On a new method of series analysis in lattice statistics

1972 J. Phys. A: Gen. Phys. 5 L81

(http://iopscience.iop.org/0022-3689/5/9/001)

J. Phys. A: Gen. Phys., Vol. 5, September 1972. Printed in Great Britain. © 1972.

LETTER TO THE EDITOR

On a new method of series analysis in lattice statistics†

A J GUTTMANN‡ and G S JOYCE§

‡School of Mathematics, University of Newcastle, Newcastle, NSW 2308, Australia
§Wheatstone Physics Laboratory, King's College, Strand, London, WC2R 2LS, UK

MS received 14 July 1972

Abstract. A new recurrence relation method for analysing the singular behaviour of series expansions is described. It is shown using plausible nonrigorous arguments that the method can resolve logarithmic singularities and finite cusp singularities.

A basic problem in the lattice statistical theories of critical phenomena is the determination of the behaviour of a given thermodynamic function $\psi(T)$ in the neighbourhood of its physical and nonphysical singularities. In the standard approximate approach to this problem the function $\psi(T)$ is expanded as a Taylor series in the form

$$\psi(z) = \sum_{n=0}^{\infty} c_n z^n \qquad |z| < r_0 \tag{1}$$

where $z = z(T)$ is a suitable high or low temperature expansion variable, and the coefficients $c_0, c_1 \ldots c_N$ are calculated exactly. The singular behaviour of $\psi(z)$ in the complex z plane is then investigated by applying various series analysis techniques to the truncated series $\Sigma_{n=0}^{N} c_n z^n$. (For reviews of these techniques see Fisher 1967, Gaunt and Guttmann 1972.)

The main aim in this letter is to present a new general method for the analysis and study of series expansions which arise in lattice statistics. In this method we fit the available series coefficients $c_0, c_1, \ldots c_N$ in the expansion (1) to an $(M+1)$ term recurrence relation of the form

$$R_{2,M}(c_n) \equiv \sum_{i=0}^{M} \{A_{i,2}(n-i)^2 + A_{i,1}(n-i) + A_{i,0}\} c_{n-i} = 0 \qquad (n \geqslant 1) \tag{2}$$

with $A_{0,2} \equiv 1$, $A_{0,0} \equiv 0$, and $c_{-n} = 0$ $(n = 1, 2, \ldots)$. The set of unknown coefficients $\{A_{0,1};\ A_{i,2},\ A_{i,1},\ A_{i,0},\ i = 1, 2, \ldots M\}$ is determined in terms of the coefficients $c_0, c_1, \ldots c_N$ by solving the set of recurrence relations $\{R_{2,M}(c_1) = 0,\ R_{2,M}(c_2) = 0, \ldots R_{2,M}(c_{3M+1}) = 0\}$. We repeat this procedure for all values of M in the range $1 \leqslant M \leqslant [\frac{1}{3}(N-1)]$, (where $[x]$ denotes the largest integer which is not greater than x) and hence obtain a set of approximate recurrence relations $\{R_{2,M}(c_n) = 0,\ M = 1, 2, \ldots [\frac{1}{3}(N-1)]\}$ for the series coefficients c_n.

Each recurrence relation $R_{2,M}(c_n) = 0$ essentially *defines* a function $\psi_M(z)$ whose series expansion agrees with the expansion (1) through terms of order $3M+1$. Thus, we have

$$\psi(z) = \psi_M(z) + \mathrm{O}(z^{3M+2}). \tag{3}$$

† This research has been supported (in part) by the United States Department of the Army through its European Office.

The functions $\psi_M(z)$, therefore, provide a set of approximate 'representations' for the thermodynamic function $\psi(z)$. Estimates for the singular behaviour of $\psi(z)$ are then derived by investigating the appropriate singularities of the representations $\psi_M(z)$.

It may be readily verified that each representation $\psi_M(z)$ satisfies the second-order differential equation

$$L(\psi_M) \equiv Q(z)\frac{d^2\psi_M}{dz^2} + R(z)\frac{d\psi_M}{dz} + S(z)\psi_M = 0 \tag{4}$$

where

$$Q(z) = z\sum_{i=0}^{M} A_{i,2}z^i$$
$$R(z) = \sum_{i=0}^{M} (A_{i,2}+A_{i,1})z^i$$
$$S(z) = \sum_{i=1}^{M} A_{i,0}z^{i-1}. \tag{5}$$

We can now determine the non-analytic behaviour of the representation $\psi_M(z)$ by applying standard techniques to this differential equation (see Whittaker and Watson 1927, Ince 1927). In order to simplify the discussion we shall assume that the zeros $z_0 \equiv 0, z_1, \ldots z_M$ of the polynomial $Q(z)$ are all *distinct* (with $A_{M,2} \neq 0$), and that the polynomials $Q(z)$, $R(z)$ and $S(z)$ have no common factors. For this 'general' case the differential equation (4) is a *Fuchsian* equation which has $M+2$ *regular singular points* at $z = z_\alpha(\alpha = 0, 1, \ldots M)$, and $z = \infty$. The *exponents* ρ_α, ξ_α at each regular singular point are calculated in the usual manner by solving the corresponding *indicial equation*. We find

$$\rho_\alpha = 1 - \lim_{z\to z_\alpha}(z-z_\alpha)\frac{R(z)}{Q(z)} \qquad (\alpha = 0, 1, \ldots M) \tag{6}$$

with $\xi_\alpha = 0$. (The regular singular point at $z = \infty$ requires a separate treatment.) The Riemannian scheme (Ince 1927) associated with the differential equation (4) is given by

$$P\begin{bmatrix} 0 & z_1 & z_2 & \cdots & z_M & \infty & \\ 0 & 0 & 0 & \cdots & 0 & \xi_\infty & z \\ \rho_0 & \rho_1 & \rho_2 & \cdots & \rho_M & \rho_\infty & \end{bmatrix}. \tag{7}$$

It is interesting to note that the exponents in this scheme *always* satisfy the relation

$$(\xi_\infty+\rho_\infty)+\sum_{\alpha=0}^{M}\rho_\alpha = M. \tag{8}$$

The behaviour of the representation $\psi_M(z)$ in the neighbourhood of each regular singular point $z_\alpha(\alpha = 1, \ldots M)$ is, *in general*, described by an analytic continuation of the form

$$\begin{aligned}\psi_M(z) &= \phi_1(z)+(z_\alpha-z)^{\rho_\alpha}\phi_2(z) && (\rho_\alpha \neq 0, \pm 1, \pm 2, \ldots)\\ &= \phi_3(z)+\phi_4(z)\ln(z_\alpha-z) && (\rho_\alpha = 0)\\ &= \phi_5(z)+\epsilon_1(z_\alpha-z)^{\rho_\alpha}\phi_6(z)\ln(z_\alpha-z) && (\rho_\alpha = 1, 2, \ldots)\\ &= \{1+\epsilon_2\ln(z_\alpha-z)\}\phi_7(z)+(z_\alpha-z)^{\rho_\alpha}\phi_8(z) && (\rho_\alpha = -1, -2, \ldots)\end{aligned} \tag{9}$$

where the functions $\phi_i(z)$ are *analytic* and nonzero at $z = z_\alpha$, and ϵ_1, ϵ_2 are contants which are *not necessarily different from zero* (see Whittaker and Watson 1927). In order to establish a link between equation (9) and the non-analytic properties of the thermodynamic function $\psi(z)$ we *assume* that $\psi(z)$ displays physical and nonphysical singularities at $z = \omega_i(i = 1, 2, \ldots q)$, and that the structure of each singularity is given by equation (9) with an exponent $\lambda_i(i = 1, 2, \ldots q)$. Under these circumstances it is reasonable to *conjecture* that a subset of the set $\{z_\alpha, \rho_\alpha; \alpha = 1, \ldots M\}$ will yield approximations for the required set of positions and exponents $\{\omega_i, \lambda_i; i = 1, \ldots q\}$, provided that $M \geqslant q$. This conjecture forms the basis for the recurrence relation method of series analysis.

From the above discussion it is evident that the recurrence relation method can deal *directly* with finite *cusp* singularities ($\lambda_i > 0$), and with 'weak' *nonfactorizable* divergent singularities ($\lambda_i \leqslant 0$). Furthermore, the method can be used to analyse functions $\psi(z)$ which have several physical and nonphysical singularities on or *outside* the circle of convergence $|z| = r_0$. We see, therefore, that the recurrence relation technique is, *at least in principle*, more powerful than any other method of series analysis which is currently available. In addition, the method provides one with a mathematical tool for deducing *exact* recurrence relations and differential equations in lattice statistics and in the theory of special functions. For example, if the recurrence relation procedure is applied to the low temperature expansion of the Onsager expression (Onsager 1944) for the internal energy of the two dimensional Ising model one obtains an *exact* recurrence relation of the type (2) with $M = 8$ (Joyce, unpublished work).

A straightforward generalization of the recurrence relation method can be achieved by fitting the coefficients $c_0, c_1, \ldots c_N$ to an $(M+1)$ term recurrence relation of the type

$$R_{K,M}(c_n) = \sum_{i=0}^{M} \left(\sum_{k=0}^{K} A_{i,k}(n-i)^k \right) c_{n-i} = 0 \qquad (n \geqslant 1) \tag{10}$$

with $A_{0,K} \equiv 1$, $A_{0,0} \equiv 0$, and $c_{-n} = 0, (n = 1, 2, \ldots)$. In this scheme the representations $\psi_M(z)$ satisfy a Kth order Fuchsian differential equation. The singular behaviour of $\psi_M(z)$ can be readily found using standard techniques (Ince 1927). When $K = 1$ the representation $\psi_M(z)$ satisfies the equation

$$\left(\sum_{i=0}^{M} A_{i,1} z^i \right) \frac{\mathrm{d}\psi_M}{\mathrm{d}z} + \left(\sum_{i=1}^{M} A_{i,0} z^{i-1} \right) \psi_M = 0 \tag{11}$$

with $A_{0,1} \equiv 1$. This differential equation can also be constructed by forming the $[M, M-1]$ Padé approximant to the logarithmic derivative of the series (1). We see, therefore, that the recurrence relation method for $K \geqslant 2$ is a *natural generalization* of the standard $[M, M-1]$ Padé approximant method of series analysis (Baker 1961). An extension of the recurrence relation scheme (10) can be made by formally defining $A_{i,k} \equiv 0$, for $i > M_k$ $(M_k \leqslant M, k = 0, 1 \ldots K)$. This procedure leads to a $(K+1)$ dimensional array of representations $\psi_K[M_0, M_1 \ldots M_K; z]$, which in general satisfy non-Fuchsian Kth order differential equations. It is also possible to fit the coefficients $c_0, c_1 \ldots c_N$ to an *inhomogeneous* Kth order recurrence relation. A detailed account of of these generalizations will be given elsewhere.

The recurrence relation method is currently being applied to a wide variety of series expansions in lattice statistics. We hope to discuss these applications in future publications.

We are extremely grateful to Dr M F Sykes for proposing various recurrence relation problems in the theory of the Ising model, from which the recurrence relation method evolved.

References

Baker G A Jr 1961 *Phys. Rev.* **124** 768–74

Fisher M E 1967 *Rep. Prog. Phys.* **30** 615–730

Gaunt D S and Guttman A J 1972 *Phase Transitions and Critical Phenomena* ed C Domb and M S Green (London: Academic Press) to be published

Ince E L 1927 *Ordinary Differential Equations* (London: Longmans)

Onsager L 1944 *Phys. Rev.* **65** 117–49

Whittaker E T and Watson G N 1927 *A Course of Modern Analysis* (London: Cambridge University Press)