literature values. The successful application of this method to some recently studied ferrimagnet series expansions is demonstrated. (iii) A hybrid approach employing the PET and the ε-convergence algorithm (Shanks 1955; Wynn 1956) that was studied by us is also very successful, in predicting the higher order coefficients as demonstrated by us in the known two-dimensional Ising model series expansion for magnetisation.

References

Abramovitz M and Stegun I A 1964 (eds) *Handbook of mathematical functions* (New York: National Bureau of Standards)
Alder B J and Wainright J E 1960 *J. Chem. Phys.* **33** 1439
Baker G A Jr 1971 *Rev. Mod. Phys.* **43** 479
Baker G A Jr and Hunter D L 1973 *Phys. Rev.* **137** 3377
Baker G A Jr and Graves Moris P 1981 in *Encyclopaedia of mathematics* (ed) Gran Carlo Rota (Reading, Massachusetts: Addison Wesley) Vol 13
Baker G A Jr, Benofy L A, Fortes M, Llano M, Peltier S M and Plastind A 1982 *Phys. Rev.* **A26** 3575
Baram A and Luban M 1978 *J. Phys.* **C12** L659
Bhattacharyya K 1982 *Int. J. Quantum Chem.* **22** 307
Bowers R G and Yousif B Y 1983 *Phys. Lett.* **A96** 49
Carnahan N F and Starling K E 1969 *J. Chem. Phys.* **51** 635
Chisholm J S R 1973 *Math. Comp.* **27** 841
Croxton C A 1975 *Introduction to liquid state physics* (New York: John Wiley)
Darboux G 1878 *J. Math. 'ele'm* **6** 1 377
Domb C and Sykes M F 1957 *Proc. R. Soc. London* **A240** 214
Domb C and Sykes M F 1961 *J. Math. Phys.* **2** 63
Fisher M E and Styer D F 1982 *Proc. R. Soc. London* **A384** 259
Gaunt D S and Guttman A J 1974 in *Phase transitions and critical phenomena* (eds) C Domb and M S Green (London: Academic Press) Vol 3 p 181
Hunter T L and Baher G A Jr 1973 *Phys. Rev.* **B7** 3346
Knopp K 1949 *Theory and applications of infinite series* (London: Blackie and Sons)
Morse P M and Feshbach M 1953 *Methods of theoretical physics* (New York: McGraw-Hill)
Ninham B W 1963 *J. Math. Phys.* **4** 679
Rangarajan S K 1984 (Unpublished)
Roberts D E, Griffiths H P and Wood D W 1975 *J. Phys.* **A8** 1365

Sangaranarayanan M V and Rangarajan S K 1983a *Phys. Lett.* **A96** 339
Sangaranarayanan M V and Rangarajan S K 1984 *Pramana* **22**
Shanks D 1955 *J. Math. Phys.* **34** 1
Stilck T J F and Salinas S R 1981 *J. Phys. A.* **14** 2027
Thompson C J *Mathematical statistical mechanics* (London: Macmillan Co.)
van Dyke M 1975 *SIAM J. Appl. Math.* **28** 720
Wynn P 1956 *Math. Tables* **10** 91