PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A
MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

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Phil. Trans. R. Soc. Lond. A 1988 **325**, 643-702
doi: 10.1098/rsta.1988.0077

Phil. Trans. R. Soc. Lond. A **325**, 643–702 (1988) [643]
Printed in Great Britain

ON THE HARD-HEXAGON MODEL AND THE THEORY OF MODULAR FUNCTIONS

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(*Communicated by R. J. Baxter, F.R.S. – Received* 6 *October* 1987)

CONTENTS

The mathematical properties of the exact solution of the hard-hexagon lattice gas model are investigated by using the Klein–Fricke theory of modular functions. In particular, it is shown that the order-parameter R and the reciprocal activity z' for the model can be expressed in terms of hauptmoduls that are associated with certain congruence subgroups of the full modular group Γ. Known modular equations are then used to prove that $R(z')$ is an *algebraic* function of z'. A connection is established between the singular points of this function and the geometrical properties of the *icosahedron*. Various algebraic and hypergeometric closed-form expressions are also derived for the order-parameter $R(z')$ in terms of the fundamental modular invariant J. Next the simple relation

$$\Xi_+^6 = (z')^{-2}[1-11z'-(z')^2]^{-1}R^9, \quad (0 < z' < z'_c)$$

is derived, where Ξ_+ is the grand partition function per site and $z'_c = \frac{1}{2}(5\sqrt{5}-11)$ denotes the critical value of z'. This important result forms the basis for a detailed analysis of the properties of the mean density $\rho(z')$ and the isothermal compressibility $\kappa_T(z')$ in the ordered region. It is shown that the mean density $\rho(z')$ is a solution of the algebraic equation

$$3[1-11z'-(z')^2]\rho^4-[1-66z'-11(z')^2]\rho^3-15z'(3+z')\rho^2 + 3z'(4+3z')\rho-z'(1+2z') = 0.$$

From this relation we obtain the following simple closed-form expressions for the inverse function $z'(\rho)$ and the isothermal compressibility $\kappa_T(\rho)$:

$$z'(\rho) = -\tfrac{1}{2}(2-3\rho)^{-1}(1-\rho)^{-3}[(1-12\rho+45\rho^2-66\rho^3+33\rho^4) + (-1+5\rho-5\rho^2)^{\frac{3}{2}}(-1+9\rho-9\rho^2)^{\frac{1}{2}}],$$

and

$$k_B T\rho\kappa_T(\rho) = \frac{1}{15\rho}[(1-2\rho)(-1+9\rho-9\rho^2)^{\frac{1}{2}}(-1+5\rho-5\rho^2)^{-\frac{1}{2}}-(-1+9\rho-9\rho^2)],$$

where $\rho_c < \rho \leqslant \frac{1}{3}$, and $\rho_c = \frac{1}{10}(5-\surd 5)$. The formula for $\kappa_T(\rho)$ is used to write the equation of state of the lattice gas

$$pa_0/k_B T = \ln \Xi_+(\rho) \equiv \Gamma_+(\rho)$$

in terms of a certain pseudo-elliptic integral, which is evaluated exactly to give a further closed-form expression for $\Gamma_+(\rho)$. (The quantity a_0 is the area of a unit cell in the lattice.) Finally, the properties of the hard-hexagon model in the disordered region $0 < \rho < \rho_c$ are studied with further modular equations derived by Hermite, and Klein and Fricke. This work leads to a closed-form expression for the generating function of the irreducible cluster sums β_l, $l = 1, 2, 3, \ldots$, and an asymptotic formula for the virial coefficients B_l as $l \to \infty$. It is also proved that the radius of convergence ρ_r of the virial series for the pressure p is given by

$$\rho_r = \tfrac{1}{10}\surd 5[(4\surd 10-5\surd 5+5)-\surd 10(4\surd 10-5\surd 5-4\surd 2+7)^{\frac{1}{2}}]^{\frac{1}{2}}.$$

A striking feature of this result is that ρ_r is *less* than the critical density

$$\rho_c = \tfrac{1}{10}(5-\surd 5).$$

1. Introduction

Various lattice gas models have been studied to gain insight into the melting transition and the phase transitions that occur in the mathematically intractable continuum systems of hard spheres and discs. (For a general review of lattice gas models, see Runnels 1972.) In this paper we shall be concerned with a lattice gas model in which the particles are restricted to lie on the sites of a two-dimensional triangular lattice with a lattice spacing a (Gaunt & Fisher 1965; Runnels & Combs 1966; Gaunt 1967). The interaction potential between two particles with lattice site positions $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ is assumed to be equal to $+\infty$ for $0 \leqslant |\boldsymbol{r}_i - \boldsymbol{r}_j| \leqslant a$, and zero otherwise. Thus the model forbids the multiple occupancy of lattice sites, and also does not allow the simultaneous occupation of nearest-neighbour sites. If each particle is surrounded by a regular hexagon that covers the six adjacent nearest-neighbour faces in the lattice we see that each configuration of particles on the lattice can be associated with a set of *non-overlapping* 'hard' hexagons.

For a lattice of N sites, the grand partition function for the hard-hexagon model is (Gaunt & Fisher 1965; Gaunt 1967)

$$\Xi(N, z) = \sum_{n=0}^{[\frac{1}{3}N]} g(n, N) z^n, \tag{1.1}$$

where $g(n, N)$ is the number of *allowed* ways of placing n particles on the lattice, z is the activity of the lattice gas and $[\frac{1}{3}N]$ is the largest integer that is less than or equal to $\frac{1}{3}N$. To determine the thermodynamic properties of the hard-hexagon model we must evaluate the limit

$$\Gamma_-(z) \equiv \ln \Xi_-(z) = \lim_{N\to\infty} \frac{1}{N} \ln \Xi(N, z), \tag{1.2}$$

where $\Gamma_-(z)$ denotes the *low-activity* branch of the reduced grand potential for the model. We can now find the particle number density ρ for the model by using the standard formula

$$\rho = \rho(z) = z(\mathrm{d}/\mathrm{d}z)\Gamma_-(z). \tag{1.3}$$

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It is also possible to develop a similar formulation that is valid for large values of z. Following Gaunt & Fisher (1965) we shall take the *high-activity* branch of the reduced grand potential $\Gamma_+(z')$ to be a function of $z' = 1/z$.

The early work on the hard-hexagon model involved the use of approximate numerical methods. In particular, Runnels & Combs (1966) calculated the maximum eigenvalue of the transfer matrix for lattices of finite width, whereas Gaunt (1967) derived and analysed various series expansions for the model. From these studies convincing evidence was found to indicate that the hard-hexagon model underwent a continuous order–disorder transition at a critical activity $z_c = 11.09 \pm 0.13$.

Further finite width lattice calculations were carried out by Metcalf & Yang (1978) for the special case $z = 1$. On the basis of their numerical result $\Gamma_-(1) \approx 0.3333$ they conjectured that the exact value of $\Gamma_-(1)$ was equal to $\frac{1}{3}$. However, this conjecture was shown to be incorrect by Baxter & Tsang (1980) who used the corner transfer matrix method to obtain the extremely accurate value

$$\Gamma_-(1) \approx 0.333\,242\,721\,976. \tag{1.4}$$

More importantly, these authors also observed that the eigenvalues of the corner transfer matrices had certain limiting properties, which suggested that the hard-hexagon model may be exactly solvable.

Following this work an exact solution of the hard-hexagon model was in fact soon established by Baxter (1980, 1982). It was found that the order–disorder transition occurred at a critical activity

$$z_c = \tfrac{1}{2}(11 + 5\sqrt{5}) = 11.091\,699\ldots, \tag{1.5}$$

which is in good agreement with the earlier numerical estimates for z_c. The reduced grand potential Γ and various thermodynamic quantities such as z and ρ were also evaluated by Baxter (1980, 1982) for $z < z_c$ and $z > z_c$ in terms of certain infinite products which were functions of a *non-physical parameter* x, with $-1 < x < 1$. In particular, the following simple product forms were derived for the order-parameter R and the reciprocal activity $z' = 1/z$:

$$R = \prod_{n=1}^{\infty} (1-x^n)(1-x^{5n})(1-x^{3n})^{-2}, \tag{1.6}$$

$$z' = x \prod_{n=1}^{\infty} \frac{(1-x^{5n-4})^5 (1-x^{5n-1})^5}{(1-x^{5n-3})^5 (1-x^{5n-2})^5}, \tag{1.7}$$

where $0 \leqslant x < 1$. It is possible, at least in principle, to eliminate the parameter x from these two equations and hence obtain the physically important thermodynamic function $R = R(z')$. Baxter (1982) carried out this elimination procedure *locally* in the neighbourhood of $x = 1$ to determine the critical behaviour of $R(z')$ as $z \to z_c+$. However, no attempt was made to establish the *global* structure and properties of the function $R(z')$ in the z'-plane.

In §§2 and 3*a* of the present paper we shall use the theory of modular functions as developed by Klein & Fricke (1890, 1892) to prove that the thermodynamic function $R = R(z')$ satisfies an *algebraic* equation of the type

$$\sum_{t=0}^{4} Q_t(z')\, R^{3t} = 0, \tag{1.8}$$

where $Q_0(z') \ldots Q_4(z')$ are polynomials in z', with $Q_1(z') \equiv 0$. It is shown in §3*b* that there exists a remarkable connection between the zeros of the polynomials $Q_t(z')$ and the geometrical properties of the *icosahedron* (Klein 1913), whereas in §3*d* the detailed analytic properties of $R(z')$ in the z'-plane are investigated by applying the methods of *algebraic function* theory (Bliss 1966) to equation (1.8). Various closed-form algebraic expressions and hypergeometric formulae for the order-parameter $R(z')$ are given in §6.

In §7 these results for $R(z')$ and the simple relation

$$\Xi_+(z') = (z')^{-\frac{1}{3}}[1-11z'-(z')^2]^{-\frac{1}{6}}[R(z')]^{\frac{5}{2}} \tag{1.9}$$

are used to establish the analytic properties of the grand partition function per site $\Xi_+(z')$. A detailed study of the thermodynamic functions of the hard-hexagon model is then carried out in §§8, 9 and 10 for $z > z_c$. In particular, it is shown in §8*b* that the mean number density $\rho = \rho(z')$ satisfies the algebraic equation

$$3[1-11z'-(z')^2]\rho^4-[1-66z'-11(z')^2]\rho^3-15z'(3+z')\rho^2+3z'(4+3z')\rho-z'(1+2z') = 0. \tag{1.10}$$

This relation is of considerable significance because, as is demonstrated in §10, it forms the basis for the derivation of closed-form expressions for the inverse function $z' = z'(\rho)$, the isothermal compressibility $\kappa_T = \kappa_T(\rho)$ and the equation of state $\Gamma_+ = \Gamma_+(\rho)$ in the high-density region $\rho_c < \rho < \frac{1}{3}$. In the remaining sections of the paper modular function theory is used to investigate the properties of the hard-hexagon model for $0 < z < z_c$.

Modular functions and modular equations have previously been employed in the theory of critical phenomena by Joyce (1975*a*, *b*) to study the analytic properties of the Ising model with pure triplet interactions on the triangular lattice. The present work on the application of modular functions to the hard-hexagon model was begun in 1980 and has been carried out over a period of several years. Some of the early results obtained for the order-parameter $R(z')$ and the virial series for $\Gamma_-(\rho)$ have already been reported by Baxter (1982, p. 451) and Gaunt & Joyce (1980) respectively. After the completion of the work, my attention was drawn to the independent work of Tracy *et al.* (1987) and Richey & Tracy (1987), which is also concerned with the application of modular function techniques to the hard-hexagon model.

In particular, Tracy *et al.* (1987) have proved in Theorem (2.1) that the physical quantities computed by Baxter (1980, 1982) are modular functions with respect to certain congruence groups. This theorem and general results from Riemann surface theory are then used to establish the existence of polynomial modular relations of the type (1.8) and (1.10) between the various physical quantities. The special role of the Klein icosahedral function $\zeta(\tau)$ in the hard-hexagon model is also discussed, and the analytic structure of Ξ and ρ in the complex z-plane is determined for the ordered and disordered régimes. In the present paper similar results for the analytic properties of Ξ and ρ in the z-plane are derived in §§7*b*, 8*b* and 12*b*. Richey & Tracy (1987) have used a general group theoretic algorithm to compute the detailed form of the polynomial relation between Ξ and ρ in the *disordered* régime. The corresponding result for the *ordered* régime is given in equation (10.48) of the present paper.

The group theoretic methods extensively used by Tracy *et al.* (1987) and Richey & Tracy (1987) are more sophisticated and modern than those used in the present paper, which are based on the hauptmodul functions of Klein & Fricke (1890, 1892). The main advantage of the hauptmodul method is that it leads more naturally to *explicit* algebraic and hypergeometric *closed-form* expressions for the various properties of the model.

2. Modular functions

We begin by considering the set of matrices

$$\left\{ M \equiv \begin{pmatrix} a & b \\ c & d \end{pmatrix} \middle| a, b, c, d \in \mathbb{Z}, ad - bc = 1 \right\}, \tag{2.1}$$

where $\mathbb{Z}$ denotes the set of integers. Under the binary operation of matrix multiplication this set of integral unimodular matrices forms a group called the homogeneous modular group Γ' (see Schoeneberg 1974; Apostol 1976). With each matrix $M \in \Gamma'$ we can associate a fractional linear transformation

$$\tau' = M(\tau) \equiv (a\tau + b)/(c\tau + d), \tag{2.2}$$

where $\tau \in \mathbb{C}^+$ and $\mathbb{C}^+$ denotes the set of complex numbers in the upper half-plane $\mathrm{Im}\,(\tau) > 0$. The transformations (2.2) also form a group called the inhomogeneous modular group Γ, which is homomorphic with the group Γ'. (The groups Γ' and Γ are not simply isomorphic because the matrices $\pm M$ are both associated with the same transformation in Γ.)

We now introduce the class of modular functions $f(\tau)$ that satisfy the following conditions:

(i) $f(\tau)$ is meromorphic in $\mathbb{C}^+$;

(ii) $f(M(\tau)) = f(\tau)$ for all $M(\tau) \in \Gamma$ and all $\tau \in \mathbb{C}^+$;

(iii) there is a constant $v_0 > 0$, such that for $\mathrm{Im}\,(\tau) > v_0$, $f(\tau)$ has a Fourier expansion of the form

$$f(\tau) = \sum_{n=m}^{\infty} a_n \exp\,(2\pi i n\tau), \tag{2.3}$$

where $m \in \mathbb{Z}$ and $a_m \neq 0$. (It is readily seen from condition (ii) and equation (2.2) with $a = b = d = 1$ and $c = 0$ that a modular function must be a periodic function of τ with a period 1.)

The fundamental modular function (or 'hauptmodul') for Γ can be defined as (Klein & Fricke 1890, p. 154)

$$J(\tau) = \frac{1}{1728}[\eta(\tau)]^{-24}\left[1 + 240 \sum_{n=1}^{\infty} \frac{n^3 \exp\,(2\pi i n\tau)}{1 - \exp\,(2\pi i n\tau)}\right]^3, \tag{2.4}$$

where
$$\eta(\tau) = \exp\,(\tfrac{1}{12}\pi i\tau) \prod_{n=1}^{\infty} [1 - \exp\,(2\pi i n\tau)], \tag{2.5}$$

is the Dedekind eta function, and $\tau \in \mathbb{C}^+$. The modular invariant $J(\tau)$ is of basic importance because it can be shown that every modular function is expressible as a *rational* function of $J(\tau)$. It is found by expanding equation (2.4) that the Fourier expansion (2.3) for $J(\tau)$ is given by

$$\begin{aligned} 1728 J(\tau) = \sum_{n=-1}^{\infty} j_n x^n &= x^{-1} + 744 + 196\,884x + 21\,493\,760x^2 \\ &+ 864\,299\,970x^3 + 20\,245\,856\,256x^4 + 333\,202\,640\,600x^5 + \ldots, \end{aligned} \tag{2.6}$$

where
$$x = \exp\,(2\pi i\tau), \tag{2.7}$$

and $0 < |x| < 1$. (This expansion is just a Laurent series for J about the origin in the x-plane.) The higher-order coefficients j_n in (2.6) have been calculated by Zuckerman (1939) for

$h \leqslant 24$. Petersson (1932) and Rademacher (1939) have derived the following asymptotic formula for the Fourier coefficients j_n in (2.6):

$$j_n \sim 2^{-\frac{1}{2}} n^{-\frac{3}{4}} \exp(4\pi n^{\frac{1}{2}}), \quad \text{as} \quad n \to \infty. \tag{2.8}$$

Recently, it has been shown (Thompson 1979) that there exists a remarkable connection between the coefficients j_n and the degrees of the irreducible characters of the Fischer–Griess 'monster' group.

Subgroups of the full modular group Γ can be constructed by requiring that the integers a, b, c, d involved in the transformation (2.2) satisfy certain congruence relations. For any subgroup G of finite index in Γ we can define a new class of modular functions $f(\tau)$ that satisfy the conditions:

(i) $f(\tau)$ is meromorphic in $\mathbb{C}^+$;

(ii) $f(S(\tau)) = f(\tau)$ for all transformations $S(\tau) \in G$ and all $\tau \in \mathbb{C}^+$;

(iii) at each cusp s of G choose a transformation $M(\tau) \in \Gamma$, which has $M(\infty) = s$, then there is a constant $v_0 > 0$ such that, for $\operatorname{Im}(\tau) > v_0$, $f(M(\tau))$ has a Fourier expansion of the form

$$f(M(\tau)) = \sum_{n=m}^{\infty} b_n \exp(2\pi i n\tau/h), \tag{2.9}$$

where h is the least positive integer such that the transformation $M\sigma M^{-1}(\tau) \in G$, with $\sigma(z) = z+h$.

An important subgroup $\Gamma_0(N)$ of the modular group is defined to be the set of transformations (2.2), which satisfy the additional congruence relation $c \equiv 0 \bmod N$, where N is any positive integer. When $N \leqslant 10$ or $N = 12$, 13, 16 and 25 there exists a univalent modular function (or hauptmodul) for $\Gamma_0(N)$. For the prime number cases $N = 2$, 3, 5, 7 and 13 it can be proved that the hauptmodul for $\Gamma_0(N)$ can be written as

$$\omega_N(\tau) = e_N[\eta(N\tau)/\eta(\tau)]^{24/(N-1)}, \tag{2.10}$$

where $\eta(\tau)$ is the Dedekind eta function and e_N is an arbitrary constant (see Klein & Fricke 1892, p. 64 and Apostol 1976, p. 87). In particular, we have

$$\omega_2(\tau) = 64x \prod_{n=1}^{\infty} [(1-x^{2n})/(1-x^n)]^{24}, \tag{2.11}$$

$$\omega_3(\tau) = 27x \prod_{n=1}^{\infty} [(1-x^{3n})/(1-x^n)]^{12}, \tag{2.12}$$

$$\omega_5(\tau) = 125x \prod_{n=1}^{\infty} [(1-x^{5n})/(1-x^n)]^{6}, \tag{2.13}$$

where $x = \exp(2\pi i\tau)$. (The constants e_N have been defined to give agreement with the work of Klein and Fricke. However, we have changed the modular function notation used by Klein and Fricke from τ_N to ω_N in order to avoid confusion with the variable τ defined in equation (2.7).)

When $N = 2$, 3, 5, 7 and 13 every modular function $f(\tau)$ for the congruence subgroup $\Gamma_0(N)$ can be expressed as a rational function of the hauptmodul $\omega_N(\tau)$. Because the modular invariant $J(\tau)$ is a modular function for all the subgroups of Γ it must be possible to write $J(\tau)$

as a rational function of $\omega_N(\tau)$, provided $N = 2, 3, 5, 7$ and 13. When $N = 2, 3$ and 5 we find from the work of Klein & Fricke (1892, pp. 60, 61) that

$$J = (4\omega_2+1)^3/27\omega_2 = (\omega_3+1)(9\omega_3+1)^3/64\omega_3$$
$$= (\omega_5^2+10\omega_5+5)^3/1728\omega_5, \tag{2.14}$$

where $J = J(\tau)$ and $\omega_N = \omega_N(\tau)$. Klein & Fricke also give the following alternative form for the relations (2.14):

$$J-1 = (\omega_2+1)(8\omega_2-1)^2/27\omega_2 = (27\omega_3^2+18\omega_3-1)^2/64\omega_3$$
$$= (\omega_5^2+22\omega_5+125)(\omega_5^2+4\omega_5-1)^2/1728\omega_5. \tag{2.15}$$

Next we consider the set of transformations (2.2) which satisfy the congruence relations

$$a \equiv d \equiv 1, \quad b \equiv c \equiv 0 \quad \mathrm{mod}\, N, \tag{2.16}$$

where N is any positive integer. These transformations form a subgroup $\Gamma(N)$ of the modular group Γ, which is called the principal congruence subgroup of level N. When $N = 2, 3, 4, 5$ there exists a univalent modular function (or hauptmodul) for the subgroup $\Gamma(N)$. For the particular case $\Gamma(5)$ it can be shown that the hauptmodul may be defined as

$$\zeta(\tau) = x^{\frac{1}{5}} \prod_{n=1}^{\infty} \frac{(1-x^{5n-4})(1-x^{5n-1})}{(1-x^{5n-3})(1-x^{5n-2})}, \tag{2.17}$$

where $x = \exp(2\pi i\tau)$ (see Klein & Fricke 1892, p. 383; Mordell 1922). The modular function $\zeta(\tau)$ has a Fourier expansion of the type (2.9) with $h = 5$. It is interesting to note that the factor group $\Gamma/\Gamma(5)$ is isomorphic with the icosahedral rotation group. The basic hauptmodul for the subgroup $\Gamma(2)$ is the well-known elliptic modular function

$$\lambda(\tau) \equiv k^2(\tau) = 16x^{\frac{1}{2}} \prod_{n=1}^{\infty} [(1+x^n)/(1+x^{n-\frac{1}{2}})]^8. \tag{2.18}$$

(In the theory of elliptic functions it is usual to write $x \equiv q^2$.)

The function $\omega_5(\tau)$ is also a modular function for the principal congruence subgroup $\Gamma(5)$, because $\Gamma(5)$ is a subgroup of $\Gamma_0(5)$. It follows, therefore, that $\omega_5(\tau)$ can be expressed as a rational function of the hauptmodul $\zeta(\tau)$. From the work of Klein & Fricke (1890, p. 639), we find

$$\omega_5 = 125\theta/(1-11\theta-\theta^2), \tag{2.19}$$

where $\omega_5 = \omega_5(\tau)$ and

$$\theta = \theta(\tau) \equiv [\zeta(\tau)]^5. \tag{2.20}$$

For the function $\omega_2(\tau)$ we have the rational relation

$$\omega_2 = \tfrac{1}{4}\lambda^2(1-\lambda)^{-1}, \tag{2.21}$$

where $\lambda = \lambda(\tau)$ is the hauptmodul (2.18).

We can also express $J(\tau)$ as a rational function of $\zeta(\tau)$ because $J(\tau)$ is a modular function for all the subgroups of Γ. The particular form of this rational relation may be obtained by substituting equation (2.19) in equations (2.14) and (2.15). This procedure gives (Klein & Fricke 1890, pp. 105, 106)

$$1728J = \Omega_2^3(\theta)/\theta\Omega_1^5(\theta), \tag{2.22}$$

and
$$1728(J-1) = \Omega_3^2(\theta)/\theta\Omega_1^5(\theta), \tag{2.23}$$
where
$$\left.\begin{aligned}\Omega_1(\theta) &= 1-11\theta-\theta^2,\\ \Omega_2(\theta) &= 1+228\theta+494\theta^2-228\theta^3+\theta^4,\\ \Omega_3(\theta) &= 1-522\theta-10005\theta^2-10005\theta^4+522\theta^5+\theta^6.\end{aligned}\right\} \tag{2.24}$$
In §3 we shall discuss the connection between these polynomials and the geometrical properties of the icosahedron.

3. Order-parameter of the hard-hexagon model

Baxter (1980, 1982) has shown that the order-parameter R of the hard-hexagon model has the following parametric representation:
$$R = \prod_{n=1}^{\infty} (1-x^n)(1-x^{5n})(1-x^{3n})^{-2}, \tag{3.1}$$
$$z^{-1} = x\prod_{n=1}^{\infty} \frac{(1-x^{5n-4})^5(1-x^{5n-1})^5}{(1-x^{5n-3})^5(1-x^{5n-2})^5}, \tag{3.2}$$
where z is the activity and $0 \leqslant x < 1$. As the parameter x increases from 0 to 1 the activity z decreases from ∞ to its critical value
$$z_c = \tfrac{1}{2}(11+5\surd 5), \tag{3.3}$$
while R decreases from 1 to 0.

The elimination of the parameter x from equations (3.1) and (3.2) gives the order-parameter R as a function of the reciprocal activity $z' = 1/z$. Our main purpose in this section is to use the theory of modular functions to investigate the properties of the function $R(z')$ in the z'-plane.

(a) *Algebraic equations for R*

We begin by applying the results (2.12), (2.13) and (2.17) to equations (3.1) and (3.2). In this manner we obtain the alternative τ-parametric representation
$$R^6 = (\tfrac{3}{5})^3[\omega_5(\tau)/\omega_3(\tau)], \tag{3.4}$$
$$z' = \zeta^5(\tau) \equiv \theta(\tau), \tag{3.5}$$
where $\omega_3(\tau)$, $\omega_5(\tau)$ and $\zeta(\tau)$ are the hauptmoduls for the congruence subgroups $\Gamma_0(3)$, $\Gamma_0(5)$ and $\Gamma(5)$ respectively. The physically significant range for the parameter τ is $0 < \mathrm{Im}\,(\tau) < \infty$ with $\mathrm{Re}\,(\tau) = 0$.

Next we use equation (3.4) to eliminate ω_3 from the modular relation (2.14). This procedure gives
$$5^9R^{18}(\omega_5^2+10\omega_5+5)^3 = (27\omega_5+125R^6)(243\omega_5+125R^6)^3. \tag{3.6}$$

The elimination of ω_3 from the alternative result (2.15) yields the further algebraic equation
$$5^9R^{18}(\omega_5^2+22\omega_5+125)(\omega_5^2+4\omega_5-1)^2 = (19683\omega_5^2+60750\omega_5R^6-15625R^{12})^2. \tag{3.7}$$

It may be readily verified that equations (3.6) and (3.7) can both be written in the *same* expanded form

$$5^{12}R^{24}-5^{9}(\omega_5^6+30\omega_5^5+315\omega_5^4+1300\omega_5^3+1575\omega_5^2-6\omega_5+125)\,R^{18}$$
$$+2\cdot 3^9\cdot 5^7\omega_5^2R^{12}+2^2\cdot 3^{14}\cdot 5^3\omega_5^3R^6+3^{18}\omega_5^4=0. \quad (3.8)$$

We see from equation (3.8) that the order-parameter R is an algebraic function of the hauptmodul ω_5.

If we substitute the modular relation (2.19) in equations (3.6) and (3.7), and apply equation (3.5) we obtain

$$\Omega_2^3(z')\,R^{18}=\Omega_1^2(z')\,[27z'+\Omega_1(z')\,R^6]\,[243z'+\Omega_1(z')\,R^6]^3, \quad (3.9)$$

and the alternative form

$$\Omega_3^2(z')\,R^{18}=\Omega_1^2(z')\,[19\,683(z')^2+486z'\Omega_1(z')\,R^6-\Omega_1^2(z')\,R^{12}]^2, \quad (3.10)$$

where the polynomials Ω_j $(j=1,2,3)$ are defined in equation (2.24). From equations (3.9) and (3.10) it is found that

$$\Omega_1^6(z')\,R^{24}-\Lambda(z')\,R^{18}+196\,830(z')^2\Omega_1^4(z')\,R^{12}+19\,131\,876(z')^3\Omega_1^3(z')\,R^6$$
$$+387\,420\,489(z')^4\Omega_1^2(z')=0, \quad (3.11)$$

where $$\Lambda(z')=\Omega_2^3(z')-756z'\Omega_1^5(z')=\Omega_3^2(z')+972z'\Omega_1^5(z'). \quad (3.12)$$

We see directly from equation (3.11) that the order-parameter R is an algebraic function of the reciprocal activity $z'=1/z$.

It should be noted that the algebraic equation (3.11) is not irreducible because it can be factorized by using the equivalent equation (3.10). In this manner we obtain the *reduced* equation

$$\Omega_1^3(z')\,R^{12}-\Omega_3(z')\,R^9-486z'\Omega_1^2(z')\,R^6-19\,683(z')^2\Omega_1(z')=0 \quad (3.13)$$

for the order-parameter R.

(*b*) *Connection with the icosahedron*

In this section we shall use the work of Klein (1913) to establish a link between the hard-hexagon model and the geometrical properties of the icosahedron. Consider a three-dimensional space with orthogonal coordinate axes (u,v,ω), and suppose that the (u,v) plane is used to represent the set of complex numbers $\zeta=u+\mathrm{i}v$. A Riemann unit sphere is now placed with its centre at the origin of the ζ-plane, and an icosahedron is inscribed within the sphere. To fix the orientation of the inscribed icosahedron we suppose that there is a vertex at each of the poles $(0,0,\pm 1)$ and that one of the vertices nearest the pole $(0,0,1)$ lies in the positive quadrant of the (u,ω)-plane. Next all the points on the surface of the icosahedron are projected radially outwards onto the unit sphere. In this manner we obtain an icosahedral pattern on the Riemann sphere. Finally, we make a stereographic projection of this pattern onto the ζ-plane as shown in figure 1.

The 12 vertices of the icosahedron have stereographic images in the ζ-plane at $0,\infty$ and

$$\zeta_1=\{\tfrac{1}{2}(-1+\surd 5)\exp(\tfrac{2}{5}\pi\mathrm{i}n),\ \tfrac{1}{2}(1+\surd 5)\exp[\tfrac{1}{5}\pi\mathrm{i}(2n+1)]\}, \quad (3.14)$$

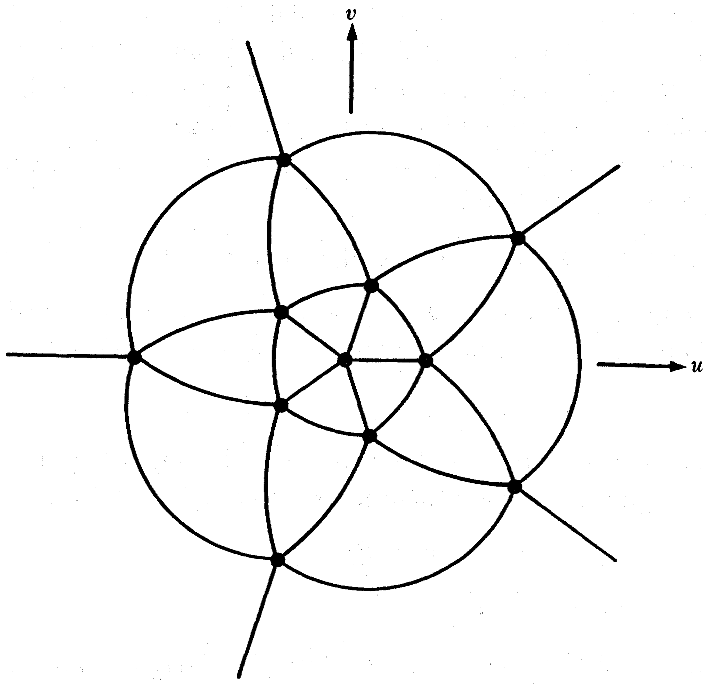

FIGURE 1. Stereographic projection of the icosahedron onto the ζ-plane.

where $n = 0, 1, 2, 3, 4$. For the 20 face-centres of the icosahedron we find that the stereographic images are given by

$$\zeta_2 = \{[\tfrac14\sqrt{6}(5\pm\sqrt{5})^{\frac12}+\tfrac14(3\pm\sqrt{5})]\exp(\tfrac25\pi i n),\\ [\tfrac14\sqrt{6}(5\pm\sqrt{5})^{\frac12}-\tfrac14(3\pm\sqrt{5})]\exp[\tfrac15\pi i(2n+1)]\}, \tag{3.15}$$

where $n = 0, 1, 2, 3, 4$. The 30 mid-points of the edges of the icosahedron have stereographic images

$$\zeta_3 = \{[\tfrac12\sqrt{2}(5\pm\sqrt{5})^{\frac12}-\tfrac12(1\pm\sqrt{5})]\exp(\tfrac25\pi i n),\\ [\tfrac12\sqrt{2}(5\pm\sqrt{5})^{\frac12}+\tfrac12(1\pm\sqrt{5})]\exp[\tfrac15\pi i(2n+1)],\\ \exp[\tfrac{1}{10}\pi i(2m+1)]\}, \tag{3.16}$$

where $n = 0, 1, 2, 3, 4$ and $m = 0, 1, 2, \ldots, 9$. It can be shown (Klein 1913, pp. 60, 61) that the sets of image points ζ_1, ζ_2 and ζ_3 are the zeros of the basic polynomials $\Omega_1(\theta)$, $\Omega_2(\theta)$ and $\Omega_3(\theta)$ respectively, with θ replaced by ζ^5. We see, therefore, that there is a close connection between the order-parameter of the hard-hexagon model and the geometrical properties of the icosahedron.

An interesting feature of this connection can be established by calculating the $\theta = \zeta^5$ values associated with the stereographic image points ζ_1, ζ_2 and ζ_3. The final results are

$$\left.\begin{aligned}
\theta_1 &= \{\tfrac12(-11\pm5\sqrt{5})\},\\
\theta_2 &= \{(57\pm25\sqrt{5})+5(255\pm114\sqrt{5})^{\frac12},\ (57\pm25\sqrt{5})-5(255\pm114\sqrt{5})^{\frac12}\},\\
\theta_3 &= \{-\tfrac12(261\pm125\sqrt{5})+\tfrac{15}{2}(650\pm290\sqrt{5})^{\frac12},\ -\tfrac12(261\pm125\sqrt{5})-\tfrac{15}{2}(650\pm290\sqrt{5})^{\frac12},\ \pm i\}.
\end{aligned}\right\} \tag{3.17}$$

The sets θ_1, θ_2 and θ_3 are the zeros of the polynomials $\Omega_1(\theta)$, $\Omega_2(\theta)$ and $\Omega_3(\theta)$ respectively. From the results (3.17) and (3.3) we see that the critical point $z'_c = 1/z_c$ of the hard-hexagon model and the non-physical singularity at $z' = -z_c$ are associated with the stereographic images of the non-polar vertices of the inscribed icosahedron!

The values of ω_5 associated with the image points ζ_1, ζ_2 and ζ_3 may be determined by using equations (2.19) and (3.17). We find that

$$\omega_{5,1} = \{\pm\infty\}, \quad \omega_{5,2} = \{-5\pm 2\sqrt{5}\}, \quad \omega_{5,3} = \{-2\pm\sqrt{5},\ -11\pm 2\mathrm{i}\}. \tag{3.18}$$

It is seen that the 10 non-polar vertices of the icosahedron are all associated with the point at infinity in the ω_5-plane, while the 2 polar vertices are associated with the origin $\omega_5 = 0$.

(c) *Behaviour of R in the ω_5-plane*

We now use the algebraic equation (3.8) to investigate the singularity structure of the order-parameter R in the ω_5-plane. For convenience, we introduce the notation

$$y \equiv \left(\tfrac{125}{81}\right) R^6, \tag{3.19}$$

and rewrite (3.8) in the quartic form

$$f(\omega_5, y) \equiv 3y^4 - 4\omega_5(16J-7)\,y^3 + 90\omega_5^2 y^2 + 108\omega_5^3 y + 27\omega_5^4 = 0, \tag{3.20}$$

where

$$J = (\omega_5^2 + 10\omega_5 + 5)^3/1728\omega_5. \tag{3.21}$$

The standard method for studying the properties of a function $y(x)$ that satisfies the general algebraic equation

$$f(x,y) \equiv \sum_{k=0}^{n} a_{n-k}(x)\, y^k = 0, \tag{3.22}$$

where $a_l(x)$, $(l = 0, 1, \ldots, n)$ are polynomials in x, is to use the Sylvester determinant to eliminate y from the two equations $f = 0$ and $\partial f/\partial y = 0$ (Goursat 1959; Bliss 1966). This procedure gives the resultant polynomial in x, which we shall denote by

$$\operatorname{Res}(f, \partial f/\partial y;\, y). \tag{3.23}$$

The zeros x_i $(i = 1, \ldots, h)$ of this resultant polynomial are called the *singular* points of the equation (3.22). At any *non-singular* point in the finite x-plane the n branches of the algebraic function $y(x)$ are all analytic functions, whereas at a singular point x_i one usually finds that at least one of the branches of $y(x)$ is not analytic. However, in exceptional circumstances it is possible for *all* the branches of $y(x)$ to be *analytic* even at a *singular* point x_i. We shall call a singular point of this special type an *apparent singular* point.

For the particular quartic equation (3.20) the resultant (3.23) is found to be

$$\operatorname{Res}(f, \partial f/\partial y;\, y) = -2^{24}\cdot 3^{10}\omega_5^{12} J^2 (J-1)^2. \tag{3.24}$$

The application of equations (2.15) and (3.21) to this result gives the explicit polynomial form

$$\operatorname{Res}(f, \partial f/\partial y;\, y) = -(\omega_5^8/9)\,(\omega_5^2+10\omega_5+5)^6(\omega_5^2+4\omega_5-1)^4(\omega_5^2+22\omega_5+125)^2. \tag{3.25}$$

It follows from formula (3.25) that equation (3.20) has *singular* points in the finite ω_5-plane at

$$\omega_5 = 0,\ -5\pm 2\sqrt{5},\ -2\pm\sqrt{5} \quad\text{and}\quad -11\pm 2\mathrm{i}. \tag{3.26}$$

There is also a *singular* point at $\omega_5 = \infty$ (see Goursat 1959, p. 241), which is associated with the *physical* critical point of the hard-hexagon model. We see from these results and equation (3.18) that the *singular* points in the extended ω_5-plane can be associated with the stereographic image points ζ_1, ζ_2 and ζ_3 for the icosahedron!

It can be shown that the *physical* branch of $y(\omega_5)$ is *analytic* at the *singular* point $\omega_5 = 0$, whereas the three non-physical branches form a single cyclic system of non-analytic functions at $\omega_5 = 0$. We also find that all the branches of $y(\omega_5)$ exhibit a square-root branch-point at the *singular* points $\omega_5 = -11 \pm 2\mathrm{i}$. However, the *singular* points $-5 \pm 2\sqrt{5}$ and $-2 \pm \sqrt{5}$ are all *apparent singular* points. At the point $\omega_5 = \infty$ the physical branch and 2 non-physical branches form a single cyclic system of non-analytic functions.

From the above singularity analysis it is clear that we can represent the *physical* branch of $y(\omega_5)$ as a Taylor series in powers of ω_5. In particular, we obtain

$$R^6 = (\tfrac{81}{125})\,y = 1 - 6v + 45v^2 - 356v^3 + 2844v^4 - 22\,380v^5 + 169\,190v^6$$
$$- 1\,180\,980v^7 + 6\,928\,416v^8 - 22\,202\,424v^9 - 232\,534\,962v^{10} + 6\,688\,362\,132v^{11}$$
$$- 108\,259\,550\,865v^{12} + 1\,467\,755\,129\,538v^{13} - \dots, \tag{3.27}$$

where $v = \frac{1}{125}\omega_5$. This series is convergent provided that $|\omega_5| \leqslant 5\sqrt{5}$.

The application of the Puiseux method to the singular point $\omega_5 = \infty$ of the algebraic equation (3.20) enables one to establish an analytic continuation of the physical branch (3.27) which is valid in the interval $5\sqrt{5} \leqslant |\omega_5| < \infty$. In particular, we find that

$$R^6 = (\tfrac{81}{125})\,y = \left(\frac{3^6}{5^3}\right)|\omega_5|^{-\frac{2}{3}} \sum_{n=0}^{\infty} (\pm 1)^n A_n\,|\omega_5|^{-\frac{1}{3}n}, \tag{3.28}$$

where the upper sign is taken in the interval $5\sqrt{5} \leqslant \omega_5 < \infty$, and the lower sign is taken for $-\infty < \omega_5 \leqslant -5\sqrt{5}$. A list of the coefficients A_n is given in table 1 for $n \leqslant 31$. It follows from equation (3.28) that

$$R^6 = \left(\frac{3^6}{5^3}\right)|\omega_5|^{-\frac{2}{3}}[F_0(\omega_5) \pm |\omega_5|^{-\frac{5}{3}}F_1(\omega_5) + |\omega_5|^{-\frac{10}{3}}F_2(\omega_5)], \tag{3.29}$$

TABLE 1. COEFFICIENTS A_n IN THE EXPANSION (3.28)

n	A_n	n	A_n
0	1	16	52650
1	0	17	528900
2	0	18	734635
3	−10	19	−846000
4	0	20	−6027657
5	12	21	−6504120
6	95	22	12163500
7	0	23	66476850
8	−240	24	54261625
9	−900	25	−162598212
10	90	26	−713394075
11	3480	27	−407922250
12	8525	28	2063030220
13	−2700	29	7466547000
14	−44400	30	2442173375
15	−79994	31	−25146798840

where the functions $F_k(\omega_5)$, $(k = 0, 1, 2)$ are analytic at $\omega_5 = \infty$ with Taylor series representations:

$$F_k(\omega_5) = \sum_{n=0}^{\infty} A_{3n+5k}\, \omega_5^{-n}, \tag{3.30}$$

where $k = 0, 1, 2$ and $5\sqrt{5} \leqslant |\omega_5| < \infty$. These Taylor series exhibit branch-point singularities on the circle of convergence at $\omega_5 = -11 \pm 2\mathrm{i}$. We see from equation (3.29) that the corrections to the dominant critical behaviour

$$R \sim (3/\sqrt{5})\, \omega_5^{-\frac{1}{6}}, \quad \text{as} \quad \omega_5 \to +\infty, \tag{3.31}$$

have a rather complicated confluent singularity structure.

(d) *Behaviour of R in the z′-plane*

It can be shown by analysing the resultant (3.23) that the algebraic equation (3.13) for the function $R(z')$ has proper *singular* points in the z'-plane at $z' = 0$, ∞, z'_c and $-1/z'_c$, and 4 *apparent singular* points at $z' = \theta_2$, where the set of values θ_2 is defined in equation (3.17). At the *singular* point $z' = 0$ the *physical* branch of $R(z')$ is an analytic function. It is possible, therefore, to expand the order-parameter in the form

$$R = \sum_{n=0}^{\infty} r_n (z')^n, \tag{3.32}$$

where $|z'| \leqslant z'_c$. The coefficients r_n, which were obtained by substituting the relation

$$\omega_5 = 125z'/[1 - 11z' - (z')^2] \tag{3.33}$$

in the Taylor series (3.27), are given in table 2 for $n \leqslant 24$. The first few coefficients $r_0, \ldots, r_5$ in table 2 are in agreement with the earlier calculations of Gaunt (1967).

We can determine the behaviour of the order-parameter R in the neighbourhood of the branch-points z'_c and $-1/z'_c$ by using equations (3.28) and (3.33). In this manner we obtain

$$R = 3 \cdot 5^{-\frac{5}{6}} [(z'_c - z')(z_c + z')/|z'|]^{\frac{1}{6}} \sum_{n=0}^{\infty} (\pm 1)^n C_n 5^{-n} [(z'_c - z')(z_c + z')/|z'|]^{\frac{1}{2}n}, \tag{3.34}$$

where the upper sign is taken for $z' \lesssim z'_c$ and the lower sign is taken for $z' \gtrsim -1/z'_c$. The coefficients C_n in (3.34) are defined by the relation

$$\left[\sum_{n=0}^{\infty} A_n x^n\right]^{\frac{1}{6}} \equiv \sum_{n=0}^{\infty} C_n x^n, \tag{3.35}$$

and the coefficients A_n are defined in equation (3.28). A list of the coefficients C_n is given in table 3 for $n \leqslant 23$.

To investigate the behaviour of R in the neighbourhood of the *physical* critical point $z' = z'_c$, we first use the variable

$$t' \equiv 5^{-\frac{3}{2}}[1 - (z'/z'_c)], \tag{3.36}$$

to write equation (3.34) in the alternative form

$$R = (3/\sqrt{5})\,(t')^{\frac{1}{6}} [G_0(t') + (t')^{\frac{5}{3}} G_1(t') + (t')^{\frac{10}{3}} G_2(t')], \tag{3.37}$$

TABLE 2. COEFFICIENTS r_n IN THE EXPANSION (3.32)

n	r_n
0	1
1	−1
2	−6
3	−43
4	−347
5	−3002
6	−27165
7	−253625
8	−2423014
9	−23559091
10	−232269858
11	−2315845513
12	−23305516673
13	−236370993938
14	−2413311489567
15	−24780942112943
16	−255732635182579
17	−2650669372188184
18	−27580891652646375
19	−287979786719182165
20	−3016215679346417804
21	−31679462052621305651
22	−333576121312242893841
23	−3520592195120956837214
24	−37235270065999873219081

TABLE 3. COEFFICIENTS C_n IN THE EXPANSION (3.35)

n	C_n	n	C_n
0	1	12	110075/243
1	0	13	−325/3
2	0	14	−195650/81
3	−5/3	15	−2568911/729
4	0	16	14950/9
5	2	17	5796700/243
6	80/9	18	180895760/6561
7	0	19	−1790750/81
8	−70/3	20	−169872988/729
9	−4900/81	21	−4158538360/19683
10	5	22	66196000/243
11	2170/9	23	14764754500/6561

where the functions

$$G_k(t') = \sum_{n=0}^{\infty} C_{3n+5k}(t')^n[(1-z_c' t')/(1-5^{\frac{3}{2}}t')]^{n+\frac{5}{3}k+\frac{1}{9}}, \tag{3.38}$$

$(k = 0, 1, 2)$, are all analytic at $t' = 0$, and $t' \gtrsim 0$. We now expand (3.38) in powers of t' by using the Taylor series

$$[(1-z_c' t')/(1-5^{\frac{3}{2}}t')]^{\lambda} = \sum_{m=0}^{\infty} E_m(\lambda)\,(t')^m, \tag{3.39}$$

where the coefficients $E_m(\lambda)$ satisfy the recurrence relation

$$2(m+1)\,E_{m+1}(\lambda) - [\lambda(11+5\sqrt{5}) + (-11+15\sqrt{5})\,m]\,E_m(\lambda) + 5(25-11\sqrt{5})\,(m-1)\,E_{m-1}(\lambda) = 0, \tag{3.40}$$

with the initial conditions $E_0(\lambda) = 1$ and $E_{-1}(\lambda) \equiv 0$. In this manner we find that

$$G_k(t') = \sum_{n=0}^{\infty} D_n^{(k)} (t')^n, \tag{3.41}$$

where $k = 0, 1, 2$; $t' \gtrsim 0$ and

$$D_n^{(k)} = \sum_{m=0}^{n} C_{3m+5k} E_{n-m}(m + \tfrac{5}{3}k + \tfrac{1}{9}). \tag{3.42}$$

Next we calculate the coefficients $D_n^{(k)}$ by using the recurrence relation (3.40) and the results in table 3, and then substitute equation (3.41) in the formula (3.37). This procedure yields the following basic expansion for R about the *physical* critical point $z' = z'_c$:

$$\begin{aligned} R = {} & (3/\sqrt{5})\,(t')^{\frac{1}{9}}[1-(1/18)\,(19-5\sqrt{5})\,t' + 2(t')^{\frac{5}{3}} - (1/162)\,(-423+475\sqrt{5})\,(t')^2 \\ & + (1/9)\,(-34+80\sqrt{5})\,(t')^{\frac{8}{3}} - (1/2187)\,(108604-15295\sqrt{5})\,(t')^3 + 5(t')^{\frac{10}{3}} \\ & + (1/81)\,(15543-2125\sqrt{5})\,(t')^{\frac{11}{3}} - (1/39366)\,(-4275491+7307685\sqrt{5})\,(t')^4 \\ & + (1/18)\,(-245+775\sqrt{5})\,(t')^{\frac{13}{3}} + (1/2187)\,(-1583363+1838465\sqrt{5})\,(t')^{\frac{14}{3}} + O((t')^5)], \end{aligned} \tag{3.43}$$

where $t' \gtrsim 0$.

The behaviour of the order-parameter R in the neighbourhood of the non-physical singularity $z' = -1/z'_c$ can be determined from equation (3.34) in a similar manner by introducing the expansion variable

$$t^* = 5^{-\frac{3}{2}}(1 + z'_c z'). \tag{3.44}$$

It is found that the final expansion for R is

$$\begin{aligned} R = {} & (3/\sqrt{5})\,(t^*)^{\frac{1}{9}}[1+(1/18)\,(19+5\sqrt{5})\,t^* - 2(t^*)^{\frac{5}{3}} + (1/162)\,(423+475\sqrt{5})\,(t^*)^2 \\ & - (1/9)\,(34+80\sqrt{5})\,(t^*)^{\frac{8}{3}} + (1/2187)\,(108604+15295\sqrt{5})\,(t^*)^3 + 5(t^*)^{\frac{10}{3}} \\ & - (1/81)\,(15543+2125\sqrt{5})\,(t^*)^{\frac{11}{3}} + (1/39366)\,(4275491+7307685\sqrt{5})\,(t^*)^4 \\ & + (1/18)\,(245+775\sqrt{5})\,(t^*)^{\frac{13}{3}} - (1/2187)\,(1583363+1838465\sqrt{5})\,(t^*)^{\frac{14}{3}} + O((t^*)^5)], \end{aligned} \tag{3.45}$$

where $t^* \gtrsim 0$.

An asymptotic representation for the series coefficients r_n in equation (3.32) can now be derived by applying the Darboux theorem (see Ninham 1963) to the critical point expansion (3.43). The final result is

$$\begin{aligned} r_n \sim {} & -3^{-1}\cdot 5^{-\frac{2}{3}}[\Gamma(8/9)]^{-1} n^{-\frac{10}{9}} (z'_c)^{-n} \{1 + \sqrt{5}(19/405)\,n^{-1} \\ & - \sqrt{5}(224/1125)\,\Gamma(8/9)\,[\Gamma(2/9)]^{-1} n^{-\frac{5}{3}} - (1463/164025)\,n^{-2} \\ & - (3808/18225)\,\Gamma(8/9)\,[\Gamma(2/9)]^{-1} n^{-\frac{8}{3}} \\ & - \sqrt{5}(2898469/996451875)\,n^{-3} \\ & - (35464/455625)\,\Gamma(8/9)\,[\Gamma(5/9)]^{-1} n^{-\frac{10}{3}} \\ & - \sqrt{5}(163744/36905625)\,\Gamma(8/9)\,[\Gamma(2/9)]^{-1} n^{-\frac{11}{3}} \\ & - (213010406/403563009375)\,n^{-4} \\ & - \sqrt{5}(6950944/184528125)\,\Gamma(8/9)\,[\Gamma(5/9)]^{-1} n^{-\frac{13}{3}} \\ & + (1700808928/44840334375)\,\Gamma(8/9)\,[\Gamma(2/9)]^{-1} n^{-\frac{14}{3}} + O(n^{-5})\}, \end{aligned} \tag{3.46}$$

as $n \to \infty$, where $\Gamma(x)$ denotes the gamma function. On general grounds one would expect the coefficients in the expansion (3.46) to be of the form $a + b\sqrt{5}$, where a and b are *non-zero* real numbers. However, a remarkable cancellation occurs in the derivation of the expansion (3.46), which leads to an alternating *zero* value for the constants a and b. A check on the calculation has been made by evaluating (3.46) for a range of values $n = 1, 2, 3, \ldots$. For the case $n = 24$ one finds that

$$r_{24} \approx -3.723\,527\,013 \times 10^{22}.$$

This asymptotic representation for r_{24} is in excellent agreement with the exact value given in table 2. The asymptotic formula (3.46) also gives a surprisingly accurate approximation for r_n when n is *small*. For example, if the asymptotic value for r_n is rounded to the nearest integer one obtains the *exact* value for r_n, provided $n = 1, 2, \ldots, 7$!

4. Hauptmodul analysis in the τ-plane

In this section we shall analyse the behaviour of the hauptmoduls $\omega_3(\tau)$, $\omega_5(\tau)$ and $\zeta(\tau)$ in the upper half of the τ-plane. The elimination of the parameter τ from these results gives one an alternative method for establishing the singular behaviour of R in the ω_5- and z'-planes.

(a) *Properties of the hauptmoduls $\omega_3(\tau)$ and $\omega_5(\tau)$*

We begin by applying the standard transformation formula (Ayoub 1963, p. 158)

$$\eta(\tau) = \exp\left(\tfrac{1}{4}\pi \mathrm{i}\right) \tau^{-\frac{1}{2}} \eta(-1/\tau), \quad \tau \in \mathbb{C}^+ \tag{4.1}$$

to the hauptmodul (2.10). This procedure gives

$$[\omega_3(\tau)]^{-1} = \omega_3(-1/3\tau), \tag{4.2}$$

$$[\omega_5(\tau)]^{-1} = (1/125)\, \omega_5(-1/5\tau). \tag{4.3}$$

If we apply equations (2.12) and (2.13) to these results we obtain

$$[\omega_3(\tau)]^{-1} = 27X \prod_{n=1}^{\infty} [(1-X^{3n})/(1-X^n)]^{12}, \tag{4.4}$$

and
$$[\omega_5(\tau)]^{-1} = \Delta \prod_{n=1}^{\infty} [(1-\Delta^{5n})/(1-\Delta^n)]^{6}, \tag{4.5}$$

where
$$\Delta = \exp(-2\pi \mathrm{i}/5\tau), \tag{4.6}$$

and
$$X \equiv \Delta^{\frac{5}{3}} = \exp(-2\pi \mathrm{i}/3\tau). \tag{4.7}$$

Next we expand the products in (4.4) and (4.5) in powers of X and Δ respectively. In this manner we find that

$$[\omega_3(\tau)]^{-1} = 27 \sum_{n=0}^{\infty} f_n X^{n+1}, \quad |X| < 1 \tag{4.8}$$

where $f_0 = 1, f_1 = 12, f_2 = 90$; and

$$[\omega_5(\tau)]^{-1} = \sum_{n=0}^{\infty} g_n \Delta^{n+1}, \quad |\Delta| < 1 \tag{4.9}$$

where $g_0 = 1$, $g_1 = 6$, $g_2 = 27$, $g_3 = 98$, $g_4 = 315$. It can be shown by using an identity derived by Ramanujan (see Rademacher 1973, p. 241) that the coefficients g_n satisfy the relations

$$g_n = \tfrac{1}{5}p(5n+4), \quad (n \leqslant 4) \tag{4.10}$$

$$g_n = \tfrac{1}{5}p(5n+4) - \sum_{l=1}^{[\frac{1}{5}n]} p(l)\, g_{n-5l}, \quad (n \geqslant 5) \tag{4.11}$$

where $p(l)$ is the number of unrestricted partitions of the integer l, and $[\frac{1}{5}n]$ denotes the largest integer that is less than or equal to $\frac{1}{5}n$. Because extensive tabulations of $p(l)$ are available in the literature the recurrence relation (4.11) provides one with a convenient method for calculating the coefficient g_n.

We now use the expansion (4.8) to write the order-parameter (3.4) in the alternative form

$$R^6 = (3/\sqrt{5})^6 \omega_5(\tau) \sum_{n=0}^{\infty} f_n X^{n+1}, \quad |X| < 1. \tag{4.12}$$

The expansions (4.9) and (4.12), which are valid for all $\tau \in \mathbb{C}^+$, are the basic results in this section. They provide one with an implicit parametric representation for the *physical* branch of the algebraic function $R(\omega_5)$, which is particularly useful in the neighbourhood of the critical point $\omega_5 = +\infty$, $\tau = +\mathrm{i}0$. An *explicit* representation for $R(\omega_5)$ can be established by first reverting the series (4.9). In this manner we obtain

$$\Delta = \omega_5^{-1} - 6\omega_5^{-2} + 45\omega_5^{-3} - 368\omega_5^{-4} + 3132\omega_5^{-5} - \ldots. \tag{4.13}$$

From this expansion we find that

$$X \equiv \Delta^{\frac{5}{3}} = \omega_5^{-\frac{5}{3}} \sum_{m=0}^{\infty} e_m \omega_5^{-m}, \tag{4.14}$$

where $e_0 = 1$, $e_1 = -10$, $e_2 = 95$, $e_3 = -900$ and $e_4 = 8525$. The substitution of the expansion (4.14) in equation (4.12) yields the required explicit representation

$$R^6(\omega_5) = (3/\sqrt{5})^6 \omega_5^{-\frac{2}{3}} [F_0(\omega_5) + \omega_5^{-\frac{5}{3}} F_1(\omega_5) + \omega_5^{-\frac{10}{3}} F_2(\omega_5)], \tag{4.15}$$

where
$$F_j(\omega_5) = \sum_{l=0}^{\infty} f_{3l+j}\, \omega_5^{-5l} \left(\sum_{m=0}^{\infty} e_m \omega_5^{-m} \right)^{3l+j+1}, \tag{4.16}$$

$j = 0, 1, 2$ and $5\sqrt{5} \leqslant \omega_5 < \infty$. From (4.16) it is readily found that

$$\left.\begin{aligned} F_0(\omega_5) &= 1 - 10\omega_5^{-1} + 95\omega_5^{-2} - 900\omega_5^{-3} + 8525\omega_5^{-4} - \ldots, \\ F_1(\omega_5) &= 12 - 240\omega_5^{-1} + 3480\omega_5^{-2} - 44\,400\omega_5^{-3} + 528\,900\omega_5^{-4} - \ldots, \\ F_2(\omega_5) &= 90 - 2700\omega_5^{-1} + 52\,650\omega_5^{-2} - 846\,000\omega_5^{-3} + 12\,163\,500\omega_5^{-4} - \ldots. \end{aligned}\right\} \tag{4.17}$$

These results are in agreement with those derived in §3*c*.

To determine the behaviour of R in the neighbourhood of the singular point $\omega_5 = -\infty$, $\tau = \frac{1}{2} + \mathrm{i}0$, we make the substitution

$$\tau = \tfrac{1}{2} + \tfrac{1}{2}\tau^*, \quad \mathrm{Im}\,(\tau^*) > 0 \tag{4.18}$$

in equation (2.10), and then apply the standard transformation formulae (Ayoub 1963, pp. 159, 200),

$$\eta(\tau+1) = \exp(\tfrac{1}{12}i\pi)\,\eta(\tau), \tag{4.19}$$

$$\eta(\tfrac{1}{2}+\tfrac{1}{2}\tau) = \exp(\tfrac{1}{4}\pi i)\,\tau^{-\frac{1}{2}}\eta(\tfrac{1}{2}-\tfrac{1}{2}\tau^{-1}). \tag{4.20}$$

This procedure gives

$$[\omega_3(\tau)]^{-1} = \omega_3(\tfrac{1}{2}-\tfrac{1}{6}(\tau^*)^{-1}), \tag{4.21}$$

$$[\omega_5(\tau)]^{-1} = \tfrac{1}{125}\omega_5(\tfrac{1}{2}-\tfrac{1}{10}(\tau^*)^{-1}), \tag{4.22}$$

where $\tau = \frac{1}{2}+\frac{1}{2}\tau^*$. From these results we readily obtain the basic expansions

$$[\omega_5(\tau)]^{-1} = \sum_{n=0}^{\infty} g_n(-\Delta^*)^{n+1}, \quad |\Delta^*| < 1 \tag{4.23}$$

and

$$R^6 = (3/\sqrt{5})^6\omega_5(\tau)\sum_{n=0}^{\infty} f_n(-X^*)^{n+1}, \quad |X^*| < 1 \tag{4.24}$$

where

$$\Delta^* \equiv \exp(-\pi i/5\tau^*), \tag{4.25}$$

$$X^* \equiv (\Delta^*)^{\frac{5}{3}} = \exp(-\pi i/3\tau^*), \tag{4.26}$$

and the coefficients g_n and f_n are defined in equations (4.9) and (4.8) respectively. The expansions (4.23) and (4.24) give a parametric representation for the order-parameter $R(\omega_5)$, which is particularly useful in the neighbourhood of the singular point $\omega_5 = -\infty$, $\tau = \frac{1}{2}+i0$.

An explicit representation for $R(\omega_5)$ can be derived by first reverting the series (4.23). Hence we find that

$$X^* \equiv (\Delta^*)^{\frac{5}{3}} = (-\omega_5)^{-\frac{5}{3}}\sum_{m=0}^{\infty} e_m\,\omega_5^{-m}, \tag{4.27}$$

where the coefficients e_m are defined in equation (4.14). If the expansion (4.27) is now substituted in equation (4.24), we obtain the required explicit representation

$$R^6(\omega_5) = (3/\sqrt{5})^6(-\omega_5)^{-\frac{2}{3}}[F_0(\omega_5)-(-\omega_5)^{-\frac{5}{3}}F_1(\omega_5)+(-\omega_5)^{-\frac{10}{3}}F_2(\omega_5)], \tag{4.28}$$

where $-\infty < \omega_5 < -5\sqrt{5}$, and the functions $F_j(\omega_5), j = 0, 1, 2$ are defined in equations (4.15) and (4.16). The result (4.28) is in agreement with that derived in §3 (see equation (3.29)).

(b) *Properties of the hauptmodul* $\zeta(\tau)$

The hauptmodul $\zeta(\tau)$, which is defined by the infinite product (2.17), can be expressed in the alternative form (Klein & Fricke 1892, p. 383)

$$\zeta(\tau) = x^{\frac{1}{5}}\sum_{n=-\infty}^{\infty}(-1)^n x^{\frac{1}{2}n(5n+3)}\Big/\sum_{n=-\infty}^{\infty}(-1)^n x^{\frac{1}{2}n(5n+1)}, \tag{4.29}$$

where $x = \exp(2\pi i\tau)$. It is also possible to write $\zeta(\tau)$ as the continued fraction

$$\zeta(\tau) = \frac{x^{\frac{1}{5}}}{1+}\,\frac{x}{1+}\,\frac{x^2}{1+}\,\frac{x^3}{1+}\cdots \tag{4.30}$$

If the infinite product (2.17) is expanded in powers of x we obtain the Fourier series

$$\zeta(\tau) = x^{\frac{1}{5}}(1-x+x^2-x^4+x^5-x^6+x^7-x^9+2x^{10}-3x^{11}+2x^{12}-2x^{14}+4x^{15}-4x^{16}+\ldots), \tag{4.31}$$

where $|x| < 1$.

The behaviour of $\zeta(\tau)$ in the neighbourhood of $\tau = 0$ can be determined by using a modular transformation formula given by Klein & Fricke (1890, p. 615). In this manner we find that

$$\zeta(\tau) = \tfrac{1}{2}(\surd 5 - 1)\left[1 - \frac{\surd 5\,\zeta(-1/\tau)}{1 + \frac{1}{2}(\surd 5 - 1)\,\zeta(-1/\tau)}\right]. \tag{4.32}$$

This result may also be derived by applying one of Ramanujan's theorems to the continued fraction (4.30) (see Ramanujan 1927, p. xxviii). If the expansion (4.31) with τ replaced by $-1/\tau$ is substituted in equation (4.32) we obtain the simple result

$$\zeta(\tau) = \tfrac{1}{2}(\surd 5 - 1)\left[1 - \frac{\surd 5\,\Delta}{1 + \frac{1}{2}(\surd 5 - 1)\,\Delta}\right] + O(\Delta^6), \tag{4.33}$$

where Δ is defined in equation (4.6).

We shall now show how equation (4.33) can be used to determine the critical behaviour of $R(z')$ as $z' \to z'_c$, where z' is the reciprocal activity for the hard-hexagon model. From (4.33) we readily obtain the expansion

$$\begin{aligned} z' = \zeta^5(\tau) = z'_c[1 - 5\surd 5\Delta + \tfrac{5}{2}\surd 5(5\surd 5 - 1)\,\Delta^2 - \tfrac{5}{2}\surd 5(43 - 5\surd 5)\,\Delta^3 \\ + 5\surd 5(30\surd 5 - 32)\,\Delta^4 - \tfrac{5}{2}\surd 5(377 - 115\surd 5)\,\Delta^5 + \dots], \end{aligned} \tag{4.34}$$

where $z'_c = 1/z_c$. Next we carry out a reversion of the expansion (4.34). This procedure leads to the important result

$$\Delta = t' + \tfrac{1}{2}(5\surd 5 - 1)\,(t')^2 + \tfrac{1}{2}(83 - 5\surd 5)\,(t')^3 + (155\surd 5 - 57)\,(t')^4 + \tfrac{1}{2}(6177 - 515\surd 5)\,(t')^5 + \dots, \tag{4.35}$$

where the variable t' is defined in equation (3.36) and $|t'| < 5^{-\frac{3}{2}}$.

An expansion for $R(\tau)$ in powers of the parameter Δ may be derived by using equations (3.4), (4.4) and (4.5). It is found that

$$R(\tau) = (3/\surd 5)\,\Delta^{\frac{1}{9}} \prod_{n=1}^{\infty} (1 - \Delta^n)\,(1 - \Delta^{5n})\,(1 - \Delta^{\frac{5}{3}n})^{-2}, \tag{4.36}$$

$$= (3/\surd 5)\,\Delta^{\frac{1}{9}}[1 - \Delta + 2\Delta^{\frac{5}{3}} - \Delta^2 - 2\Delta^{\frac{8}{3}} + 5\Delta^{\frac{10}{3}} - 2\Delta^{\frac{11}{3}} - 5\Delta^{\frac{13}{3}} + O(\Delta^5)]. \tag{4.37}$$

The required critical behaviour of R is obtained by substituting the expansion (4.35) in equation (4.37). The final result is in complete agreement with equation (3.43), which was derived by a direct analysis of the algebraic function $R(z')$.

Next we determine the behaviour of the hauptmodul $\zeta(\tau)$ in the neighbourhood of $\tau = \frac{1}{2}$. First we define the modular transformations

$$\left.\begin{aligned} \tau' &= \tau + 1 \equiv M_1\tau, \\ \tau' &= -1/\tau \equiv M_2\tau, \\ \tau' &= (\tau - 1)/(2\tau - 1) \equiv M_3\tau, \end{aligned}\right\} \tag{4.38}$$

where

$$M_3\tau = M_1(M_2(M_1^2(M_2\tau))). \tag{4.39}$$

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We then evaluate $\zeta(M_3\tau)$ using (4.39) and the basic transformation formulae

$$\zeta(M_1\tau) = \exp\left(\tfrac{2}{5}\pi i\right)\zeta(\tau), \tag{4.40}$$

$$\zeta(M_2\tau) = \tfrac{1}{2}(\sqrt{5}-1)\left[1-\frac{\sqrt{5}\,\zeta(\tau)}{1+\frac{1}{2}(\sqrt{5}-1)\,\zeta(\tau)}\right]. \tag{4.41}$$

If we make the substitution $\tau = \frac{1}{2}-\frac{1}{2}(\tau^*)^{-1}$ in the final result we obtain the required relation

$$\exp\left(-\tfrac{1}{5}i\pi\right)\zeta\left(\tfrac{1}{2}+\tfrac{1}{2}\tau^*\right) = \tfrac{1}{2}(\sqrt{5}+1)\left[1-\frac{\sqrt{5}\exp\left(-\frac{1}{5}i\pi\right)\zeta\left(\frac{1}{2}-\frac{1}{2}(\tau^*)^{-1}\right)}{1+\frac{1}{2}(\sqrt{5}+1)\exp\left(-\frac{1}{5}i\pi\right)\zeta\left(\frac{1}{2}-\frac{1}{2}(\tau^*)^{-1}\right)}\right], \tag{4.42}$$

where $\operatorname{Im}(\tau^*) > 0$. The application of expansion (4.31) with $\tau = \frac{1}{2}-\frac{1}{2}(\tau^*)^{-1}$ to this formula gives the simple expression

$$\exp\left(-\tfrac{1}{5}i\pi\right)\zeta\left(\tfrac{1}{2}+\tfrac{1}{2}\tau^*\right) = \tfrac{1}{2}(\sqrt{5}+1)\left[1-\frac{\sqrt{5}\,\Delta^*}{1+\frac{1}{2}(\sqrt{5}+1)\,\Delta^*}\right]+O[(\Delta^*)^6], \tag{4.43}$$

where Δ^* is defined in equation (4.25).

We conclude this section with an analysis of the singular behaviour of the order-parameter $R(z')$ as $z' \to (-z_c)+$. From equation (4.43) we readily find that

$$\begin{aligned} z' = \zeta^5(\tau) = -z_c[1&-5\sqrt{5}\Delta^*+\tfrac{5}{2}\sqrt{5}(5\sqrt{5}+1)(\Delta^*)^2-\tfrac{5}{2}\sqrt{5}(43+5\sqrt{5})(\Delta^*)^3 \\ &+5\sqrt{5}(30\sqrt{5}+32)(\Delta^*)^4-\tfrac{5}{2}\sqrt{5}(377+115\sqrt{5})(\Delta^*)^5+\ldots], \end{aligned} \tag{4.44}$$

where $\tau = \frac{1}{2}+\frac{1}{2}\tau^*$. The reversion of this expansion gives

$$\begin{aligned} \Delta^* = t^* &+\tfrac{1}{2}(5\sqrt{5}+1)(t^*)^2+\tfrac{1}{2}(83+5\sqrt{5})(t^*)^3 \\ &+(155\sqrt{5}+57)(t^*)^4+\tfrac{1}{2}(6177+515\sqrt{5})(t^*)^5+\ldots, \end{aligned} \tag{4.45}$$

where the variable t^* is defined in equation (3.44), and $|t^*| < 5^{-\frac{3}{2}}$.

An expansion for $R(\tau)$ in powers of Δ^* may be derived by using equations (3.4), (4.21) and (4.22). We find that

$$\begin{aligned} R(\tau) = (3/\sqrt{5})(\Delta^*)^{\frac{1}{9}}[1&+\Delta^*-2(\Delta^*)^{\frac{5}{3}}-(\Delta^*)^2-2(\Delta^*)^{\frac{8}{3}} \\ &+5(\Delta^*)^{\frac{10}{3}}+2(\Delta^*)^{\frac{11}{3}}+5(\Delta^*)^{\frac{13}{3}}+O((\Delta^*)^5)], \end{aligned} \tag{4.46}$$

where $\tau = \frac{1}{2}+\frac{1}{2}\tau^*$. If the expansion (4.45) is substituted in (4.46) we obtain the singular behaviour of $R(z')$ as $z' \to (-z_c)+$. The final result is in agreement with equation (3.45).

5. Analysis of the algebraic function $\omega_3(J)$

The second modular relation in equation (2.14) provides one with an implicit definition of an algebraic function $\omega_3(J)$ with four branches. In this section we shall derive various closed-form expressions for $\omega_3(J)$ and investigate the analytic properties of $\omega_3(J)$ in the J-plane. The results will be used to obtain closed-form expressions for the order-parameter $R(z')$.

(*a*) *Algebraic formulae*

Although it is possible to analyse the function $\omega_3(J)$ by using the relation in equation (2.14) it is simpler and more instructive to take the alternative form

$$J-1 = (27\omega_3^2+18\omega_3-1)^2/64\omega_3 \tag{5.1}$$

as our basic result. We shall assume (at least initially) that J is real, with $J \geqslant 1$. If we make the substitution $\omega_3 = (\frac{1}{3}\Theta)^2$ in equation (5.1), we find that the function $\Theta(J)$ is determined by the reduced equations

$$\Theta^4+6\Theta^2 \pm 8(J-1)^{\frac{1}{2}}\Theta-3 = 0. \tag{5.2}$$

This quartic equation may be solved by following the standard procedure (see Merriman 1906). In this manner we find that the four solutions of (5.1) are

$$\left.\begin{aligned}
\omega_3^{(1)}(J) &= \tfrac{1}{9}[-(J^{\frac{1}{3}}-1)^{\frac{1}{2}}+\{-(2+J^{\frac{1}{3}})+2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}\}^{\frac{1}{2}}]^2,\\
\omega_3^{(2)}(J) &= \tfrac{1}{9}[+(J^{\frac{1}{3}}-1)^{\frac{1}{2}}+\{-(2+J^{\frac{1}{3}})+2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}\}^{\frac{1}{2}}]^2,\\
\omega_3^{(3)}(J) &= -\tfrac{1}{9}[-\mathrm{i}(J^{\frac{1}{3}}-1)^{\frac{1}{2}}+\{+(2+J^{\frac{1}{3}})+2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}\}^{\frac{1}{2}}]^2,\\
\omega_3^{(4)}(J) &= -\tfrac{1}{9}[+\mathrm{i}(J^{\frac{1}{3}}-1)^{\frac{1}{2}}+\{+(2+J^{\frac{1}{3}})+2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}\}^{\frac{1}{2}}]^2,
\end{aligned}\right\} \tag{5.3}$$

where $1 \leqslant J < \infty$.

When $-\infty < J < 1$ we make the substitution $\omega_3 = -(\frac{1}{3}\bar{\Theta})^2$ in equation (5.1) to obtain the reduced equations

$$\bar{\Theta}^4-6\bar{\Theta}^2 \pm 8(1-J)^{\frac{1}{2}}\bar{\Theta}-3 = 0. \tag{5.4}$$

If we solve equation (5.4) we find that the four solutions of (5.1) for $-\infty < J < 1$ can be written down from the results (5.3) by making the formal replacements

$$\left.\begin{aligned}
(J^{\frac{1}{3}}-1)^{\frac{1}{2}} &\equiv \mathrm{i}(1-J^{\frac{1}{3}})^{\frac{1}{2}}, && 0 \leqslant J < 1\\
&\equiv \mathrm{i}[1+(-J)^{\frac{1}{3}}]^{\frac{1}{2}}, && -\infty < J < 0\\
\text{and}\qquad J^{\frac{1}{3}} &\equiv -(-J)^{\frac{1}{3}}, && -\infty < J < 0.
\end{aligned}\right\} \tag{5.5}$$

It is interesting to note that the quartic equation (5.4) with $-\infty < J \leqslant 0$ also plays a key role in the exact solution of the Ising model with pure triplet interactions on the triangular lattice (Baxter & Wu 1973, 1974; Baxter 1974; Joyce 1975*a*, *b*). More recently the quartic equation (5.4) has occurred in the theory of cusped caustics and rainbows (Peregrine & Smith 1979; Connor & Farrelly 1981)! This surprising connection leads one to speculate that modular functions may have important applications in the theory of caustics.

For *complex* values of J we can consider the results (5.3) to be the four branches of an algebraic function $\omega_3(J)$ with branch points at $J = 0, 1$ and ∞. Each branch will be a single-valued analytic function in the J-plane provided we make cuts along the real axis from $-\infty$ to 0, and 0 to 1. (For the branch $\omega_3^{(1)}(J)$ it is only necessary to cut the J-plane from 0 to 1, because $\omega_3^{(1)}(J)$ is in fact analytic at $J = \infty$.)

The Riemann surface for $\omega_3(J)$ may be constructed in the usual manner by joining together the cut-edges on different sheets that are associated with the same set of function values. The genus of the surface is given by the general formula (Bliss 1966)

$$g = \tfrac{1}{2}\sum_k (c_k-1)-n+1, \tag{5.6}$$

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where n is the degree of the algebraic function and c_k is the cycle number at the kth branch point on the Riemann surface. For the algebraic function $\omega_3(J)$ there is a branch point with cycle number $c = 3$ above $J = 0$ and $J = \infty$, and *two* branch points with $c = 2$ above $J = 1$. It follows, therefore, that the genus g is zero. If we encircle $J = 0$ once in the positive-sense with $|J| > 1$, we find that the branches (5.3) undergo the permutation cycles (1) (234). In a similar manner the encirclement of $J = 1$, without enclosing $J = 0$, yields the permutation cycles (12) (34).

(*b*) *Hypergeometric formulae*

It has been shown (Joyce 1975*a*) that the Lagrange inversion formula can be used to solve the algebraic equation (5.4) in terms of ${}_2F_1$ hypergeometric functions. From this work we find that

$$\omega_3^{(1)}(J) = -\frac{1}{64(1-J)}\left[{}_2F_1\left(\frac{1}{4}, \frac{3}{4}; \frac{4}{3}; \frac{1}{1-J}\right)\right]^4. \tag{5.7}$$

The application of the transformation formula (Erdélyi *et al.* 1953, p. 105)

$${}_2F_1(a, b; c; z) = (1-z)^{-a}{}_2F_1[a, c-b; c; z/(z-1)] \tag{5.8}$$

to equation (5.7) gives the simplified expression

$$\omega_3^{(1)}(J) = \tfrac{1}{64}J^{-1}[{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1})]^4, \tag{5.9}$$

where $|J| \geqslant 1$. A comparison of this result with (5.3) yields the interesting relation

$$[{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; I)]^2 = \tfrac{8}{3}I^{-\frac{2}{3}}[-(1-I^{\frac{1}{3}})^{\frac{1}{2}}+\{-(1+2I^{\frac{1}{3}})+2(1+I^{\frac{1}{3}}+I^{\frac{2}{3}})^{\frac{1}{2}}\}^{\frac{1}{2}}], \tag{5.10}$$

where $|I| \leqslant 1$. It is also clear from the hypergeometric formula (5.9) that the branch $\omega_3^{(1)}(J)$ is *analytic* at $J = \infty$.

Next we determine the behaviour of $\omega_3^{(1)}(J)$ in the neighbourhood of the branch point $J = 1$ using standard ${}_2F_1$ analytic continuation formulae (Erdélyi *et al.* 1953, pp. 105, 108). The final result is

$$\omega_3^{(1)}(J) = \frac{3^{-\frac{3}{2}}}{2}(\surd 3-1)^2[{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{1}{2}; 1-J)-2^{-\frac{3}{2}}\cdot 3^{-\frac{3}{4}}(\surd 3+1)(J-1)^{\frac{1}{2}}{}_2F_1(\tfrac{5}{12}, \tfrac{3}{4}; \tfrac{3}{2}; 1-J)]^4, \tag{5.11}$$

where $|J-1| < 1$ and $|\arg(J-1)| < \pi$. It is readily seen by encircling the point $J = 1$ that a hypergeometric formula for the branch $\omega_3^{(2)}(J)$ can now be obtained from equation (5.11) by simply making the replacement $(J-1)^{\frac{1}{2}} \rightarrow -(J-1)^{\frac{1}{2}}$. The behaviour of the branch $\omega_3^{(2)}(J)$ in the neighbourhood of $J = \infty$ is found from this result by reversing the analytic continuation procedure used to derive (5.11). In this manner we find

$$\omega_3^{(2)}(J) = \tfrac{4}{9}J^{\frac{1}{3}}\left[{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J^{-1})-\frac{1}{4J^{\frac{1}{3}}}{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1})\right]^4, \tag{5.12}$$

where $|J| \geqslant 1$ and $|\arg(J)| < \pi$. Similar hypergeometric formulae for the remaining branches $\omega_3^{(3)}(J)$ and $\omega_3^{(4)}(J)$ are obtained from equation (5.12) by making the replacements

$$J^{\frac{1}{3}} \rightarrow J^{\frac{1}{3}}\exp(\tfrac{2}{3}\pi i) \quad \text{and} \quad J^{\frac{1}{3}} \rightarrow J^{\frac{1}{3}}\exp(-\tfrac{2}{3}\pi i)$$

respectively.

Analytic continuation formulae that are valid for $|J| < 1$ can be constructed from equations (5.9) and (5.12) in a standard manner (Erdélyi *et al.* 1953, p. 108). It is found that

$$\omega_3^{(3)}(J) = -[{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J)]^4, \tag{5.13}$$

$$\omega_3^{(4)}(J) = -\tfrac{1}{9}[{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J) + \tfrac{1}{2}J^{\frac{1}{3}}{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J)]^4, \tag{5.14}$$

where $0 \leqslant |J| \leqslant 1$ and $0 < \arg(J) < \pi$. Similar formulae for the branches $\omega_3^{(1)}(J)$ and $\omega_3^{(2)}(J)$ are obtained from equation (5.14) by making the substitutions $J^{\frac{1}{3}} \to J^{\frac{1}{3}}\exp(\frac{2}{3}\pi i)$ and $J^{\frac{1}{3}} \to J^{\frac{1}{3}}\exp(-\frac{2}{3}\pi i)$ respectively. When $-\pi < \arg(J) < 0$ these analytic continuations for the branches $\omega_3^{(k)}(J)$, $(k = 1, \ldots, 4)$ undergo the permutation cycles (12) (34). For the branch $\omega_3^{(1)}(J)$ we also have the alternative combined form

$$\omega_3^{(1)}(J) = -\tfrac{1}{9}[{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J) - \tfrac{1}{2}(-J)^{\frac{1}{3}}{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J)]^4, \tag{5.15}$$

where $0 \leqslant |J| \leqslant 1$ and $|\arg(-J)| < \pi$. We see clearly from this result and equation (5.9) that the branch $\omega_3^{(1)}(J)$ has a real value for $-\infty < J \leqslant 0$ and $1 \leqslant J < \infty$. A comparison of (5.13) with (5.3) leads to the relation

$$[{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J)]^2 = \tfrac{1}{3}(1 - J^{\frac{1}{3}})^{\frac{1}{2}} + \tfrac{1}{3}[(2 + J^{\frac{1}{3}}) + 2(1 + J^{\frac{1}{3}} + J^{\frac{2}{3}})^{\frac{1}{2}}]^{\frac{1}{2}}, \tag{5.16}$$

where $|J| \leqslant 1$.

The analysis presented in this section is essentially a special case of a general theory of algebraic hypergeometric functions which was first developed by Schwarz (1873). It is interesting to note that in this work an alternative algebraic formula is given for the hypergeometric function ${}_2F_1(\frac{1}{4}, -\frac{1}{12}; \frac{2}{3}; J)$ in equation (5.16). This particular ${}_2F_1$ function was also discussed by Cayley (1879).

(c) *Properties of the function* $1/\omega_3(J)$

It is worthwhile investigating the reciprocal algebraic function $1/\omega_3(J)$ because this function basically determines the behaviour of the order-parameter R. From the quartic equation (5.1) we readily see that the four branches of the reciprocal function $1/\omega_3(J)$ satisfy the relations

$$1/\omega_3^{(i)}(J) = 729 \prod_{k=1}^{4}{}' \omega_3^{(k)}(J), \tag{5.17}$$

where $i = 1, \ldots, 4$ and the prime indicates that the term $k = i$ should be omitted from the product. We can now analyse the reciprocal function by applying the various hypergeometric formulae for $\omega_3(J)$ to equation (5.17). For example, in the neighbourhood of $J = \infty$ we find from (5.12) that

$$1/\omega_3^{(1)}(J) = 64J\left[{}_2F_1^3(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J^{-1}) - \tfrac{1}{64}J^{-1}\,{}_2F_1^3(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1})\right]^4, \tag{5.18}$$

where $|J| \geqslant 1$.

We can rewrite equation (5.18) in the alternative form

$$1/\omega_3^{(1)}(J) = \xi^3(J) - 1, \tag{5.19}$$

where

$$\xi(J) = 4J^{\frac{1}{3}}\frac{{}_2F_1(\frac{1}{4}, -\frac{1}{12}; \frac{2}{3}; J^{-1})}{{}_2F_1(\frac{1}{4}, \frac{7}{12}; \frac{4}{3}; J^{-1})}, \tag{5.20}$$

and $|J| \geqslant 1$. It is clear from equations (2.14) and (5.19) that $\xi(J)$ and its analytic continuations define an algebraic schwarzian function of degree 12 whose branches satisfy the rational relation

$$J = \xi^3(8+\xi^3)^3/64(\xi^3-1)^3. \tag{5.21}$$

The geometrical significance of this result is discussed by Klein & Fricke (1890, p. 104). If the substitution $J = J(\tau)$ is made in equation (5.20) then we obtain a modular function $\xi(J(\tau)) \equiv \xi(\tau)$, which is a hauptmodul for the principal congruence subgroup $\Gamma(3)$. (An explicit formula for $\xi(\tau)$ is given by Klein & Fricke (1892, p. 375).)

The modular equations (2.19) and (5.19) enable one to write the order-parameter in the form

$$R^6(\tau) = 27(\xi^3-1)/(\zeta^{-5}-11-\zeta^5), \tag{5.22}$$

where $\xi = \xi(\tau)$ and $\zeta = \zeta(\tau)$ are the hauptmoduls for the subgroups $\Gamma(3)$ and $\Gamma(5)$ respectively. A striking feature of this result is that the factor groups $\Gamma/\Gamma(3)$ and $\Gamma/\Gamma(5)$ are isomorphic with the tetrahedral and icosahedral rotation groups respectively.

It can be shown (Forsyth 1902, p. 44) that any algebraic function of degree n must satisfy a homogeneous *linear* differential equation of nth order. The differential equation for the particular algebraic function $1/\omega_3(J)$ can be determined by applying the recurrence relation method (Guttmann & Joyce 1972) to the hypergeometric series in equation (5.18). In this manner we obtain the fourth-order equation

$$72J^2(J-1)^2\mathrm{D}^4y+72J(J-1)(7J-4)\mathrm{D}^3y+2(332J^2-385J+80)\mathrm{D}^2y + (16J-7)\mathrm{D}y-16y = 0, \tag{5.23}$$

where $\mathrm{D} \equiv \mathrm{d}/\mathrm{d}J$ and $y = 1/\omega_3$. It is readily verified that the differential equation (5.23) is a fuchsian equation (Ince 1927; Poole 1936) with three regular singular points at $J = 0, 1$ and ∞.

The Riemann P-symbol (see Ince 1927, p. 370) associated with equation (5.23) is

$$P\begin{bmatrix} 0 & 1 & \infty & \\ 0 & 0 & -1 & \\ 1 & 1 & 1 & J \\ \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \\ \frac{2}{3} & \frac{3}{2} & \frac{2}{3} & \end{bmatrix}. \tag{5.24}$$

In this scheme the singular points are placed in the first row with the roots of the corresponding indicial equations beneath them. For an *arbitrary* fourth-order fuchsian equation with a regular singularity at $J = \infty$ and ν regular singular points in the finite J-plane it can be shown (Ince 1927, p. 371) that the sum of all the exponents in the riemannian scheme is an *invariant* equal to $6(\nu-1)$. We see directly from (5.24) that the differential equation (5.23) has the correct fuchsian invariant of 6. Finally, we note that the function $[\omega_3(J)]^{-\alpha}$ with $\alpha > 0$ also satisfies a fuchsian differential equation of fourth order when $\alpha = \frac{1}{2}$ and $\frac{1}{4}$.

6. Closed-form expressions for $R(z')$

The results given in §5 will now be used to derive various explicit formulae for the order-parameter $R(z')$.

(a) *Formulae for* $0 < z' < z'_c$

For this physically important case we find from equations (2.19), (3.4) and (5.3) that

$$R^6(z') = \frac{3^5 z'}{\Omega_1(z')}[\pm(J^{\frac{1}{3}}-1)^{\frac{1}{2}}+\{-(2+J^{\frac{1}{3}})+2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}\}^{\frac{1}{2}}]^{-2}, \tag{6.1}$$

where

$$J = (12)^{-3}\Omega_2^3(z')/z'\Omega_1^5(z'), \tag{6.2}$$

and $\Omega_i(z')$, $(i = 1, 2)$ are the icosahedral polynomials defined in equation (2.24). The upper and lower signs in (6.1) are valid for $\theta_3(+) < z' < z'_c$ and $0 < z' < \theta_3(+)$ respectively, where

$$\theta_3(+) = -\tfrac{1}{2}(261+125\sqrt{5})+\tfrac{15}{2}(650+290\sqrt{5})^{\frac{1}{2}} \tag{6.3}$$

is one of the zeros of the icosahedral polynomial $\Omega_3(\theta)$, (see §3*b*). When $z' = \theta_3(+)$ the function $J(z')$ has the value $J = 1$, and it would appear from (6.1) that $R(z')$ has a branch point at $z' = \theta_3(+)$. However, we see from equation (2.23) that $J(z')$ has a minimum value at $z' = \theta_3(+)$, and as a result the function $R(z')$ is in fact analytic at $z' = \theta_3(+)$.

Hypergeometric representations for $R(z')$ can also be obtained by using equations (5.9) and (5.12). It is found that

$$R^6(z') = [\Omega_2^3(z')/\Omega_1^6(z')]\,[{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};J^{-1})]^{-4}, \tag{6.4}$$

where $0 \leqslant z' \leqslant \theta_3(+)$ and the function $J = J(z')$ is defined in equation (6.2). In the neighbourhood of the critical point z'_c we have the alternative formula

$$R^6(z') = 3^6(z')^{\frac{4}{3}}\Omega_1^{\frac{2}{3}}(z')\,\Omega_2^{-1}(z')\left[{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};J^{-1})-\frac{1}{4J^{\frac{1}{3}}}\,{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};J^{-1})\right]^{-4}, \tag{6.5}$$

where $\theta_3(+) \leqslant z' < z'_c$.

The application of the quadratic transformation (see Erdélyi *et al.* 1953, p. 111)

$${}_2F_1(a,b;a+b+\tfrac{1}{2};z) = {}_2F_1[2a,2b;a+b+\tfrac{1}{2};\tfrac{1}{2}-\tfrac{1}{2}(1-z)^{\frac{1}{2}}] \tag{6.6}$$

to equations (6.4) and (6.5) yields the further results

$$R^6(z') = [\Omega_2^3(z')/\Omega_1^6(z')]\,[{}_2F_1(\tfrac{1}{2},\tfrac{7}{6};\tfrac{4}{3};\beta_-(z'))]^{-4}, \tag{6.7}$$

and

$$R^6(z') = 3^6(z')^{\frac{4}{3}}\Omega_1^{\frac{2}{3}}(z')\,\Omega_2^{-1}(z')\,[{}_2F_1(\tfrac{1}{2},-\tfrac{1}{6};\tfrac{2}{3};\beta_+(z')) - 3(z')^{\frac{1}{3}}\Omega_1^{\frac{5}{3}}(z')\,\Omega_2^{-1}(z')\,{}_2F_1(\tfrac{1}{2},\tfrac{7}{6};\tfrac{4}{3};\beta_+(z'))]^{-4}, \tag{6.8}$$

where

$$\beta_\pm(z') = \tfrac{1}{2}\pm\tfrac{1}{2}\Omega_3(z')\,\Omega_2^{-\frac{3}{2}}(z'). \tag{6.9}$$

These representations are of particular interest because they are valid for *all* values of z' in the physical range $0 < z' < z'_c$. It is also clear from equation (6.7) that $R(z')$ does *not* have a singularity at $\theta_3(+)$. Finally, we note that the values of $\beta_+(z')$ and $\beta_-(z')$ at the critical point z'_c are 0 and 1 respectively.

(*b*) *Formulae for* $-z_c < z' < 0$

When $-z_c < z' < 0$ we find from equations (5.3), (5.5) and (6.2) that the analytic continuation of the order-parameter $R(z')$ can be written in the algebraic form

$$R^6(z') = 3^5\,|z'|\,\Omega_1^{-1}(z')\,[\pm(1-J^{\frac{1}{3}})^{\frac{1}{2}}+\{(2+J^{\frac{1}{3}})+2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}\}^{\frac{1}{2}}]^{-2}, \tag{6.10}$$

where

$$J^{\frac{1}{3}} \equiv \operatorname{sgn}(J)\cdot|J|^{\frac{1}{3}} = -(12)^{-1}\Omega_2(z')/|z'|^{\frac{1}{3}}\Omega_1^{\frac{5}{3}}(z'). \tag{6.11}$$

The upper and lower signs in equation (6.10) are valid for $-z_c < z' < \theta_3(-)$ and $\theta_3(-) < z' < 0$ respectively, where

$$\theta_3(-) = -\tfrac{1}{2}(261-125\sqrt{5})-\tfrac{15}{2}(650-290\sqrt{5})^{\frac{1}{2}} \tag{6.12}$$

is one of the zeros of the icosahedral polynomial $\Omega_3(\theta)$. The function $J(z')$ takes the value $J = 1$ when $z' = \theta_3(-)$. However, the order-parameter $R(z')$ does not exhibit a branch-point singularity at $z' = \theta_3(-)$ because $J(z')$ has a maximum value at $\theta_3(-)$. In the interval $-z_c < z' < 0$ the function $J(z')$ also has the value $J = 0$ at the two points

$$\theta_2(\pm) = (57\pm25\sqrt{5})-5(255\pm114\sqrt{5})^{\frac{1}{2}}, \tag{6.13}$$

where $\theta_2(\pm)$ are zeros of the polynomial $\Omega_2(\theta)$, (see §3*b*). We readily see from (6.11) that the order-parameter $R(z')$ is an analytic function at the apparent singular points $z' = \theta_2(\pm)$, (see §3*d*).

The results in §5*b* enable one to derive various hypergeometric representations for $R(z')$ that are valid in the interval $-z_c < z' < 0$. For example, we find from equation (5.7) that

$$R^6(z') = [\Omega_3^2(z')/\Omega_1^6(z')]\left[{}_2F_1\left(\frac{1}{4},\frac{3}{4};\frac{4}{3};\frac{1}{1-J}\right)\right]^{-4}, \tag{6.14}$$

where

$$(1-J)^{-1} = (12)^3\,|z'|\,\Omega_1^5(z')/\Omega_3^2(z'), \tag{6.15}$$

and $\theta_2(+) \leqslant z' \leqslant 0$. In a similar manner we obtain from equations (5.13) and (5.14) the further representations:

$$R^6(z') = 3^5\,|z'|\,\Omega_1^{-1}(z')\,[{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};J)+\tfrac{1}{2}J^{\frac{1}{3}}{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};J)]^{-4}, \tag{6.16}$$

for values of z' in the interval $\theta_3(-) \leqslant z' \leqslant \theta_2(+)$; and

$$R^6(z') = 3^3\,|z'|\,\Omega_1^{-1}(z')\,[{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};J)]^{-4}, \tag{6.17}$$

for the interval $\theta_2(-) \leqslant z' \leqslant \theta_3(-)$. The functions $J^{\frac{1}{3}} = J^{\frac{1}{3}}(z')$ and $J = J(z')$ in these formulae are defined in equations (6.11) and (6.2) respectively. In the final interval $-z_c < z' < \theta_2(-)$ we find by using (5.8) and (5.12) that

$$R^6(z') = 3^6\,|z'|^{\frac{4}{3}}\Omega_1^{\frac{2}{3}}(z')\,\Omega_2^{-1}(z')\,[(J-1)/J]\left[{}_2F_1\left(\frac{1}{4},\frac{3}{4};\frac{2}{3};\frac{1}{1-J}\right)-\frac{1}{4J^{\frac{1}{3}}}\,{}_2F_1\left(\frac{1}{4},\frac{3}{4};\frac{4}{3};\frac{1}{1-J}\right)\right]^{-4}, \tag{6.18}$$

where $(1-J)^{-1}$ is defined as a function of z' in (6.15). The representation (6.18) shows clearly the *confluent singularity* structure of $R(z')$ as $z' \to -z_c+$, and $J \to -\infty$.

The representation (6.17) becomes slowly convergent as $z' \to \theta_3(-)$. We can overcome this

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problem by applying the quadratic transformation formula (6.6) to the hypergeometric series in (6.17). This procedure gives

$$R^6(z') = 3^3\,|z'|\,\Omega_1^{-1}(z')\,[{}_2F_1(\tfrac{1}{2}, -\tfrac{1}{6}; \tfrac{2}{3}; \alpha_+(z'))]^{-4}, \tag{6.19}$$

where
$$\alpha_+(z') = \tfrac{1}{2}+\tfrac{1}{2}(12)^{-\frac{3}{2}}|z'|^{-\frac{1}{2}}\Omega_1^{-\frac{5}{4}}(z')\,\Omega_3(z'). \tag{6.20}$$

The transformed representation (6.19) is convergent for all z' in the interval $\theta_2(-) \leqslant z' \leqslant \theta_2(+)$. It is also possible to apply the quadratic transformation to equation (6.16).

All the hypergeometric representations derived so far have a restricted range of validity in the interval $-z_c < z' < 0$. We can improve this situation by first applying the cubic transformation formula (Goursat 1881, S137, equation (113))

$${}_2F_1\left(\frac{1}{4}, \frac{3}{4}; \frac{4}{3}; \frac{1}{1-J}\right) = (1-8\omega_2)^{\frac{1}{4}}(1+\omega_2)^{\frac{1}{4}}{}_2F_1(\tfrac{3}{4}, \tfrac{1}{12}; \tfrac{4}{3}; -\omega_2) \tag{6.21}$$

to equation (6.14), where $\omega_2 = \omega_2(\tau)$ is the hauptmodul for the congruence subgroup $\Gamma_0(2)$ and $J = J(\tau)$ is the fundamental modular invariant. (For the interval $-z_c < z' < 0$ of interest we must have $\tau = \frac{1}{2}+\frac{1}{2}\tau^*$, with $\mathrm{Re}\,(\tau^*) = 0$ and $\mathrm{Im}\,(\tau^*) > 0$.) The quadratic transformation (6.6) is now applied to equation (6.21), and an explicit formula for $\omega_2 = \omega_2(J)$ is derived by solving the modular relation given in equation (2.14). This procedure finally yields the representation

$$R^6(z') = \frac{64z'}{\Omega_1(z')\,\omega_2}[{}_2F_1(\tfrac{3}{2}, \tfrac{1}{6}; \tfrac{4}{3}; k_\pm^2)]^{-4}, \tag{6.22}$$

where
$$k_\pm^2 = \tfrac{1}{2}\pm\tfrac{1}{2}(1+\omega_2)^{\frac{1}{2}}, \tag{6.23}$$

$$\omega_2 = -\tfrac{1}{4}+\tfrac{3}{8}J^{\frac{1}{3}}[(1-J)^{\frac{1}{2}}-1]^{\frac{1}{3}}-\tfrac{3}{8}J^{\frac{1}{3}}[(1-J)^{\frac{1}{2}}+1]^{\frac{1}{3}}, \tag{6.24}$$

and the function $J = J(z')$ is defined in equation (6.2). The upper and lower signs in this result are valid for $-z_c < z' < \theta_3(-)$ and $\theta_3(-) < z' < 0$ respectively, and we define $X^{\frac{1}{3}} \equiv \mathrm{sgn}\,(X)\cdot|X|^{\frac{1}{3}}$.

The quantities $k_\pm^2$ provide one with a natural parametrization for the hard-hexagon model for $z' < 0$, because the representation (6.22) is convergent for all z' in the interval $-z_c < z' < 0$. When $z' \to -z_c+$ the parameter $k_+^2 \to 1-$, and the hypergeometric series in (6.22) becomes very slowly convergent. The singular behaviour of $R(z')$ at $z' = -z_c$ is associated with the divergence of this series at $k_+^2 = 1$. A similar mathematical mechanism is responsible for the phase transition in the two-dimensional Ising model (Onsager 1944).

It can be shown by applying the transformation $\tau = \frac{1}{2}+\frac{1}{2}\tau^*$ to the modular equation (2.21) that

$$\omega_2(\tau) = -4k^2(\tau^*)\,[k'(\tau^*)]^2, \tag{6.25}$$

where $k(\tau^*)$ in the standard elliptic modular function and $k'(\tau^*)$ is the complementary modular function. If this result is substituted in equation (6.23) we readily see that the quantities $k_\pm^2$ can be written in the modular form $k_-^2 = k^2(\tau^*)$ and $k_+^2 = [k'(\tau^*)]^2$.

7. Grand partition function for $0 < z' < z'_c$

When $0 < z' < z'_c$, Baxter (1980) has shown that for a large lattice the grand partition function per site Ξ of the hard-hexagon model has the parametric representation

$$\Xi(x) = x^{-\frac{1}{3}} \prod_{n=1}^{\infty} \frac{(1-x^{3n-2})(1-x^{3n-1})(1-x^{5n-3})^2(1-x^{5n-2})^2(1-x^{5n})^2}{(1-x^{3n})^2(1-x^{5n-4})^3(1-x^{5n-1})^3}, \tag{7.1}$$

$$z'(x) = x \prod_{n=1}^{\infty} \frac{(1-x^{5n-4})^5(1-x^{5n-1})^5}{(1-x^{5n-3})^5(1-x^{5n-2})^5}, \tag{7.2}$$

where $0 < x < 1$. The elimination of the parameter x from these two equations gives the grand partition function Ξ as a function of z'. We shall denote this explicit function by $\Xi_+(z')$.

Our aim in the present section is to show that there exists a surprisingly simple algebraic relation between the grand partition function $\Xi_+(z')$ and the order-parameter $R(z')$. We shall then use the results derived in the previous sections to investigate the properties of $\Xi_+(z')$.

(a) *Relation between $\Xi_+(z')$ and $R(z')$*

We begin by substituting the product identities

$$\prod_{n=1}^{\infty} (1-x^{5n-3})(1-x^{5n-2})(1-x^{5n}) = \prod_{n=1}^{\infty} \frac{(1-x^n)}{(1-x^{5n-4})(1-x^{5n-1})} \tag{7.3}$$

and

$$\prod_{n=1}^{\infty} (1-x^{3n-2})(1-x^{3n-1}) = \prod_{n=1}^{\infty} (1-x^n)(1-x^{3n})^{-1} \tag{7.4}$$

in equation (7.1). In this manner we obtain

$$\Xi^2(x) = x^{-\frac{2}{3}} \prod_{n=1}^{\infty} \frac{(1-x^n)^6}{(1-x^{3n})^6(1-x^{5n-4})^{10}(1-x^{5n-1})^{10}}. \tag{7.5}$$

Next we use (7.2) and (7.3) to write the formula (7.5) in the form

$$\Xi^4 = \frac{x^{\frac{2}{3}}}{(z')^2} \prod_{n=1}^{\infty} \left(\frac{1-x^n}{1-x^{3n}}\right)^{12} \left(\frac{1-x^{5n}}{1-x^n}\right)^{10}. \tag{7.6}$$

We can now apply the definitions (2.12) and (2.13) to the expression (7.6). This procedure gives

$$\Xi^4 = 27\omega_5^{\frac{5}{3}}/[5^5(z')^2\omega_3], \tag{7.7}$$

where $\omega_3 = \omega_3(\tau)$ and $\omega_5 = \omega_5(\tau)$ are the hauptmoduls for the congruence subgroups $\Gamma_0(3)$ and $\Gamma_0(5)$ respectively. We obtain the required relation between $\Xi_+(z')$ and $R(z')$ by eliminating ω_3 and ω_5 from the formula (7.7) by using the order-parameter equation (3.4) and the modular equation (2.19) with $\theta = z'$. The final result is

$$\Xi_+^4(z') = (z')^{-\frac{4}{3}}\Omega_1^{-\frac{2}{3}}(z')\, R^6(z'), \tag{7.8}$$

where $0 < z' < z'_c$. This algebraic relation will form the basis for our analysis of the properties of $\Xi_+(z')$.

(*b*) *Algebraic equation for* $\Xi_+(z')$

If we use the relation (7.8) to eliminate the order-parameter R from equation (3.13) we find that $\Xi_+(z')$ is a solution of the algebraic equation

$$f(z',y) \equiv (z')^2\Omega_1^{10}(z')\,y^4 - \Omega_3(z')\,[1458z'\Omega_1^5(z') + \Omega_3^2(z')]\,y^3$$
$$-3^{10}[2430z'\Omega_1^5(z') + \Omega_3^2(z')]\,y^2 - 3^{19}\Omega_3(z')\,y - 3^{27} = 0, \qquad (7.9)$$

where
$$y \equiv \Xi_+^6. \qquad (7.10)$$

The resultant polynomial in z' for this quartic equation is found to be

$$\mathrm{Res}\,(f, \partial f/\partial y;\, y) = -3^{69}(z')^4\Omega_1^{20}(z')\,\Omega_2^6(z')\,P_1^2(z'), \qquad (7.11)$$

where
$$P_1(z') = 8[(z')^{12}+1] + 3789[(z')^{11} - z'] + 1\,768\,827[(z')^{10} + (z')^2]$$
$$-89\,060\,175[(z')^9 - (z')^3] + 740\,910\,450[(z')^8 + (z')^4]$$
$$-401\,086\,467[(z')^7 - (z')^5] + 982\,326\,229(z')^6. \qquad (7.12)$$

We see from this resultant and the known analytic properties of the order-parameter that the algebraic function $\Xi_+^6(z')$ has proper singular points at $z' = 0$, ∞, z_c' and $-z_c$, and apparent singular points at the zeros of the polynomials $\Omega_2(z')$ and $P_1(z')$.

It follows from the algebraic equation (7.9) and the work of Forsyth (1902, p. 44) that the function $\Xi_+^6(z')$ must satisfy a homogeneous linear differential equation of fourth order. Unfortunately, it has not been possible to determine the detailed form of this differential equation because of the formidable amount of algebra involved in its derivation. However, one would expect the differential equation to have a complicated structure with four regular singular points in the z'-plane at $z' = 0$, ∞, z_c', $-z_c$ and at least 16 apparent regular singular points (see Poole 1936, p. 68) at the zeros of the polynomials $\Omega_2(z')$ and $P_1(z')$.

(*c*) *Closed-form expressions for* $\Xi_+(z')$

An algebraic formula for $\Xi_+(z')$ follows directly from the relation (7.8) and equation (6.1). We find that

$$\Xi_+(z') = 3^{\frac{5}{4}}(z')^{-\frac{1}{12}}\Omega_1^{-\frac{5}{12}}(z')\,[\pm(J^{\frac{1}{3}}-1)^{\frac{1}{2}} + \{-(2+J^{\frac{1}{3}}) + 2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}\}^{\frac{1}{2}}]^{-\frac{1}{2}}, \qquad (7.13)$$

where the function $J = J(z')$ is defined in (6.2), and the upper and lower signs are valid for $\theta_3(+) < z' < z_c'$ and $0 < z' < \theta_3(+)$ respectively.

The behaviour of $\Xi_+(z')$ in the neighbourhood of $z' = 0$ may be established by using (7.8) and the hypergeometric representation (6.4). In this manner we obtain

$$\Xi_+(z') = (z')^{-\frac{1}{3}}\Omega_1^{-\frac{5}{3}}(z')\,\Omega_2^{\frac{3}{4}}(z')\,[{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1})]^{-1}, \qquad (7.14)$$

where $0 < z' \leqslant \theta_3(+)$. The application of (5.9) and (5.18) to the hypergeometric function in this result yields the alternative formula

$$\Xi_+(z') = (z')^{-\frac{1}{3}}\Omega_1^{-\frac{5}{3}}(z')\,\Omega_2^{\frac{3}{4}}(z')\,[{}_2F_1^3(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J^{-1}) - \tfrac{1}{64}J^{-1}\,{}_2F_1^3(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1})], \qquad (7.15)$$

where $0 < z' \leqslant \theta_3(+)$. It follows from (7.15) and a theorem of Appell (1880) that the function $\Xi_+(z')$ must also satisfy a homogeneous linear differential equation of fourth order with polynomial coefficients.

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In the neighbourhood of the critical point z'_c we can use equations (7.8) and (6.5) to obtain the representation

$$\Xi_+(z') = 3^{\frac{3}{8}}\Omega_2^{-\frac{1}{4}}(z')\,[{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J^{-1}) - \tfrac{1}{4}J^{-\frac{1}{3}}{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1})]^{-1}, \tag{7.16}$$

where $\theta_3(+) \leqslant z' \leqslant z'_c$. If we take the limit $z' \to z'_c-$, the function $J(z')$ tends to $+\infty$, and (7.16) gives

$$\Xi_+(z'_c) = 3^{\frac{3}{8}}\Omega_2^{-\frac{1}{4}}(z'_c) = (27\sqrt{5}/125z'_c)^{\frac{1}{8}}, \tag{7.17}$$

which is in agreement with the work of Baxter (1980). The application of equation (5.12) and the reciprocal relation (5.17) to the representation (7.16) enables one to completely resolve the confluent singularity structure at z'_c into the additive form

$$\Xi_+(z') = \psi_0(z') + [1-(z'/z'_c)]^{\frac{5}{3}}\psi_1(z') + [1-(z'/z'_c)]^{\frac{10}{3}}\psi_2(z'), \tag{7.18}$$

where

$$\left.\begin{aligned}
\psi_0(z') &= 3^{\frac{3}{8}}\Omega_2^{-\frac{1}{4}}(z')\,[{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J^{-1})]^2\,{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1}),\\
\psi_1(z') &= 3^{\frac{5}{8}}(z')^{\frac{1}{3}}(1+z'_c z')^{\frac{5}{3}}\Omega_2^{-\frac{5}{4}}(z')\,{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; J^{-1})\,[{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1})]^2,\\
\psi_2(z') &= 3^{\frac{7}{8}}(z')^{\frac{2}{3}}(1+z'_c z')^{\frac{10}{3}}\Omega_2^{-\frac{9}{4}}(z')\,[{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1})]^3,
\end{aligned}\right\} \tag{7.19}$$

and $\theta_3(+) \leqslant z' \leqslant z'_c$.

It is clear that the functions $\psi_i(z')$, $(i = 0, 1, 2)$ are analytic at the critical point z'_c and therefore can be expanded as Taylor series about z'_c. From these expansions and equation (7.18) we find that

$$\begin{aligned}
\Xi_+(z') = \Xi_+(z'_c)\,[1 &+ \tfrac{5}{2}(-1+\sqrt{5})\,t' + 3(t')^{\frac{5}{3}} + \tfrac{5}{2}(19-5\sqrt{5})\,(t')^2 + 10(-1+2\sqrt{5})\,(t')^{\frac{8}{3}}\\
&+ 5(-59+40\sqrt{5})\,(t')^3 + 9(t')^{\frac{10}{3}} + \tfrac{5}{3}(339-55\sqrt{5})\,(t')^{\frac{11}{3}} + \tfrac{5}{2}(1763-555\sqrt{5})\,(t')^4\\
&+ \tfrac{15}{2}(-5+13\sqrt{5})\,(t')^{\frac{13}{3}} + \tfrac{5}{27}(-16702+16345\sqrt{5})\,(t')^{\frac{14}{3}} + O((t')^5)],
\end{aligned} \tag{7.20}$$

where
$$t' = 5^{-\frac{3}{8}}[1-(z'/z'_c)], \tag{7.21}$$

and $t' \gtrsim 0$.

Finally, it should be noted that the range of validity of the hypergeometric representations (7.14), (7.15), (7.16) and (7.19) can be extended to $0 < z' < z'_c$ by using the quadratic transformation (6.6).

(*d*) *Properties of* $\ln \Xi_+(z')$

The thermodynamic properties of a lattice gas system can usually be expressed directly in terms of the reduced grand potential $\Gamma \equiv \ln \Xi$ (see Gaunt & Fisher 1965; Gaunt 1967). For the hard-hexagon model we see from the relation (7.8) that

$$pa_0/k_B T = \Gamma_+(z') \equiv \ln \Xi_+(z') = -\tfrac{1}{3}\ln(z') - \tfrac{1}{6}\ln[1-11z'-(z')^2] + \tfrac{3}{2}\ln R(z'), \tag{7.22}$$

where p is the pressure of the lattice gas, a_0 is the area of a unit cell in the lattice and $0 < z' < z'_c$. It is also convenient to introduce the modified reduced potential

$$\Gamma^*_+(z') \equiv \Gamma_+(z') + \tfrac{1}{3}\ln(z'), \tag{7.23}$$

where $0 < z' < z'_c$.

The modified potential (7.23) is an analytic function at $z' = 0$, and we can therefore expand it as a Mayer-type series

$$\Gamma_+^*(z') = \frac{1}{3}\sum_{l=1}^{\infty} \frac{G_l}{l}(z')^l, \tag{7.24}$$

where $0 < z' < z'_c$. (In the notation of Gaunt & Fisher 1965 we have $G_l \equiv 3lb'_l$.) To determine the integer coefficients G_l we first use the results in table 2 and the identity

$$\ln R(z') = \ln\left[\sum_{n=0}^{\infty} r_n(z')^n\right] \equiv -\sum_{l=1}^{\infty} \frac{L_l}{l}(z')^l \tag{7.25}$$

to generate the set of coefficients $\{L_l\}$. The substitution of this identity in equation (7.22) then yields the relation

$$G_l = \tfrac{1}{2}(H_l - 9L_l), \quad (l \geqslant 1) \tag{7.26}$$

where the coefficients H_l satisfy the recurrence relation

$$H_{l+1} - 11H_l - H_{l-1} = 0, \quad (l \geqslant 2) \tag{7.27}$$

with the initial conditions $H_1 = 11$ and $H_2 = 123$. A list of the coefficients G_l obtained by using (7.26) is given in table 4 for $l \leqslant 24$. For large values of n this procedure becomes numerically ill-conditioned, because $H_l \sim 9L_l$ as $l \to \infty$.

Table 4. Coefficients G_l in the expansion (7.24)

l	G_l
1	1
2	3
3	16
4	107
5	806
6	6534
7	55679
8	491923
9	4466824
10	41441118
11	391183255
12	3745534346
13	36293268662
14	355253577675
15	3507807526121
16	34899845984947
17	349541143227319
18	3521491734372588
19	35663981440936927
20	362887730308910042
21	3708116440249430666
22	38036506785075251247
23	391529796047179549874
24	4043113138126578563002

The behaviour of $\Gamma_+(z')$ in the neighbourhood of the critical point z'_c may be derived directly from (7.20). In particular, we find that

$$\begin{aligned}\Gamma_+(z') = \Gamma_+(z'_c) &+ \tfrac{5}{2}(-1+\sqrt{5})\,t' + 3(t')^{\frac{5}{3}} + \tfrac{5}{4}(23-5\sqrt{5})\,(t')^2 + \tfrac{5}{2}(-1+5\sqrt{5})\,(t')^{\frac{8}{3}} \\ &+ \tfrac{5}{3}(-62+55\sqrt{5})\,(t')^3 + \tfrac{9}{2}(t')^{\frac{10}{3}} + \tfrac{10}{3}(78-5\sqrt{5})\,(t')^{\frac{11}{3}} + \tfrac{5}{8}(2667-615\sqrt{5})\,(t')^4 \\ &+ \tfrac{15}{2}(-1+5\sqrt{5})\,(t')^{\frac{13}{3}} + \tfrac{5}{27}(-2428+5995\sqrt{5})\,(t')^{\frac{14}{3}} + O((t')^5).\end{aligned} \tag{7.28}$$

An alternative approach is to evaluate the logarithm of the expansion (3.43), and then use the relation (7.22). This indirect procedure provides one with an excellent check on the accuracy of (7.28).

We can derive an asymptotic representation for the series coefficients G_l in equation (7.24) by applying the Darboux theorem (see Ninham 1963) to the critical-point expansion (7.28). The final result is

$$G_l \sim \frac{2\sqrt{5}(z_c')^{-l}}{25\Gamma(\frac{1}{3})\, l^{\frac{5}{3}}}\left[1+\frac{4\sqrt{5}}{45l}+\frac{14\sqrt{5}}{375}\cdot\frac{\Gamma(\frac{1}{3})}{\Gamma(\frac{2}{3})}\cdot\frac{1}{l^{\frac{5}{3}}}-\frac{22}{2025l^2}+\frac{182}{3375}\cdot\frac{\Gamma(\frac{1}{3})}{\Gamma(\frac{2}{3})}\cdot\frac{1}{l^{\frac{8}{3}}}-\frac{11704\sqrt{5}}{1366875l^3}+\ldots\right], \tag{7.29}$$

as $l \to \infty$, where $\Gamma(x)$ denotes the gamma function. This asymptotic representation gives a very accurate approximation for G_l when l is *small*. For example, if the asymptotic value for G_l is rounded to the nearest integer one obtains the exact value for G_l, provided $l \leqslant 7$! This result provides, at least for the hard-hexagon model, a precise justification for the series analysis method for investigating critical behaviour (Gaunt 1967). When $n = 24$ the representation (7.29) gives

$$G_{24} \approx 4.04311279 \times 10^{21},$$

which is in excellent agreement with the exact value in table 4.

8. Mean densities for $0 < z' < z_c'$

When $z' < z_c'$ the hard-hexagon model undergoes an ordering process in which the particles preferentially occupy one of the three basic triangular sub-lattices S_1, S_2, S_3 in the triangular lattice. We can gain insight into this phenomenon by studying the behaviour of the mean number density $\rho_k(z')$ on the sub-lattice S_k, where $k = 1, 2, 3$. For convenience we shall assume that S_1 is the preferred sub-lattice, so that at close-packing ($z' = 0$) we have $\rho_1(0) = 1$ and $\rho_2(0) = \rho_3(0) = 0$. It should be noted that the sub-lattice densities satisfy the relations

$$\rho_1(z') \neq \rho_2(z') = \rho_3(z'), \tag{8.1}$$

$$R(z') = \rho_1(z') - \rho_2(z') = \rho_1(z') - \rho_3(z'), \tag{8.2}$$

where $0 \leqslant z' < z_c'$.

The mean number density $\rho(z')$ for the whole lattice is given by the thermodynamic equation

$$\rho(z') = -z'\frac{\mathrm{d}}{\mathrm{d}z'}\Gamma_+(z'), \tag{8.3}$$

where the reduced grand potential $\Gamma_+(z')$ is defined in equation (7.22). We can also write the density $\rho(z')$ in the form

$$\rho(z') = \tfrac{1}{3}[\rho_1(z') + \rho_2(z') + \rho_3(z')]. \tag{8.4}$$

It follows from (8.2) and (8.4) that the sub-lattice densities can be expressed in terms of $R(z')$ and $\rho(z')$. In particular, we have the relations

$$\left.\begin{aligned} \rho_2(z') = \rho_3(z') &= \rho(z') - \tfrac{1}{3}R(z'), \\ \rho_1(z') &= \rho(z') + \tfrac{2}{3}R(z'). \end{aligned}\right\} \tag{8.5}$$

Our main aim in the remainder of this section is to determine the properties of $\rho(z')$. We shall then use (8.5) and the known results for $R(z')$ to analyse the behaviour of $\rho_k(z')$, $k = 1, 2, 3$.

(a) Hypergeometric representations for $\rho(z')$

To determine $\rho(z')$ we first use equations (2.22) and (7.14) to write the reduced potential (7.22) in the hypergeometric form

$$\Gamma_+(z') = -\tfrac{1}{12}\ln(z') + \tfrac{3}{4}\ln(12) - \tfrac{5}{12}\ln[1-11z'-(z')^2] - \ln[I^{\frac{1}{4}}{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};I)], \tag{8.6}$$

where $I = I(z') = 1/J(z')$, and $0 < z' \leqslant \theta_3(+)$. We now evaluate the derivative in the thermodynamic formula (8.3) by applying the standard result (Erdélyi *et al.* 1953, p. 102)

$$\frac{\mathrm{d}}{\mathrm{d}I}[I^a{}_2F_1(a,b;c;I)] = aI^{a-1}{}_2F_1(a+1,b;c;I), \tag{8.7}$$

and the elegant relation

$$\frac{z'}{I}\cdot\frac{\mathrm{d}I}{\mathrm{d}z'} = \frac{\Omega_3(z')}{\Omega_1(z')\,\Omega_2(z')}. \tag{8.8}$$

In this manner we find that

$$\rho(z') = \tfrac{1}{12}[1-66z'-11(z')^2][\Omega_1(z')]^{-1} + \tfrac{1}{4}\Omega_3(z')[\Omega_1(z')\,\Omega_2(z')]^{-1} \times [{}_2F_1(\tfrac{5}{4},\tfrac{7}{12};\tfrac{4}{3};I)/{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};I)], \tag{8.9}$$

where $0 \leqslant z' \leqslant \theta_3(+)$.

A considerable simplification of the result (8.9) can be achieved by considering the properties of the hypergeometric differential equation

$$I(1-I)\frac{\mathrm{d}^2y}{\mathrm{d}I^2} + [c-(a+b+1)\,I]\frac{\mathrm{d}y}{\mathrm{d}I} - aby = 0, \tag{8.10}$$

with $a = \frac{1}{4}$, $b = -\frac{1}{12}$ and $c = \frac{2}{3}$. In the neighbourhood of $I = 0$ this differential equation has two independent solutions,

$$y_1(I) = {}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};I) \tag{8.11}$$

and

$$y_2(I) = I^{\frac{1}{3}}{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};I). \tag{8.12}$$

If we define the function $Y(I) \equiv y_1(I)/y_2(I)$ then we can write

$$\mathrm{d}Y/\mathrm{d}I = -[y_2(I)]^{-2}W(y_1,y_2), \tag{8.13}$$

where $W(y_1,y_2)$ is the wronskian for the solutions y_1 and y_2. The application of the Abel formula (Poole 1936) to (8.13) gives

$$\mathrm{d}Y/\mathrm{d}I = -\tfrac{1}{3}[y_2(I)]^{-2}I^{-\frac{2}{3}}(1-I)^{-\frac{1}{2}}. \tag{8.14}$$

We now use the function $Y(I)$ and equation (5.9) to express the relation (5.19) in the alternative form

$$64[I^{\frac{1}{4}}{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};I)]^{-4} = 64[Y(I)]^3 - 1. \tag{8.15}$$

Next we differentiate (8.15) and apply the formulae (8.7) and (8.14). This procedure yields the unusual hypergeometric identity

$$[{}_2F_1(\tfrac{5}{4},\tfrac{7}{12};\tfrac{4}{3};I)/{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};I)] = (1-I)^{-\frac{1}{2}}[{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};I)]^2. \tag{8.16}$$

The substitution of this identity in equation (8.9) gives the required simplified result

$$\rho(z') = \tfrac{1}{12}[1-66z'-11(z')^2]\,[\Omega_1(z')]^{-1}+\tfrac{1}{4}[\Omega_2^{\frac{1}{2}}(z')/\Omega_1(z')]\,[{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};J^{-1})]^2, \qquad (8.17)$$

where the function $J = J(z')$ is defined in (6.2), and $0 \leqslant z' \leqslant \theta_3(+)$.

It is possible to extend the range of validity of the representation (8.17) by using the quadratic transformation (6.6). We find that

$$\rho(z') = \tfrac{1}{12}[1-66z'-11(z')^2]\,[\Omega_1(z')]^{-1}+\tfrac{1}{4}[\Omega_2^{\frac{1}{2}}(z')/\Omega_1(z')]\,[{}_2F_1(\tfrac{1}{2},-\tfrac{1}{6};\tfrac{2}{3};\beta_-(z'))]^2, \qquad (8.18)$$

where $\beta_-(z')$ is defined in (6.9), and $0 \leqslant z' < z'_c$. It is also interesting to note that the Clausen theorem (Erdélyi *et al.* 1953, p. 185)

$$[{}_2F_1(a,b;a+b+\tfrac{1}{2};I)]^2 = {}_3F_2(2a,a+b,2b;a+b+\tfrac{1}{2},2a+2b;I) \qquad (8.19)$$

enables one to express the representation (8.17) in terms of a *generalized* hypergeometric function.

(*b*) *Properties of the density* $\rho(z')$

We see by inspection of the basic result (8.17) that $\rho(z')$ can be expanded as a Taylor series about $z' = 0$. The detailed form of this expansion is readily obtained by using equations (7.24) and (8.3). We find

$$\rho(z') = \frac{1}{3}\left[1-\sum_{l=1}^{\infty} G_l(z')^l\right], \qquad (8.20)$$

where $|z'| \leqslant z'_c$. An asymptotic representation for the coefficients G_l is given in (7.29).

The behaviour of $\rho(z')$ in the neighbourhood of the critical point z'_c may be established by comparing the representation (8.17) with equations (5.13) and (5.14) for the branches of the algebraic function $\omega_3(J)$. In this manner we obtain

$$\rho(z') = \tfrac{1}{12}[1-66z'-11(z')^2]\,[\Omega_1(z')]^{-1}+\tfrac{1}{12}[\Omega_2^{\frac{1}{2}}(z')/\Omega_1(z')]$$
$$\times\,[{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};J^{-1})+\tfrac{1}{2}J^{-\frac{1}{3}}{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};J^{-1})]^2, \qquad (8.21)$$

where $\theta_3(+) \leqslant z' < z'_c$. It follows from this result that $\rho(z')$ exhibits a confluent singularity at z'_c of the type

$$\rho(z') = \phi_0(z')+[1-(z'/z'_c)]^{\frac{2}{3}}\phi_1(z')+[1-(z'/z'_c)]^{\frac{7}{3}}\phi_2(z'), \qquad (8.22)$$

where

$$\left.\begin{aligned}
\phi_0(z') &= \tfrac{1}{12}[1-66z'-11(z')^2]\,[\Omega_1(z')]^{-1}+\tfrac{1}{12}\Omega_2^{\frac{1}{2}}(z')\,[\Omega_1(z')]^{-1}[{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};J^{-1})]^2,\\
\phi_1(z') &= (z')^{\frac{1}{3}}(1+z'_c z')^{\frac{2}{3}}[\Omega_2(z')]^{-\frac{1}{2}}{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};J^{-1})\,{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};J^{-1}),\\
\phi_2(z') &= 3(z')^{\frac{2}{3}}(1+z'_c z')^{\frac{7}{3}}[\Omega_2(z')]^{-\frac{3}{2}}[{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};J^{-1})]^2,
\end{aligned}\right\} \qquad (8.23)$$

and $\theta_3(+) \leqslant z' < z'_c$. When $z' = z'_c$ the function $\phi_0(z')$ has the indeterminate form '0/0', and we must write

$$\rho(z'_c) = \lim_{z'\to z'_c-} \phi_0(z') = \tfrac{1}{10}(5-\surd 5). \qquad (8.24)$$

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The products of ${}_2F_1$ functions in (8.23) can all be expressed in terms of ${}_3F_2$ generalized hypergeometric functions (see Erdélyi *et al.* 1953, p. 185). In particular, we find

$$\left.\begin{aligned} [{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};J^{-1})]^2 &= {}_3F_2(\tfrac{1}{2},\tfrac{1}{6},-\tfrac{1}{6};\tfrac{1}{3},\tfrac{2}{3};J^{-1}),\\ {}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};J^{-1})\,{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};J^{-1}) &= {}_3F_2(\tfrac{5}{6},\tfrac{1}{2},\tfrac{1}{6};\tfrac{4}{3},\tfrac{2}{3};J^{-1}),\\ [{}_2F_1(\tfrac{1}{4},\tfrac{7}{12};\tfrac{4}{3};J^{-1})]^2 &= {}_3F_2(\tfrac{7}{6},\tfrac{5}{6},\tfrac{1}{2};\tfrac{5}{3},\tfrac{4}{3};J^{-1}), \end{aligned}\right\} \tag{8.25}$$

where $|J| \geqslant 1$. It is also possible to extend the range of validity of the representation (8.22) to $0 < z' < z'_c$ by applying the quadratic transformation (6.6) to equation (8.23). The expansion of the formula (8.22) in powers of the variable (7.21) is most easily derived by using equations (7.28) and (8.3). The final result is

$$\begin{aligned} \rho(z') = {} & \tfrac{1}{10}(5-\sqrt{5})+\frac{\sqrt{5}}{5}(t')^{\frac{2}{3}}-\frac{\sqrt{5}}{5}t'+\tfrac{1}{15}(25-4\sqrt{5})(t')^{\frac{5}{3}}-\tfrac{1}{10}(25-\sqrt{5})(t')^2+\frac{3\sqrt{5}}{5}(t')^{\frac{7}{3}}\\ & +\tfrac{2}{45}(108\sqrt{5}-125)(t')^{\frac{8}{3}}-\tfrac{1}{10}(83\sqrt{5}-25)(t')^3+\tfrac{1}{10}(175-13\sqrt{5})(t')^{\frac{10}{3}}\\ & +\tfrac{2}{405}(16775-4621\sqrt{5})(t')^{\frac{11}{3}}+O((t')^4), \end{aligned} \tag{8.26}$$

where $t' \gtrsim 0$.

An algebraic closed-form expression for $\rho(z')$ is readily obtained by comparing (8.17) with the identity (5.16). It is found that

$$\begin{aligned} \rho(z') = {} & \tfrac{1}{12}[1-66z'-11(z')^2][\Omega_1(z')]^{-1}+\frac{1}{(12)^{\frac{1}{2}}}[z'/\Omega_1(z')]^{\frac{1}{6}}\\ & \times[\pm(J^{\frac{1}{3}}-1)^{\frac{1}{2}}+\{(2J^{\frac{1}{3}}+1)+2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}\}^{\frac{1}{2}}], \end{aligned} \tag{8.27}$$

where the function $J = J(z')$ is defined in (6.2), and the upper and lower signs are valid for $0 < z' \leqslant \theta_3(+)$ and $\theta_3(+) \leqslant z' < z'_c$ respectively. We see from equations (6.1), (7.13) and (8.27) that the quantities $R(z')$, $\Xi_+(z')$ and $\rho(z')$ are *all* expressible in terms of the various branches of the algebraic function $\omega_3(J)$.

It can be shown by using (5.4), (5.13) and (8.17) that the mean number density $\rho(z')$ is a solution of the quartic equation

$$f(z',\rho) \equiv 3\Omega_1(z')\rho^4-[1-66z'-11(z')^2]\rho^3-15z'(3+z')\rho^2+3z'(4+3z')\rho-z'(1+2z') = 0, \tag{8.28}$$

where $0 \leqslant z' < z'_c$. The resultant polynomial in z' for this quartic equation is

$$\mathrm{Res}\,(f,\partial f/\partial\rho,\rho) = -81(z')^2\Omega_1^5(z'). \tag{8.29}$$

It follows from (8.29) that the algebraic function $\rho(z')$ has singular points in the finite z'-plane at $z' = 0$, z'_c and $-z_c$. The algebraic equation (8.28) is of considerable importance because it can be used to determine the inverse function $z' = z'(\rho)$.

(c) *Sub-lattice densities*

Most of the properties of the sub-lattice densities $\rho_k(z')$, $k = 1,2,3$ can now be established by applying the known results for $\rho(z')$ and $R(z')$ to (8.5). Because this procedure is very straightforward we shall not give any further details of closed-form expressions or series expansions for $\rho_k(z')$, $k = 1,2$.

From the work of Baxter (1982, p. 437) we find that the sub-lattice densities ρ_2 and ρ_3 have the parametric representation

$$\rho_2(\tau) = \rho_3(\tau) = x^2H(x)\,H(x^9)/[G(x)\,G(x^9)+x^2H(x)\,H(x^9)], \tag{8.30}$$

where
$$G(x) = \prod_{n=1}^{\infty}[(1-x^{5n-4})\,(1-x^{5n-1})]^{-1}, \tag{8.31}$$

$$H(x) = \prod_{n=1}^{\infty}[(1-x^{5n-3})\,(1-x^{5n-2})]^{-1}, \tag{8.32}$$

and $x = \exp(2\pi i\tau)$. If the Ramanujan identity

$$G(x)\,G(x^9)+x^2H(x)\,H(x^9) = [Q(x^3)]^2/[Q(x)\,Q(x^9)], \tag{8.33}$$

where
$$Q(x) = \prod_{n=1}^{\infty}(1-x^n), \tag{8.34}$$

is applied to (8.30) we see that the densities ρ_2 and ρ_3 can be written in the simplified product form (Baxter 1982)

$$\rho_2(\tau) = \rho_3(\tau) = x^2H(x)\,H(x^9)\,Q(x)\,Q(x^9)/[Q(x^3)]^2. \tag{8.35}$$

The striking identity (8.33) was first given without proof by Ramanujan in an unpublished manuscript (see Watson 1933; Birch 1975). A proof of the identity was later published by Rogers (1921).

In the remainder of this section we shall use (8.30) and the theory of modular functions to derive an algebraic relation for the density functions $\rho_k(z')$, $k = 2, 3$. We begin by expressing equation (8.30) in the alternative form

$$\rho^* = \rho^*(\tau) = \zeta(\tau)\,\zeta(9\tau), \tag{8.36}$$

where
$$\rho^* = \rho_2/(1-\rho_2) = \rho_3/(1-\rho_3), \tag{8.37}$$

and $\zeta(\tau)$ is the hauptmodul defined in equation (2.17). It can be shown that the two functions $\zeta(\tau)$ and $\zeta(n\tau)$, where $n = 2, 3, 4, \ldots$, are connected by an algebraic modular equation (see Klein & Fricke 1892; Rogers 1921; Mordell 1922; Watson 1939). For the case $n = 9$ the detailed structure of this modular equation can be extracted with some difficulty from the work of Klein & Fricke (1892, pp. 137–139 and pp. 150, 151). The final result is

$$\begin{aligned}(\zeta_1^{10}+\zeta_9^{10})\,(1-\zeta_1\zeta_9+\zeta_1^2\zeta_9^2)+3\zeta_1\zeta_9(\zeta_1^5+\zeta_9^5)\,(3+4\zeta_1\zeta_9-10\zeta_1^2\zeta_9^2\\ +10\zeta_1^3\zeta_9^3-4\zeta_1^4\zeta_9^4-3\zeta_1^5\zeta_9^5)-\zeta_1\zeta_9(1-\zeta_1\zeta_9+10\zeta_1^2\zeta_9^2-45\zeta_1^3\zeta_9^3+108\zeta_1^4\zeta_9^4\\ -27\zeta_1^5\zeta_9^5+108\zeta_1^6\zeta_9^6-45\zeta_1^7\zeta_9^7+10\zeta_1^8\zeta_9^8-\zeta_1^9\zeta_9^9+\zeta_1^{10}\zeta_9^{10}) = 0,\end{aligned} \tag{8.38}$$

where $\zeta_1 = \zeta(\tau)$ and $\zeta_9 = \zeta(9\tau)$. The required algebraic relation for $\rho_k(z')$, $k = 2, 3$, can now be derived by substituting (3.5) and (8.36) in (8.38). We find that

$$\begin{aligned}f(z',\rho_k) \equiv{}& 3\Omega_1^2(z')\,\rho_k^{12}-3\Omega_1(z')\,[1-66z'-11(z')^2]\,\rho_k^{11}+[1-267z'+5774(z')^2\\ &+2082(z')^3+166(z')^4]\,\rho_k^{10}+5z'[18-1847z'-879(z')^2-101(z')^3]\,\rho_k^9\\ &+45z'[1+216z'+127(z')^2+23(z')^3]\,\rho_k^8-6z'[7+1172z'+754(z')^2\\ &+251(z')^3]\,\rho_k^7+3z'[3+1185z'+599(z')^2+532(z')^3]\,\rho_k^6\\ &-18(z')^2[71-11z'+69(z')^2]\,\rho_k^5+15(z')^2[23-43z'+47(z')^2]\,\rho_k^4\\ &-15(z')^2[5-23z'+19(z')^2]\,\rho_k^3+3(z')^2[4-29z'+26(z')^2]\,\rho_k^2\\ &-(z')^2[1-9z'+13(z')^2]\,\rho_k+(z')^4 = 0,\end{aligned} \tag{8.39}$$

where $k = 2, 3$. This algebraic relation is much more complicated than the corresponding result (8.28) for the total density function $\rho(z')$.

The resultant polynomial in z for equation (8.39) is found to be

$$\operatorname{Res}(f, \partial f/\partial\rho_k, \rho_k) = -3^{20}(z')^{20}\Omega_1^{14}(z')\, P_2^2(z')\, P_3^2(z'), \tag{8.40}$$

where
$$P_2(z') = (z')^4 + 4(z')^3 + 46(z')^2 - 4(z') + 1, \tag{8.41}$$

$$P_3(z') = [(z')^8+1] - 33456[(z')^7-(z')] - 1511028[(z')^6+(z')^2] - 44429808[(z')^5-(z')^3] - 104379930(z')^4. \tag{8.42}$$

It is readily seen that the zeros of the polynomials $P_2(z')$ and $P_3(z')$ must be apparent singularities for the algebraic function $\rho_k(z')$, $(k = 2, 3)$.

The derivation of an algebraic equation for $\rho_1(z')$ is difficult because $\rho_1(z')$ does not appear to be expressible in terms of a *single* hauptmodul. However, we can obtain a relation $f(z', \rho_1, R) = 0$ by making the substitution $\rho = \rho_1 - \frac{2}{3}R$ in equation (8.28). We can then eliminate the order-parameter R from this relation using equation (3.13). In this manner we obtain an extremely complicated algebraic equation of the form

$$\sum_{i,j=0}^{48} c_{ij}(z')^i \rho_1^j = 0, \tag{8.43}$$

where $\{c_{ij}\}$ is a set of integers. It is not feasible in this paper to list the values of the coefficients c_{ij}.

9. Isothermal compressibility for $0 < z' < z'_c$

We shall now use the results derived in the previous section to analyse the properties of the reduced isothermal compressibility (see Gaunt & Fisher 1965)

$$\kappa_T^* \equiv k_B T \rho \kappa_T = -(z'/\rho)\,(\mathrm{d}\rho/\mathrm{d}z') \tag{9.1}$$

in the z'-plane.

(a) *Closed-form expressions for* $\kappa_T^*(z')$

We can determine the derivative in (9.1) by first writing equation (8.9) in the alternative form

$$\rho(z') = \tfrac{1}{12}[1-66z'-11(z')^2][1-11z'-(z')^2]^{-1} + \frac{3^{\frac{1}{2}}}{2}(z')^{\frac{1}{6}}[1-11z'-(z')^2]^{-\frac{1}{6}} \times [I^{\frac{1}{12}}(1-I)^{\frac{1}{2}}\,{}_2F_1(\tfrac{5}{4}, \tfrac{7}{12}; \tfrac{4}{3}; I)]\,[I^{\frac{1}{4}}\,{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; I)]^{-1}, \tag{9.2}$$

where
$$I = I(z') = (12)^3 z' \Omega_1^5(z')/\Omega_2^3(z'), \tag{9.3}$$

and $0 < z' \leqslant \theta_3(+)$. Next we apply equations (8.7), (8.8) and the hypergeometric relation (Erdélyi *et al.* 1953, p. 102)

$$\frac{\mathrm{d}}{\mathrm{d}I}[I^{c-a}(1-I)^{a+b-c}\,{}_2F_1(a,b;c;I)] = (c-a)\,I^{c-a-1}(1-I)^{a+b-c-1}\,{}_2F_1(a-1,b;c;I) \tag{9.4}$$

to (9.2). In this manner we obtain the basic result

$$48\rho(z')[1-11z'-(z')^2]^2\kappa_T^*(z') = -[1+8z'+414(z')^2-8(z')^3+(z')^4]$$
$$-2[1+(z')^2]\,\Omega_2^{\frac{1}{2}}(z')\,[{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};I)]^2$$
$$+3\Omega_2(z')\,[{}_2F_1(\tfrac{1}{4},-\tfrac{1}{12};\tfrac{2}{3};I)]^4, \tag{9.5}$$

where $0 \leqslant z' \leqslant \theta_3(+)$, and the function $\rho(z')$ is defined in equation (8.17).

The range of validity of (9.5) can be extended by using the quadratic transformation (6.6). Hence we find that

$$48\rho(z')[1-11z'-(z')^2]^2\kappa_T^*(z') = -[1+8z'+414(z')^2-8(z')^3+(z')^4]$$
$$-2[1+(z')^2]\,\Omega_2^{\frac{1}{2}}(z')\,[{}_2F_1(\tfrac{1}{2},-\tfrac{1}{6};\tfrac{2}{3};\beta_-(z'))]^2$$
$$+3\Omega_2(z')\,[{}_2F_1(\tfrac{1}{2},-\tfrac{1}{6};\tfrac{2}{3};\beta_-(z'))]^4, \tag{9.6}$$

where $0 \leqslant z' < z_c'$, and the function $\beta_-(z')$ is defined in equation (6.9). An algebraic closed-form expression for $\kappa_T^*(z')$ can also be derived by applying the relation (5.16) to equation (9.5). This procedure gives

$$144\rho(z')\,\Omega_1^2(z')\,\kappa_T^*(z') = -3[1+8z'+414(z')^2-8(z')^3+(z')^4]$$
$$-2[1+(z')^2]\,\Omega_2^{\frac{1}{2}}(z')\,\{\pm(1-I^{\frac{1}{3}})^{\frac{1}{2}}+[(2+I^{\frac{1}{3}})+2(1+I^{\frac{1}{3}}+I^{\frac{2}{3}})^{\frac{1}{2}}]^{\frac{1}{2}}\}$$
$$+\Omega_2(z')\,\{\pm(1-I^{\frac{1}{3}})^{\frac{1}{2}}+[(2+I^{\frac{1}{3}})+2(1+I^{\frac{1}{3}}+I^{\frac{2}{3}})^{\frac{1}{2}}]^{\frac{1}{2}}\}^2, \tag{9.7}$$

where the upper and lower signs are valid for $0 \leqslant z' \leqslant \theta_3(+)$ and $\theta_3(+) \leqslant z' < z_c'$ respectively, and the function $I = I(z')$ is defined in (9.3).

Finally, we note that if (8.17) is used to eliminate the ${}_2F_1$ function from (9.5) we obtain the further simple relation

$$3[1-11z'-(z')^2]\,\kappa_T^*(z') = -[1-33z'-5(z')^2]+3[1-11z'-(z')^2]\,\rho(z')-2z'[3+z']\,[\rho(z')]^{-1}. \tag{9.8}$$

The elimination of $\rho(z')$ from equations (8.28) and (9.8) yields an algebraic equation $f(z',\kappa_T^*) = 0$ for $\kappa_T^*(z')$.

(*b*) *Expansions for* $\kappa_T^*(z')$ *about* $z' = 0$ *and* z_c'

It follows from the definition (9.1) and equation (8.20) that we can expand $\kappa_T^*(z')$ in the form

$$\kappa_T^*(z') = \sum_{n=1}^{\infty} D_n (z')^n, \tag{9.9}$$

where $|z'| < z_c'$, and $D_1 = 1$. The coefficients D_n satisfy the recurrence relation

$$D_n = nG_n + \sum_{l=1}^{n-1} G_l D_{n-l}, \tag{9.10}$$

where $n \geqslant 2$, and the coefficients G_l are defined in table 4. A list of the coefficients D_n obtained by using (9.10) is given in table 5.

TABLE 5. COEFFICIENTS D_n IN THE EXPANSION (9.9)

n	D_n
1	1
2	7
3	58
4	523
5	4946
6	48202
7	479543
8	4842795
9	49465480
10	509778772
11	5291515351
12	55251365026
13	579764738372
14	6109170895765
15	64606835249033
16	685385220087771
17	7290937787914105
18	77747409201051916
19	830857606644275251
20	8896265387269157608
21	95421472378525391450
22	1025109615598963363201
23	11028552403636517493236
24	118805599267206863067378

An expansion for $\kappa_{\mathrm{T}}^{*}(z')$ about the physical singularity z'_c may be readily derived from (8.26) and (9.1). The final result is

$$\begin{aligned}\kappa_{\mathrm{T}}^{*}(z') = \tfrac{1}{75}(5+\sqrt{5})\,(t')^{-\frac{1}{3}}[1-\tfrac{3}{2}(t')^{\frac{1}{3}}-\tfrac{1}{2}(1+\sqrt{5})\,(t')^{\frac{2}{3}} \\ -\tfrac{1}{12}(25-5\sqrt{5})\,t'+\tfrac{1}{4}(9-\sqrt{5})\,(t')^{\frac{4}{3}}+\tfrac{1}{6}(33+\sqrt{5})\,(t')^{\frac{5}{3}} \\ -\tfrac{1}{36}(-93+221\sqrt{5})\,(t')^{2}-\tfrac{1}{4}(41-3\sqrt{5})\,(t')^{\frac{7}{3}}+\tfrac{1}{36}(-349+1009\sqrt{5})\,(t')^{\frac{8}{3}} \\ -\tfrac{1}{162}(13723-2323\sqrt{5})\,(t')^{3}+\dots],\end{aligned} \tag{9.11}$$

where t' is defined in (3.36), and $t' \gtrsim 0$. If the Darboux method is applied to this expansion we obtain the asymptotic representation

$$\begin{aligned}D_n \sim (1/15)\,(1+\sqrt{5})\,[\Gamma(\tfrac{1}{3})]^{-1}(z'_c)^{-n}n^{-\frac{2}{3}}\{1+(1/30)\,(1+\sqrt{5})\,[\Gamma(\tfrac{1}{3})/\Gamma(\tfrac{2}{3})]\,n^{-\frac{2}{3}} \\ -(1/18)\,(3-\sqrt{5})\,n^{-1}+(1/3375)\,(35+91\sqrt{5})\,[\Gamma(\tfrac{1}{3})/\Gamma(\tfrac{2}{3})]\,n^{-\frac{5}{3}} \\ -(16/2025)\,(1+3\sqrt{5})\,n^{-2}-(7/303\,750)\,(-1023+573\sqrt{5})\,[\Gamma(\tfrac{1}{3})/\Gamma(\tfrac{2}{3})]\,n^{-\frac{8}{3}} \\ -(1/1\,366\,875)\,(45045+27\,841\sqrt{5})\,n^{-3}+\dots\},\end{aligned} \tag{9.12}$$

as $n \to \infty$. When $n = 24$ the representation (9.12) gives

$$D_{24} \approx 1.188\,057\,1 \times 10^{23},$$

which is in good agreement with the exact value in table 5.

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10. Analysis of properties in the ρ-plane

In the previous sections we have analysed the properties of the hard-hexagon model as a function of the reciprocal activity z'. Our main aim in this section is to use the inverse of the density function $\rho = \rho(z')$ to establish the behaviour of the model in the ρ-plane. We shall find that the thermodynamic functions for the hard-hexagon model are surprisingly simple when expressed in terms of ρ.

(a) *Inverse function* $z' = z'(\rho)$

It is readily seen from equation (8.28) that the inverse function $z' = z'(\rho)$ satisfies the quadratic equation

$$(z')^2(2-3\rho)(1-\rho)^3+z'(1-12\rho+45\rho^2-66\rho^3+33\rho^4)+\rho^3(1-3\rho) = 0. \tag{10.1}$$

This equation defines a two-branched algebraic function that has singular points in the ρ-plane at

$$\rho = \tfrac{1}{10}(5\pm\surd 5), \tfrac{1}{6}(3\pm\surd 5), \tfrac{2}{3}, 1. \tag{10.2}$$

From (10.1) we find that the required physical branch of this algebraic function is given by

$$z'(\rho) = -\tfrac{1}{2}(2-3\rho)^{-1}(1-\rho)^{-3}[(1-12\rho+45\rho^2-66\rho^3+33\rho^4) + (-1+5\rho-5\rho^2)^{\frac{3}{2}}(-1+9\rho-9\rho^2)^{\frac{1}{2}}], \tag{10.3}$$

where $\rho_c \leqslant \rho \leqslant \frac{1}{3}$, and $\rho_c = \frac{1}{10}(5-\surd 5)$.

Hunter & Baker (1979) have shown that if a function $\omega(x)$ is a solution of the quadratic equation

$$P\omega^2+Q\omega+R = 0, \tag{10.4}$$

where P, Q and R are polynomials in x, then $\omega(x)$ also satisfies the first-order *inhomogeneous* differential equation

$$(PQ^2-4P^2R)\,\omega'+(2P^2R'-PQQ'+P'Q^2-2PP'R)\,\omega+(P'QR-2PQ'R+PQR') = 0, \tag{10.5}$$

where f' denotes the derivative $\mathrm{d}f/\mathrm{d}x$. The application of this general result to (10.1) yields the following differential equation for the function $z'(\rho)$:

$$(2-3\rho)(1-\rho)(1-9\rho+9\rho^2)(1-5\rho+5\rho^2)(\mathrm{d}z'/\mathrm{d}\rho) + 3(5-50\rho+149\rho^2-178\rho^3+75\rho^4)\,z'+6\rho^2(1-2\rho) = 0. \tag{10.6}$$

If we make the substitution

$$\rho = \tfrac{1}{3}(1-\rho') \tag{10.7}$$

in equation (10.6) we can derive a Taylor series representation for the function (10.3) in powers of ρ' about the maximum close-packing density $\rho = \frac{1}{3}$. We find that

$$z'(\rho) = \sum_{n=1}^{\infty} U_n(\rho')^n, \tag{10.8}$$

where

$$|\rho'| \leqslant \tfrac{1}{10}(-5+3\surd 5), \tag{10.9}$$

and the coefficients U_n satisfy the recurrence relation

$$2nU_n-3(3n-10)\,U_{n-1}-(19n-48)\,U_{n-2}+(11n-96)\,U_{n-3}+39(n-6)\,U_{n-4} + 25(n-6)\,U_{n-5}+5(n-6)\,U_{n-6} = 2\delta_{n,1}-6\delta_{n,3}+4\delta_{n,4}, \tag{10.10}$$

TABLE 6. COEFFICIENTS U_n IN THE EXPANSION (10.8)

n	U_n
1	1
2	−3
3	2
4	−2
5	−2
6	−10
7	−39
8	−163
9	−707
10	−3161
11	−14498
12	−67920
13	−323949
14	−1568951
15	−7699915
16	−38226703
17	−191709913
18	−970095525
19	−4948269255
20	−25421587417
21	−131448790609
22	−683678526053
23	−3574873934283
24	−18783833530317

with $n \geqslant 1$, and $U_{-m} \equiv 0$ for $m \geqslant 0$. A list of the coefficients U_n that was generated by using the relation (10.10) is given in table 6 for $n \leqslant 24$. The first few coefficients $U_1, \ldots, U_5$ were calculated by Gaunt (1967). We can also determine the coefficients U_n by reverting the series (8.20).

The series representation (10.8) exhibits a branch-point singularity on its circle of convergence at

$$\rho'_c = (1-3\rho_c) = \tfrac{1}{10}(-5+3\surd 5). \tag{10.11}$$

We can establish the detailed behaviour of z' in the neighbourhood of this singularity by deriving the series solution of the differential equation (10.6) about $\rho' = \rho'_c$. In this manner we find that

$$z'/z'_c = \xi_0(\rho') - (\tfrac{5}{12})^{\frac{3}{2}}(\surd 5-1)^3[1-(\rho'/\rho'_c)]^{\frac{3}{2}}\xi_1(\rho'), \tag{10.12}$$

where the functions $\xi_0(\rho')$ and $\xi_1(\rho')$ are analytic at $\rho' = \rho'_c$ with Taylor series representations

$$\xi_0(\rho') = 1+\tfrac{5}{12}(15-7\surd 5)[1-(\rho'/\rho'_c)]^2+\tfrac{5}{54}(505-226\surd 5)[1-(\rho'/\rho'_c)]^3 + \tfrac{5}{54}(2965-1326\surd 5)[1-(\rho'/\rho'_c)]^4+\tfrac{5}{162}(66125-29572\surd 5)[1-(\rho'/\rho'_c)]^5+\ldots, \tag{10.13}$$

and

$$\xi_1(\rho') = 1+(7/16)(3-\surd 5)[1-(\rho'/\rho'_c)]+(1/768)(10267-4583\surd 5)[1-(\rho'/\rho'_c)]^2 + (1/27648)(2271541-1015796\surd 5)[1-(\rho'/\rho'_c)]^3 + (1/1769472)(1016119447-454422541\surd 5)[1-(\rho'/\rho'_c)]^4+\ldots. \tag{10.14}$$

The application of the Darboux theorem (see Ninham 1963) to the singular part of the expression (10.12) enables one to obtain the following asymptotic representation for the series coefficients U_n in equation (10.8):

$$U_n \sim -(125/4)(5/3\pi)^{\frac{1}{2}}(\rho_c')^{4-n}n^{-\frac{5}{2}}[1+(5/32n)(-9+7\sqrt{5}) + (35/3072n^2)(9271-4163\sqrt{5}) + (35/24\,576n^3)(-1\,653\,610+737\,777\sqrt{5}) + (231/9\,437\,184n^4)(3\,638\,438\,987-1\,627\,519\,145\sqrt{5})+\ldots], \qquad (10.15)$$

as $n \to \infty$. This formula, in contrast with the expansions (3.46) and (7.29), does *not* give a good approximation for the first few coefficients $U_1, \ldots, U_5$. However, when $n = 24$ the representation (10.15) gives

$$U_{24} \approx -1.878\,399 \times 10^{13},$$

which agrees reasonably well with the exact value in table 6.

(*b*) *Isothermal compressibility* $\kappa_T(\rho)$

We shall now use the results derived in the previous section to analyse the properties of the reduced isothermal compressibility κ_T^* in the ρ-plane. First we substitute equations (9.1) and (10.3) in the differential equation (10.6). This procedure gives

$$[\kappa_T^*(\rho)]^{-1} = 3(1-3\rho)^{-1}(2-3\rho)^{-1}(1-\rho)^{-1}[(-1+5\rho-5\rho^2) + (1-2\rho)(-1+9\rho-9\rho^2)^{-\frac{1}{2}}(-1+5\rho-5\rho^2)^{\frac{1}{2}}], \qquad (10.16)$$

where $\rho_c \leqslant \rho < \frac{1}{3}$. From this result we readily obtain the basic closed-form expression

$$\kappa_T^*(\rho) = \frac{1}{15\rho}[(1-2\rho)(-1+9\rho-9\rho^2)^{\frac{1}{2}}(-1+5\rho-5\rho^2)^{-\frac{1}{2}}-(-1+9\rho-9\rho^2)]. \qquad (10.17)$$

It follows from (10.17) that the algebraic function $\kappa_T^*(\rho)$ is a solution of the quadratic equation

$$45\rho(1-5\rho+5\rho^2)(\kappa_T^*)^2-6(1-9\rho+9\rho^2)(1-5\rho+5\rho^2)\kappa_T^* + (3\rho-1)(3\rho-2)(\rho-1)(1-9\rho+9\rho^2) = 0. \qquad (10.18)$$

If we compare (10.18) with the general equation (10.4) we see that $\kappa_T^*(\rho)$ satisfies a first-order differential equation of the type (10.5). We can use this differential equation to expand formula (10.17) in powers of $\rho' = 1-3\rho$ about the close-packing density $\rho = \frac{1}{3}$. The final result is

$$\kappa_T^* = \sum_{n=1}^{\infty} V_n(\rho')^n, \quad |\rho'| < \rho_c' \qquad (10.19)$$

where the coefficients V_n satisfy the recurrence relation

$$nV_n - 5nV_{n-1} - (9n-30)V_{n-2} + (21n-60)V_{n-3} + (17n-90)V_{n-4} - (15n-60)V_{n-5} - (10n-60)V_{n-6} = \delta_{n,1} - 2\delta_{n,2} - 3\delta_{n,3} + 5\delta_{n,5} + 6\delta_{n,6} + 2\delta_{n,7}, \qquad (10.20)$$

with the initial conditions $V_{-m} \equiv 0$, $m = 0, 1, 2, \ldots$. In a similar manner we find that $1/\kappa_T^*$ can be expanded in the form

$$1/\kappa_T^* = (\rho')^{-1} \sum_{n=0}^{\infty} W_n (\rho')^n, \quad 0 < |\rho'| \leqslant \rho'_c \tag{10.21}$$

where the coefficients W_n satisfy the recurrence relation

$$\begin{aligned} 2nW_n - (5n-8)\,W_{n-1} - (37n-104)\,W_{n-2} - (27n-114)\,W_{n-3} + (61n-236)\,W_{n-4} \\ + (103n-494)\,W_{n-5} + (55n-300)\,W_{n-6} + (10n-60)\,W_{n-7} \\ = -5\delta_{n,1} + 30\delta_{n,2} + 15\delta_{n,3} - 80\delta_{n,4} - 165\delta_{n,5} - 150\delta_{n,6} - 50\delta_{n,7}, \end{aligned} \tag{10.22}$$

with the initial conditions $W_0 \equiv 1$, and $W_{-m} \equiv 0$, $m = 1, 2, \ldots$. A list of the coefficients W_n obtained by using (10.22) is given in table 7 for $n \leqslant 24$.

TABLE 7. COEFFICIENTS W_n IN THE EXPANSION (10.21)

n	W_n
0	1
1	−4
2	−2
3	−10
4	−34
5	−134
6	−572
7	−2580
8	−12114
9	−58564
10	−289492
11	−1456250
12	−7429744
13	−38351694
14	−199923012
15	−1050954170
16	−5564833874
17	−29652974374
18	−158892840932
19	−855634778490
20	−4627987878204
21	−25131711114954
22	−136965861744802
23	−748893788229110
24	−4106971889282184

The behaviour of κ_T^* in the neighbourhood of the physical singularity ρ'_c may be obtained directly from the closed-form (10.17). We find that

$$\kappa_T^* = 3^{-\frac{1}{2}}(25)^{-1}(5+3\surd 5)\,[1-(\rho'/\rho'_c)]^{-\frac{1}{2}} f_0(\rho') - (\tfrac{2}{75})\,(5+\surd 5) f_1(\rho'), \tag{10.23}$$

where the functions $f_0(\rho')$ and $f_1(\rho')$ are analytic at $\rho' = \rho'_c$ with Taylor series representations

$$\begin{aligned} f_0(\rho') = 1 - (1/48)\,(1+5\surd 5)\,[1-(\rho'/\rho'_c)] + (1/2304)\,(-3455+1531\surd 5)\,[1-(\rho'/\rho'_c)]^2 \\ + (1/27\,648)\,(9793-4256\surd 5)\,[1-(\rho'/\rho'_c)]^3 \\ - (1/5\,308\,416)\,(8\,987\,195-4\,010\,265\surd 5)\,[1-(\rho'/\rho'_c)]^4 + \ldots, \end{aligned} \tag{10.24}$$

and

$$f_1(\rho') = 1+\tfrac{1}{24}(31-13\surd 5)\,[1-(\rho'/\rho_c')]-\tfrac{1}{72}(15-5\surd 5)\,[1-(\rho'/\rho_c')]^2$$
$$+\tfrac{1}{108}(-10+5\surd 5)\,[1-(\rho'/\rho_c')]^3-\tfrac{1}{648}(35-15\surd 5)\,[1-(\rho'/\rho_c')]^4+\dots \quad (10.25)$$

The corresponding result for the reciprocal compressibility $1/\kappa_T^*$ is given by

$$1/\kappa_T^* = 3^{\frac{1}{3}}(\tfrac{5}{4})\,(-5+3\surd 5)\,[1-(\rho'/\rho_c')]^{\frac{1}{3}}g_0(\rho')+5(5-2\surd 5)\,[1-(\rho'/\rho_c')]\,g_1(\rho'), \quad (10.26)$$

where the functions $g_0(\rho')$ and $g_1(\rho')$ have Taylor series representations

$$g_0(\rho') = 1+(1/48)\,(97-27\surd 5)\,[1-(\rho'/\rho_c')]$$
$$+(1/2304)\,(36029-15281\surd 5)\,[1-(\rho'/\rho_c')]^2$$
$$+(1/27648)\,(2638075-1170048\surd 5)\,[1-(\rho'/\rho_c')]^3$$
$$+(1/5308416)\,(3572307101-1595701679\surd 5)\,[1-(\rho'/\rho_c')]^4+\dots, \quad (10.27)$$

and

$$g_1(\rho') = 1+\tfrac{1}{3}(10-3\surd 5)\,[1-(\rho'/\rho_c')]$$
$$+\tfrac{1}{18}(371-157\surd 5)\,[1-(\rho'/\rho_c')]^2$$
$$+\tfrac{1}{54}(7383-3275\surd 5)\,[1-(\rho'/\rho_c')]^3$$
$$+\tfrac{1}{162}(151595-67715\surd 5)\,[1-(\rho'/\rho_c')]^4+\dots \quad (10.28)$$

An asymptotic representation for the coefficients W_n in the expansion (10.21) can be derived by applying the Darboux theorem (see Ninham 1963) to the singular part of (10.26). The final result is

$$W_n \sim -(25/4)\,(3/\pi)^{\frac{1}{2}}n^{-\frac{3}{2}}(\rho_c')^{2-n}[1+(1/32)\,(-37+27\surd 5)\,n^{-1}$$
$$+(5/3072)\,(29729-13013\surd 5)\,n^{-2}+(35/73728)\,(-1744618+782247\surd 5)\,n^{-3}$$
$$+(7/3145728)\,(11940214297-5338544035\surd 5)\,n^{-4}+\dots], \quad (10.29)$$

as $n\rightarrow\infty$.

(c) *Reduced grand potential $\Gamma_+(\rho)$*

It is readily seen from equations (8.3) and (9.1) that the reduced grand potential Γ_+ can be written in the form

$$\Gamma_+(\rho) = \int [\kappa_T^*(\rho)]^{-1}\,d\rho+C_1, \quad (10.30)$$

where C_1 is a constant of integration. We shall use this result and the properties of $1/\kappa_T^*$ to investigate the behaviour of Γ_+ in the ρ-plane.

We begin by substituting the series (10.21) in the formula (10.30). In this manner we obtain the high-density expansion

$$3\Gamma_+(\rho) = -\ln\rho'-\sum_{n=1}^{\infty}(W_n/n)\,(\rho')^n, \quad (10.31)$$

where $\rho' = 1-3\rho$, and $0<|\rho'|\leqslant\rho_c'$. The coefficients W_n in this result satisfy the recurrence relation (10.22) and have an asymptotic representation, which is given in (10.29). The behaviour of Γ_+ in the neighbourhood of the physical singularity $\rho' = \rho'_c$ may be derived by integrating (10.26). We find that

$$\Gamma_+(\rho) = \Gamma_+(\rho_c) + 3^{-\frac{1}{2}}(\tfrac{5}{6})(7-3\sqrt{5})[1-(\rho'/\rho'_c)]^{\frac{3}{2}}h_0(\rho') + (\tfrac{5}{12})(5\sqrt{5}-11)[1-(\rho'/\rho'_c)]^2 h_1(\rho'), \tag{10.32}$$

where the functions $h_0(\rho')$ and $h_1(\rho')$ are analytic at $\rho' = \rho'_c$, with $h_0(\rho'_c) = h_1(\rho'_c) = 1$. Taylor series for $h_0(\rho')$ and $h_1(\rho')$ about $\rho' = \rho'_c$ can easily be obtained by using (10.27) and (10.28).

To establish an explicit formula for $\Gamma_+(\rho)$ we substitute the closed-form expression (10.16) in (10.30). This procedure gives

$$\Gamma_+(\rho) = -\tfrac{1}{3}(I_1+I_2)+C_2, \tag{10.33}$$

where

$$I_1 \equiv \int \frac{(1+2\rho')[1-5\rho'-5(\rho')^2]}{\rho'(1+\rho')(2+\rho')[Q(\rho')]^{\frac{1}{2}}}\,d\rho', \tag{10.34}$$

$$I_2 \equiv \int [\rho'(1+\rho')(2+\rho')]^{-1}[1-5\rho'-5(\rho')^2]\,d\rho', \tag{10.35}$$

$$Q(\rho') \equiv [1-\rho'-(\rho')^2][1-5\rho'-5(\rho')^2], \tag{10.36}$$

$\rho' = 1-3\rho$, and C_2 is a constant of integration. The indefinite integral I_2 is an elementary function given by

$$I_2 = \tfrac{1}{2}\ln[\rho'(1+\rho')^{-2}(2+\rho')^{-9}], \tag{10.37}$$

whereas I_1 is a non-trivial elliptic integral (Hancock 1958).

By following a standard *general* method (Hancock 1958, ch. 8) it is possible to express I_1 as a linear combination of an elementary integral and standard Legendre elliptic integrals of the first and third kinds. However, for our particular elliptic integral I_1 this procedure is not very useful because we know from earlier discussions that it must be possible to write the reduced grand potential $\Gamma_+(\rho)$ as the logarithm of an algebraic function $\Xi_+(\rho)$! In fact, by applying a sequence of straightforward transformations to the integrand in (10.34) we eventually obtain the explicit formula

$$\Gamma_+(\rho) = \ln \Xi_+(\rho), \tag{10.38}$$

where

$$\Xi_+^{12}(\rho) = \frac{(1+\rho')^4(2+\rho')^{18}}{5^5(\rho')^2}\left[\frac{(1+2\rho')-\sqrt{Q(\rho')}}{(1+2\rho')+\sqrt{Q(\rho')}}\right]\left\{\frac{[5-7\rho'-7(\rho')^2]-3\sqrt{Q(\rho')}}{[5-7\rho'-7(\rho')^2]+3\sqrt{Q(\rho')}}\right\}^4$$
$$\times\left\{\frac{[1-4\rho'-3(\rho')^2+2(\rho')^3+(\rho')^4]+[1-\rho'-(\rho')^2]\sqrt{Q(\rho')}}{[1-4\rho'-3(\rho')^2+2(\rho')^3+(\rho')^4]-[1-\rho'-(\rho')^2]\sqrt{Q(\rho')}}\right\}$$
$$\times\left\{\frac{[41-41\rho'-51(\rho')^2-20(\rho')^3-10(\rho')^4]+9(1+2\rho')\sqrt{Q(\rho')}}{[41-41\rho'-51(\rho')^2-20(\rho')^3-10(\rho')^4]-9(1+2\rho')\sqrt{Q(\rho')}}\right\}^2, \tag{10.39}$$

$\rho' = 1-3\rho$, and the polynomial $Q(\rho')$ is defined in (10.36). A comparison of this result with the expression for $\Gamma_+(\rho)$ in terms of Legendre elliptic integrals leads to the apparently new relation

$$9F(\varphi,\tfrac{3}{5}) - 8\Pi(\varphi,\tfrac{1}{5},\tfrac{3}{5}) = \tfrac{5}{4}\ln\left[\frac{(25-8\sin^2\varphi-\sin^4\varphi)+2\sin\varphi\cos\varphi(25-9\sin^2\varphi)^{\frac{1}{2}}}{(25-8\sin^2\varphi-\sin^4\varphi)-2\sin\varphi\cos\varphi(25-9\sin^2\varphi)^{\frac{1}{2}}}\right], \tag{10.40}$$

where
$$F(\varphi, k) = \int_0^{\varphi} (1-k^2 \sin^2\psi)^{-\frac{1}{2}} d\psi, \tag{10.41}$$
and
$$\Pi(\varphi, n, k) = \int_0^{\varphi} (1-n\sin^2\psi)^{-1}(1-k^2\sin^2\psi)^{-\frac{1}{2}} d\psi \tag{10.42}$$
are Legendre elliptic integrals of the first and third kinds respectively. If a general elliptic integral of the type (10.34) is to be expressible as the logarithm of an algebraic function then it is clear that the various polynomials in the integrand must satisfy special restrictive conditions. It is interesting to note that these conditions were investigated in great detail many years ago in a series of papers by Abel (1839) and Liouville (1833).

The basic result (10.39) can also be written in the simplified form
$$\begin{aligned}\Xi_+^6(\rho) = 2^{-7}\cdot 5^{-5}(\rho')^{-3}(1-\rho')^{-9}[(1+2\rho')-\surd Q(\rho')]\{[5-7\rho'-7(\rho')^2]-3\surd Q(\rho')\}^4 \\ \times\{[1-4\rho'-3(\rho')^2+2(\rho')^3+(\rho')^4]+[1-\rho'-(\rho')^2]\surd Q(\rho')\} \\ \times\{[41-41\rho'-51(\rho')^2-20(\rho')^3-10(\rho')^4]+9(1+2\rho')\surd Q(\rho')\}^2,\end{aligned} \tag{10.43}$$
where $\rho' = 1-3\rho$, and $0 < \rho' \leqslant \rho'_c$. A further simplification can be achieved by multiplying out all the terms in (10.43). In this manner, we finally obtain
$$\Xi_+^6(\rho) = 2^{-1}\cdot 5^{-5}(\rho')^{-2}\{S(\rho')+[1-5\rho'-5(\rho')^2]\,T(\rho')\surd Q(\rho')\}, \tag{10.44}$$
where
$$S(\rho') = \sum_{n=0}^{12} S_n(\rho')^n, \tag{10.45}$$
$$T(\rho') = \sum_{n=0}^{8} T_n(\rho')^n, \tag{10.46}$$
$\rho' = 1-3\rho$ and $0 < \rho' \leqslant \rho'_c$. The polynomial $Q(\rho')$ is defined in (10.36), and the polynomial coefficients S_n and T_n are listed in table 8.

From (10.44) and the identity
$$S^2(\rho')-[1-\rho'-(\rho')^2][1-5\rho'-5(\rho')^2]^3T^2(\rho') \equiv 2^2\cdot 5^5(\rho')^2(1+\rho')^4(2+\rho')^{18}, \tag{10.47}$$

Table 8. Polynomial coefficients S_n, T_n and Z_n in equations (10.45), (10.46) and (10.50) respectively

n	S_n	T_n	Z_n
0	3125	3125	625
1	25000	50000	3750
2	368394	228481	11250
3	1648220	510878	153572
4	2597775	656219	617949
5	−1194660	510592	756432
6	−11001870	238586	−743394
7	−19426812	61760	−3366162
8	−18739575	6820	−4563027
9	−11120900	—	−3359230
10	−4063750	—	−1440240
11	−843000	—	−339300
12	−76250	—	−34100

we readily see that $\Xi_+(\rho)$ is a solution of the 12th-degree algebraic equation

$$5^5(\rho')^2\Xi_+^{12} - S(\rho')\,\Xi_+^6 + (1+\rho')^4(2+\rho')^{18} = 0, \tag{10.48}$$

where $\rho' = 1-3\rho$. More generally, equation (10.48) specifies an algebraic function $\Xi_+^6(\rho)$, which consists of two single-valued branches defined in a cut ρ-plane. The physical branch (10.44) has (in the finite ρ-plane) a pole of order two at $\rho = \frac{1}{3}$, four branch-points at

$$\rho = \tfrac{1}{10}(5 \pm \surd 5), \tfrac{1}{6}(3 \pm \surd 5), \tag{10.49}$$

and apparently no zeros.

If the term involving the branch-point singularities in (10.44) is eliminated by using the formula (10.16) we obtain the relation

$$\rho'[1-\rho'-(\rho')^2][1-5\rho'-5(\rho')^2]\,T(\rho')\,[\kappa_T^*]^{-1} + 2(1+2\rho')(1+\rho')^3(2+\rho')^{17}[\Xi_+]^{-6} = 5\sum_{n=0}^{12} Z_n(\rho')^n, \tag{10.50}$$

where κ_T^* is the reduced isothermal compressibility, and the coefficients Z_n are defined in table 8. Because

$$[\kappa_T^*]^{-1} = -2^{-1}\cdot[\Xi_+]^{-6}\,\mathrm{d}(\Xi_+^6)/\mathrm{d}\rho', \tag{10.51}$$

it is clear that (10.50) is essentially a first-order linear differential equation for Ξ_+^6. A differential equation of this type would of course be expected on general grounds from the algebraic equation (10.48).

Finally, it follows from (10.44) that $\Xi_+^p(\rho)$ can be expanded in the form

$$\Xi_+^p(\rho) = (\rho')^{-\frac{1}{3}p}\sum_{n=0}^{\infty} X_n^{(p)}(\rho')^n, \tag{10.52}$$

where p is any real number and $\rho' = 1-3\rho$. The Taylor series in (10.52) has a radius of convergence equal to ρ'_c, where $\rho'_c = \frac{1}{10}(-5+3\surd 5)$. We can generate the values of the coefficients $X_n^{(p)}$ using the recurrence relation

$$3nX_n^{(p)} + p\sum_{k=1}^{n} W_k X_{n-k}^{(p)} = 0, \tag{10.53}$$

where $n \geqslant 1$, $X_0^{(p)} \equiv 1$ and the coefficients W_k satisfy the further relation (10.22). When $p < -0.375$ the initial coefficients $X_n^{(p)}$, $n = 0, 1, 2, \ldots$, alternate in sign before eventually all becoming negative. In particular, for $p = -12$ we find that $X_n^{(p)}$ alternates in sign for $n \leqslant 13$ with $X_n^{(p)} < 0$ for all $n > 13$.

(d) *Order-parameter* $R(\rho)$

It is now possible to establish a closed-form expression for the order-parameter $R(\rho)$ by using the basic relation (7.8) and (10.3) and (10.44). After a considerable amount of tedious algebra we find that

$$\begin{aligned} R^9(\rho) = {} & 2^2\cdot 5^{-3}(1-\rho')^6[1-5\rho'-5(\rho')^2]^{\frac{3}{2}} \\ & \times\{[1+8\rho'-3(\rho')^2-22(\rho')^3-11(\rho')^4] + [1-\rho'-(\rho')^2]^{\frac{1}{2}}[1-5\rho'-5(\rho')^2]^{\frac{3}{2}}\}^{-2} \\ & \times\{[1-\rho'-(\rho')^2]^{\frac{1}{2}}[89+228\rho'+195(\rho')^2+55(\rho')^3] \\ & -[1-5\rho'-5(\rho')^2]^{\frac{1}{2}}[39+106\rho'+91(\rho')^2+25(\rho')^3]\}^{-1} \\ & \times\{S(\rho') + [1-\rho'-(\rho')^2]^{\frac{1}{2}}[1-5\rho'-5(\rho')^2]^{\frac{3}{2}}T(\rho')\}, \end{aligned} \tag{10.54}$$

where $\rho' = 1-3\rho$ and $0 \leqslant \rho' \leqslant \rho'_c$. It follows from this result that $R^9(\rho)$ is a solution of a quadratic algebraic equation of the type (10.4). The high-density series for $R(\rho)$ in powers of ρ' can be obtained either by direct expansion of formula (10.54), or by substituting the series (10.8) in equation (3.32).

We have now completed our analysis of the hard-hexagon model in the ρ-plane. Perhaps the most surprising feature of the results is that the closed-form expressions for $z'(\rho)$, $\kappa_T^*(\rho)$, $\Xi_+^6(\rho)$ and $R^9(\rho)$ could all have been derived, at least in principle, by analysing the appropriate high-density series using the quadratic Padé approximant method (Shafer 1974) or the inhomogeneous differential approximant method (Fisher & Au-Yang 1979; Hunter & Baker 1979; Rehr *et al.* 1980).

11. Grand partition function for $0 < z < z_c$

When the activity z lies in the range $0 < z < z_c$ it can be shown (Baxter 1980) that for a large lattice the grand partition function per site Ξ of the hard-hexagon model has the parametric representation

$$\Xi(x) = \prod_{n=1}^{\infty} \frac{(1-x^{6n-4})(1-x^{6n-3})^2(1-x^{6n-2})(1-x^{5n-4})^2(1-x^{5n-1})^2(1-x^{5n})^2}{(1-x^{6n-5})(1-x^{6n-1})(1-x^{6n})^2(1-x^{5n-3})^3(1-x^{5n-2})^3}, \tag{11.1}$$

$$z(x) = -x\prod_{n=1}^{\infty} \frac{(1-x^{5n-4})^5(1-x^{5n-1})^5}{(1-x^{5n-3})^5(1-x^{5n-2})^5}, \tag{11.2}$$

where $-1 < x < 0$. The elimination of the parameter x from these equations gives the grand partition function Ξ as a function of z. We shall denote this explicit function by $\Xi_-(z)$.

Our main purpose in this section is to show that the results derived for $z > z_c$ can be used to investigate the properties of the function $\Xi_-(z)$.

(a) *Hauptmodul expression for* $\Xi(x)$

We begin by applying the following product identities:

$$\prod_{n=1}^{\infty}(1-x^{6n-4})(1-x^{6n-2}) = \prod_{n=1}^{\infty}(1-x^{2n})(1-x^{6n})^{-1}, \tag{11.3}$$

$$\prod_{n=1}^{\infty}(1-x^{6n-3}) = \prod_{n=1}^{\infty}(1-x^{3n})(1-x^{6n})^{-1}, \tag{11.4}$$

$$\prod_{n=1}^{\infty}(1-x^{6n-5})(1-x^{6n-1}) = \prod_{n=1}^{\infty}(1-x^{6n})(1-x^{3n})^{-1}(1-x^{n})(1-x^{2n})^{-1}, \tag{11.5}$$

$$\prod_{n=1}^{\infty}(1-x^{5n-3})(1-x^{5n-2}) = \prod_{n=1}^{\infty}(1-x^{n})(1-x^{5n})^{-1}(1-x^{5n-4})^{-1}(1-x^{5n-1})^{-1}, \tag{11.6}$$

to the formula (11.1). In this manner, we obtain the alternative expression

$$\Xi^2(x) = \prod_{n=1}^{\infty} \frac{(1-x^{2n})^4(1-x^{3n})^{12}(1-x^{n})^6(1-x^{5n})^5(1-x^{5n-4})^5(1-x^{5n-1})^5}{(1-x^{n})^4(1-x^{6n})^{12}(1-x^{3n})^6(1-x^{n})^5(1-x^{5n-3})^5(1-x^{5n-2})^5}. \tag{11.7}$$

If we now let $x = \exp(2\pi i\tau)$, then we can use equation (11.2) and the hauptmodul definitions (2.11), (2.12) and (2.13) to write equation (11.7) in the form

$$\Xi^{12} = (2^{12}\cdot 3^9/5^{15})\, z^6[\omega_2(\tau)/\omega_2^3(3\tau)]\,[\omega_5^5(\tau)/\omega_3^3(\tau)]. \tag{11.8}$$

To obtain values of x in the physical range $-1 < x < 0$ it is clear that we must have

$$\tau = \tfrac{1}{2} + \tfrac{1}{2}\tau^*, \tag{11.9}$$

where $\mathrm{Re}\,(\tau^*) = 0$ and $\mathrm{Im}\,(\tau^*) > 0$.

The elimination of the hauptmoduls $\omega_3(\tau)$ and $\omega_5(\tau)$ from (11.8) can be achieved by using equations (3.4) and (2.19) respectively. This procedure gives

$$\Xi^{12} = 2^{12}z^8(1+11z-z^2)^{-2}R^{18}(-z)\,[\omega_2(\tau)/\omega_2^3(3\tau)], \tag{11.10}$$

where $0 < z < z_c$. It should be carefully noted that the function $R(-z)$ in this result is the order-parameter $R(z')$ of the hard-hexagon model with the variable z' formally replaced by $-z$. A striking feature of (11.10) is that the physical behaviour of Ξ for $0 < z < z_c$ involves the non-physical behaviour of the order-parameter $R(z')$ for $-z_c < z' < 0$ (see §6*b*). We can also use equation (7.8) to write equation (11.10) in the form

$$\Xi^{12} = (2z)^{12}\Xi_+^{12}(-z)\,[\omega_2(\tau)/\omega_2^3(3\tau)], \tag{11.11}$$

where $\Xi_+(z')$ is the grand partition function per site for the ordered phase.

(*b*) *Hermite modular equation*

To establish an explicit formula for $\Xi_-(z)$ we introduce the modular functions

$$U_n(\tau^*) \equiv [k(n\tau^*)\,k'(n\tau^*)]^{\frac{1}{4}}, \quad (n = 1, 2, 3, \ldots), \tag{11.12}$$

where $k(\tau^*)$ is the standard elliptic modular function and $k'(\tau^*)$ is the complementary modular function. It follows from equation (6.25) that we can write

$$\omega_2(\tau) = -4U_1^8(\tau^*), \tag{11.13}$$

$$\omega_2(3\tau) = -4U_3^8(\tau^*), \tag{11.14}$$

where $\tau = \tfrac{1}{2} + \tfrac{1}{2}\tau^*$. Hermite (1908) has shown that the modular functions $U_1(\tau^*)$ and $U_n(\tau^*)$ are related by an algebraic modular equation. For the particular case $n = 3$ one finds that

$$U_3^4 + 4U_1^3U_3^3 - 2U_1U_3 + U_1^4 = 0. \tag{11.15}$$

(It should be noted that there is an incorrect sign in Hermite's result.)

Next we apply the transformations

$$U_3 = U_1^3/y, \tag{11.16}$$

and

$$y = -\tfrac{1}{4}(9Y+1), \tag{11.17}$$

to the Hermite equation (11.15). In this manner, we obtain the rational relation

$$(Y+1)(9Y+1)^3/64Y = 4U_1^8. \tag{11.18}$$

This formula has exactly the same *formal* structure as the basic modular equation (2.14), which relates the function $\omega_3(\tau)$ to the basic modular invariant $J(\tau)$! It follows, therefore, that we can use the results in §5 to determine the properties of the algebraic function $Y = Y(U_1)$. For example, we find from (5.13) that the required *physical* branch of $Y = Y(U_1)$ can be written as

$$Y = -[{}_2F_1(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; 4U_1^8)]^4. \tag{11.19}$$

If we express this result in terms of $\omega_2(\tau)$ and $\omega_2(3\tau)$ we obtain

$$\omega_2^3(\tau)/\omega_2(3\tau) = 2^{12}[-\tfrac{1}{8}+\tfrac{9}{8}\,{}_2F_1^4(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; -\omega_2(\tau))]^8. \tag{11.20}$$

(*c*) *Closed-form expressions for $\Xi_-(z)$*

A closed-form expression for $\Xi_-(z)$ can now be derived by eliminating $\omega_2(3\tau)$ from (11.10) and (11.20), and applying (6.24). We find that

$$\Xi_-(z) = (-64z/\omega_2)^{\frac{2}{3}}(1+11z-z^2)^{-\frac{1}{6}}R^{\frac{3}{2}}(-z)\,[-\tfrac{1}{8}+\tfrac{9}{8}\,{}_2F_1^4(\tfrac{1}{4}, -\tfrac{1}{12}; \tfrac{2}{3}; -\omega_2)]^2, \tag{11.21}$$

where

$$\omega_2 = -\tfrac{1}{4}+\tfrac{3}{8}J^{\frac{1}{3}}[(1-J)^{\frac{1}{2}}-1]^{\frac{1}{3}}-\tfrac{3}{8}J^{\frac{1}{3}}[(1-J)^{\frac{1}{2}}+1]^{\frac{1}{3}}, \tag{11.22}$$

$$J = -(12)^{-3}\Omega_2^3(-z)/z\Omega_1^5(-z), \tag{11.23}$$

and $0 < z < -\theta_3(-)$. The symbol $X^{\frac{1}{3}}$ in (11.22) denotes $\operatorname{sgn}(X)\,|X|^{\frac{1}{3}}$. We can extend the range of validity of this result by applying the quadratic transformation formula (6.6) to the ${}_2F_1$ function in (11.21). In this manner we obtain the basic hypergeometric representation

$$\Xi_-(z) = (-64z/\omega_2)^{\frac{11}{12}}(1+11z-z^2)^{-\frac{5}{12}}[{}_2F_1(\tfrac{3}{2}, \tfrac{1}{6}; \tfrac{4}{3}; k_\pm^2)]^{-1}[-\tfrac{1}{8}+\tfrac{9}{8}\,{}_2F_1^4(\tfrac{1}{2}, -\tfrac{1}{6}; \tfrac{2}{3}; k_\pm^2)]^2, \tag{11.24}$$

where

$$k_\pm^2 = \tfrac{1}{2}\pm\tfrac{1}{2}(1+\omega_2)^{\frac{1}{2}}, \tag{11.25}$$

and $0 < z < z_c$. The upper and lower signs in these equations are valid for $-\theta_3(-) < z < z_c$ and $0 < z < -\theta_3(-)$ respectively, where $\theta_3(-)$ is defined in equation (6.12).

It is also possible to derive an algebraic closed-form expression for $\Xi_-(z)$ by applying equations (5.16) and (6.10) to the formula (11.21). This procedure gives

$$\begin{aligned}\Xi_-(z) = {} & 4^{-1}\cdot 3^{\frac{5}{4}}z^{\frac{11}{12}}(1+11z-z^2)^{-\frac{5}{12}}|\omega_2|^{-\frac{2}{3}} \\ & \times\{+1\mp(1-|\omega_2|^{\frac{1}{3}})^{\frac{1}{2}}+[(2+|\omega_2|^{\frac{1}{3}})+2(1+|\omega_2|^{\frac{1}{3}}+|\omega_2|^{\frac{2}{3}})^{\frac{1}{2}}]^{\frac{1}{2}}\}^2 \\ & \times\{-1\mp(1-|\omega_2|^{\frac{1}{3}})^{\frac{1}{2}}+[(2+|\omega_2|^{\frac{1}{3}})+2(1+|\omega_2|^{\frac{1}{3}}+|\omega_2|^{\frac{2}{3}})^{\frac{1}{2}}]^{\frac{1}{2}}\}^2 \\ & \times\{\pm(1-J^{\frac{1}{3}})^{\frac{1}{2}}+[(2+J^{\frac{1}{3}})+2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}]^{\frac{1}{2}}\}^{-\frac{1}{2}},\end{aligned} \tag{11.26}$$

where $\omega_2 = \omega_2(J)$ and $J = J(z)$ are defined in (11.22) and (11.23) respectively, and $J^{\frac{1}{3}} = \operatorname{sgn}(J)\,|J|^{\frac{1}{3}}$. The upper and lower signs in (11.26) are valid for $-\theta_3(-) < z < z_c$ and $0 < z < -\theta_3(-)$ respectively.

Metcalf & Yang (1978) estimated the numerical value of $\ln\Xi_-(z)$ for $z = 1$ to be

$$\ln\Xi_-(1) \approx 0.3333\ldots. \tag{11.27}$$

On the basis of this result they conjectured that the exact value of $\ln\Xi_-(1)$ might be $\tfrac{1}{3}$. However, Baxter & Tsang (1980) used the corner transfer matrix method to obtain the more accurate estimate

$$\ln\Xi_-(1) \approx 0.333\,242\,721\,976, \tag{11.28}$$

which contradicts the conjecture of Metcalf & Yang. If we evaluate the closed-form expression (11.26) for $z = 1$ we find that

$$\ln\Xi_-(1) \approx 0.333\,242\,721\,976\,181\,887\,853\,748, \tag{11.29}$$

where $\Xi_-(1)$ is an *algebraic* number. This clearly provides a good check on the accuracy of the result (11.26).

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We can also derive from equation (11.21) a closed-form expression for $\Xi_-(z)$ that is valid in the *non-physical* interval $-1/z_c < z < 0$. The final result is

$$\begin{aligned}\Xi_-(z) = {} & 4^{-1}\cdot 3^{\frac{5}{4}}(-z)^{\frac{11}{12}}(1+11z-z^2)^{-\frac{5}{12}}\omega_2^{-\frac{2}{3}} \\ & \times\{+1+(1+\omega_2^{\frac{1}{3}})^{\frac{1}{2}}+[(2-\omega_2^{\frac{1}{3}})+2(1-\omega_2^{\frac{1}{3}}+\omega_2^{\frac{2}{3}})^{\frac{1}{2}}]^{\frac{1}{2}}\}^2 \\ & \times\{-1+(1+\omega_2^{\frac{1}{3}})^{\frac{1}{2}}+[(2-\omega_2^{\frac{1}{3}})+2(1-\omega_2^{\frac{1}{3}}+\omega_2^{\frac{2}{3}})^{\frac{1}{2}}]^{\frac{1}{2}}\}^2 \\ & \times\{\pm(J^{\frac{1}{3}}-1)^{\frac{1}{2}}+[-(2+J^{\frac{1}{3}})+2(1+J^{\frac{1}{3}}+J^{\frac{2}{3}})^{\frac{1}{2}}]^{\frac{1}{2}}\}^{-\frac{1}{2}},\end{aligned} \tag{11.30}$$

where

$$\omega_2 = -\tfrac{1}{4}+\tfrac{3}{8}J^{\frac{1}{2}}(\cos A \pm \sqrt{3}\sin A), \tag{11.31}$$

$$A = \tfrac{1}{3}\arccos(J^{-\frac{1}{2}}), \quad (0 \leqslant A < \tfrac{1}{6}\pi) \tag{11.32}$$

and $J = J(z)$ is defined in (11.23). The upper and lower signs in (11.30) and (11.31) are valid for $-1/z_c < z < -\theta_3(+)$ and $-\theta_3(+) < z < 0$ respectively, where $\theta_3(+)$ is defined in (6.3).

Our aim in this section has been to establish links between the mathematical properties of the ordered phase $z > z_c$, and the grand partition function $\Xi_-(z)$ for $0 < z < z_c$. We shall not attempt in this paper to investigate the detailed behaviour of $\Xi_-(z)$ in the neighbourhood of the singular points z_c and $-1/z_c$.

12. Mean density for $0 < z < z_c$

Baxter (1981) has shown that the mean density of the hard-hexagon model

$$\rho(z) = z(\mathrm{d}/\mathrm{d}z)\ln\Xi_-(z), \tag{12.1}$$

for $0 < z < z_c$, has the *parametric* representation

$$\rho(\tau) = -xG(x)\,H(x^6)/[H(x)\,G(x^6)-xG(x)\,H(x^6)], \tag{12.2}$$

where $x = \exp(2\pi i\tau)$, and the functions $G(x)$ and $H(x)$ are defined in equations (8.31) and (8.32) respectively. This result can be simplified by using the identity

$$H(x)\,G(x^6)-xG(x)\,H(x^6) = P(x)/P(x^3), \tag{12.3}$$

where

$$P(x) = \prod_{n=1}^{\infty}(1-x^{2n-1}). \tag{12.4}$$

The relation (12.3) was stated by Ramanujan (see Birch 1975) and proved by Rogers (1921). Hence we obtain (Baxter 1981)

$$\rho(\tau) = -xG(x)\,H(x^6)\,P(x^3)/P(x). \tag{12.5}$$

The elimination of the parameter x from (11.2) and (12.5) gives the mean density as a function of the activity z. In the next sub-section we shall use the theory of modular functions to prove explicitly that $\rho(z)$ is an algebraic function.

(*a*) *Klein–Fricke modular equation*

The application of (2.17), (8.31) and (8.32) to the formula (12.2) enables one to write $\rho(\tau)$ in the hauptmodul form

$$\rho_* = \rho_*(\tau) = -\zeta(6\tau)/\zeta(\tau), \tag{12.6}$$

where
$$\rho_*(\tau) \equiv \rho(\tau)/[1-\rho(\tau)]. \tag{12.7}$$

From the discussion in §8*c* we know that the functions $\zeta(\tau)$ and $\zeta(6\tau)$ are connected by an algebraic modular equation. The detailed structure of this modular equation can be determined from the work of Klein & Fricke (1892, pp. 137–139 and pp. 150, 151). We find that

$$\begin{aligned}187[&42\zeta_1^5\zeta_6^5(\zeta_1+\zeta_6)-42(\zeta_1+\zeta_6)+(\zeta_1^6+\zeta_6^6)+36\zeta_1\zeta_6(\zeta_1^4+\zeta_6^4)+225\zeta_1^2\zeta_6^2(\zeta_1^2+\zeta_6^2)\\ &+400\zeta_1^3\zeta_6^3]^2-882(\zeta_6-\zeta_1)^2\{374(\zeta_1^{10}\zeta_6^{10}+1)-66(\zeta_1^5\zeta_6^5-1)[21(\zeta_1^5+\zeta_6^5)\\ &+175\zeta_1\zeta_6(\zeta_1^3+\zeta_6^3)+450\zeta_1^2\zeta_6^2(\zeta_1+\zeta_6)]+(\zeta_1^{10}+\zeta_6^{10})+100\zeta_1\zeta_6(\zeta_1^8+\zeta_6^8)\\ &+2025\zeta_1^2\zeta_6^2(\zeta_1^6+\zeta_6^6)+14\,400\zeta_1^3\zeta_6^3(\zeta_1^4+\zeta_6^4)+44\,100\zeta_1^4\zeta_6^4(\zeta_1^2+\zeta_6^2)+63\,504\zeta_1^5\zeta_6^5\}\\ &+1936(\zeta_6-\zeta_1)^6[42\zeta_1^5\zeta_6^5(\zeta_1+\zeta_6)-42(\zeta_1+\zeta_6)+(\zeta_1^6+\zeta_6^6)+36\zeta_1\zeta_6(\zeta_1^4+\zeta_6^4)\\ &+225\zeta_1^2\zeta_6^2(\zeta_1^2+\zeta_6^2)+400\zeta_1^3\zeta_6^3]-1241(\zeta_6-\zeta_1)^{12}=0,\end{aligned} \tag{12.8}$$

where $\zeta_1 = \zeta(\tau)$ and $\zeta_6 = \zeta(6\tau)$.

If we make the substitutions $\zeta_6 = -\zeta_1\rho_*$ and $\zeta_1^5 = -z$ in the modular equation (12.8) we obtain, after a good deal of tedious algebra, the simplified result

$$\begin{aligned}f(\rho_*, z) \equiv\ &\rho_*^{11}z^4+\rho_*^5(\rho_*-1)(\rho_*^6-5\rho_*^5+4\rho_*^4+9\rho_*^3+4\rho_*^2-5\rho_*+1)z^3\\ &+\rho_*^2(\rho_*^8-5\rho_*^7+36\rho_*^5-59\rho_*^4+36\rho_*^3-5\rho_*+1)z^2\\ &+(\rho_*-1)(\rho_*^6-5\rho_*^5+4\rho_*^4+9\rho_*^3+4\rho_*^2-5\rho_*+1)z+\rho_*=0.\end{aligned} \tag{12.9}$$

The application of (12.7) to this *symmetric* relation yields the following algebraic equation for the physical density function $\rho(z)$:

$$\begin{aligned}f(\rho, z) \equiv\ &\rho^{11}(\rho-1)z^4-\rho^5(22\rho^7-77\rho^6+165\rho^5-220\rho^4+165\rho^3-66\rho^2+13\rho-1)z^3\\ &+\rho^2(\rho-1)^2(119\rho^8-476\rho^7+689\rho^6-401\rho^5-6\rho^4+125\rho^3-63\rho^2+13\rho-1)z^2\\ &+(\rho-1)^5(22\rho^7-77\rho^6+165\rho^5-220\rho^4+165\rho^3-66\rho^2+13\rho-1)z+\rho(\rho-1)^{11}=0.\end{aligned} \tag{12.10}$$

(*b*) *Properties of the density* $\rho(z)$

The resultant polynomial in z for the algebraic equation (12.10) is found to be

$$\operatorname{Res}(f, \partial f/\partial\rho; \rho) = -2^8\cdot 3^9 z^{22}(1+11z-z^2)^{24}. \tag{12.11}$$

We see, therefore, that the algebraic function $\rho(z)$ has singular points in the finite z-plane at $z=0$, z_c and $-1/z_c$. The physical branch of $\rho(z)$ is analytic at $z=0$ with a Taylor series representation

$$\rho(z) = \sum_{l=1}^{\infty} a_l z^l, \tag{12.12}$$

Table 9. Coefficients a_l in the expansion (12.12)

l	a_l
1	1
2	−7
3	58
4	−519
5	4856
6	−46780
7	460027
8	−4593647
9	46416730
10	−473464492
11	4866762231
12	−50346419064
13	523649493732
14	−5471647249551
15	57402510799673
16	−604310726045647
17	6381555113227479
18	−67574053536268390
19	717290150798554823
20	−7630701056990502264
21	81338708529194437456
22	−868589337931760155091
23	9290681683345015297892
24	−99526016232070896417512

where $|z| < 1/z_c$. A list of the coefficients a_l is given in table 9 for $l \leqslant 24$. It follows from (12.12) that we can expand the reduced grand potential in the form

$$pa_0/k_B T = \Gamma_-(z) \equiv \ln \Xi_-(z) = \sum_{l=1}^{\infty} b_l z^l, \tag{12.13}$$

where

$$b_l = a_l/l \tag{12.14}$$

is the lattice gas analogue of the Mayer cluster integral.

The critical behaviour of the mean density $\rho(z)$ can be established directly from the algebraic equation (12.10) by deriving the appropriate Puiseux expansion about the singular point $z = z_c$. In this manner we obtain

$$\begin{aligned}\rho(z) = {} & \tfrac{1}{10}(5-\sqrt{5}) - (1/\sqrt{5})\, t^{\frac{2}{3}} + (1/\sqrt{5})\, t - \tfrac{1}{15}(25+4\sqrt{5})\, t^{\frac{5}{3}} \\ & + \tfrac{1}{10}(25+\sqrt{5})\, t^2 - (1/\sqrt{5})\, t^{\frac{7}{3}} - \tfrac{2}{45}(125+108\sqrt{5})\, t^{\frac{8}{3}} + \tfrac{1}{10}(25+83\sqrt{5})\, t^3 \\ & - \tfrac{1}{30}(175+13\sqrt{5})\, t^{\frac{10}{3}} - \tfrac{2}{405}(16775+4621\sqrt{5})\, t^{\frac{11}{3}} + O(t^4),\end{aligned} \tag{12.15}$$

where

$$t = 5^{-\frac{3}{2}}[1-(z/z_c)], \tag{12.16}$$

and $t \gtrsim 0$. The corresponding expansion for $\Gamma_-(z)$ is

$$\begin{aligned}\Gamma_-(z) = {} & \ln \Xi_-(z_c) - \tfrac{5}{2}(\sqrt{5}-1)\, t + 3t^{\frac{5}{3}} - \tfrac{5}{4}(27-5\sqrt{5})\, t^2 + \tfrac{5}{2}(1+5\sqrt{5})\, t^{\frac{8}{3}} \\ & - \tfrac{5}{3}(-62+70\sqrt{5})\, t^3 + \tfrac{3}{2} t^{\frac{10}{3}} + \tfrac{10}{3}(78+5\sqrt{5})\, t^{\frac{11}{3}} - \tfrac{5}{8}(3583-615\sqrt{5})\, t^4 \\ & + \tfrac{5}{2}(1+5\sqrt{5})\, t^{\frac{13}{3}} + \tfrac{5}{27}(2428+5995\sqrt{5})\, t^{\frac{14}{3}} + O(t^5),\end{aligned} \tag{12.17}$$

where

$$\Xi_-(z_c) = (27 z_c \sqrt{5}/125)^{\frac{1}{2}}. \tag{12.18}$$

Finally we note that it is possible, at least in principle, to derive closed-form expressions for $\rho(z)$ by differentiating equations (11.24) and (11.26).

(*c*) *Inverse function* $z = z(\rho)$

We shall now use the basic algebraic equation (12.10) to investigate the properties of the inverse function $z = z(\rho)$ in the ρ-plane. It is found that the resultant polynomial in ρ for (12.10) is given by

$$\operatorname{Res}(f, \partial f/\partial z; z) = -\rho^{25}(1-\rho)^{15}(1-\rho+\rho^2)^2(1-5\rho+5\rho^2)^{14}P_4(\rho), \tag{12.19}$$

where $$P_4(\rho) = 1-10\rho+33\rho^2-36\rho^3+18\rho^4-70\rho^5+140\rho^6-100\rho^7+25\rho^8. \tag{12.20}$$

We see, therefore, that the inverse algebraic function $z = z(\rho)$ has singular points in the finite ρ-plane at

$$\rho = 0, 1, \exp(\pm\tfrac{1}{3}i\pi), \rho_c, (\tfrac{1}{5})\rho_c^{-1}, \boldsymbol{\rho}_s, \tag{12.21}$$

where $\boldsymbol{\rho}_s$ denotes the zeros of the polynomial $P_4(\rho)$.

The exact values of the zeros $\boldsymbol{\rho}_s$ can be determined by first applying the transformation

$$\rho = \rho_*/(1+\rho_*) \tag{12.22}$$

to the polynomial (12.20). This procedure yields the symmetric *reciprocal* equation

$$1-2\rho_*-9\rho_*^2+8\rho_*^3+53\rho_*^4+8\rho_*^5-9\rho_*^6-2\rho_*^7+\rho_*^8 = 0, \tag{12.23}$$

which can be reduced to the quartic equation

$$73+14y-13y^2-2y^3+y^4 = 0 \tag{12.24}$$

by introducing the further transformation

$$y = \rho_*+\rho_*^{-1}. \tag{12.25}$$

After solving the quartic equation (12.24) in the standard manner we find that the final expressions for the zeros $\boldsymbol{\rho}_s$ are

$$\left.\begin{aligned}
\rho_0^{\pm} &= \tfrac{1}{2}-\tfrac{1}{20}\sqrt{10}[(4\sqrt{10}-5\sqrt{5}-4\sqrt{2}+7)^{\frac{1}{2}}\pm i(4\sqrt{10}-5\sqrt{5}+4\sqrt{2}-7)^{\frac{1}{2}}],\\
\rho_1^{\pm} &= \tfrac{1}{2}-\tfrac{1}{20}\sqrt{10}[(4\sqrt{10}+5\sqrt{5}+4\sqrt{2}+7)^{\frac{1}{2}}\pm i(4\sqrt{10}+5\sqrt{5}-4\sqrt{2}-7)^{\frac{1}{2}}],\\
\rho_2^{\pm} &= \tfrac{1}{2}+\tfrac{1}{20}\sqrt{10}[(4\sqrt{10}-5\sqrt{5}-4\sqrt{2}+7)^{\frac{1}{2}}\pm i(4\sqrt{10}-5\sqrt{5}+4\sqrt{2}-7)^{\frac{1}{2}}],\\
\rho_3^{\pm} &= \tfrac{1}{2}+\tfrac{1}{20}\sqrt{10}[(4\sqrt{10}+5\sqrt{5}+4\sqrt{2}+7)^{\frac{1}{2}}\pm i(4\sqrt{10}+5\sqrt{5}-4\sqrt{2}-7)^{\frac{1}{2}}].
\end{aligned}\right\} \tag{12.26}$$

The positions of the 14 singular points in the finite ρ-plane are shown in figure 2. We see from this diagram that all the singular points have a symmetric distribution about $\rho = \frac{1}{2}$. It follows, therefore, that the polynomial (12.20) could also have been reduced to a quartic form by applying the transformation

$$\rho = \tfrac{1}{2}(1+\bar{\rho}). \tag{12.27}$$

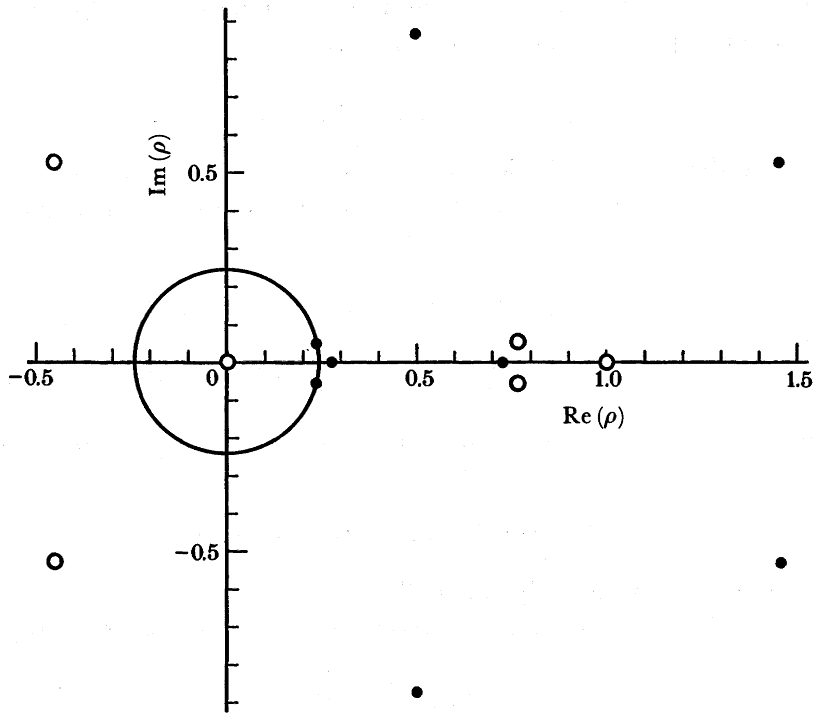

FIGURE 2. Singularity structure of the algebraic function $z = z(\rho)$ in the ρ-plane, and the circle of convergence $|\rho| = \rho_r$ for the series (12.29). The singular points marked by the symbol ● occur on the *physical* branch of $z(\rho)$, whereas the singular points denoted by the symbol ○ only occur on the *non-physical* branches.

We can establish algebraic closed-form expressions for the four branches of the function $z = z(\rho)$ by solving the symmetric quartic equation (12.9). For the *physical* branch we obtain

$$\begin{aligned} 4\rho^6(1-\rho)\,z(\rho) = {} & (1-2\rho)\,(1-11\rho+44\rho^2-77\rho^3+66\rho^4-33\rho^5+11\rho^6) \\ & +(1-\rho+\rho^2)^{\frac{1}{2}}(1-5\rho+5\rho^2)^{\frac{5}{2}}-(1-5\rho+5\rho^2)\,[2(1-16\rho \\ & +106\rho^2-378\rho^3+803\rho^4-1080\rho^5+962\rho^6-576\rho^7 \\ & +219\rho^8-50\rho^9+10\rho^{10})+2(1-2\rho)\,(1-11\rho+44\rho^2 \\ & -77\rho^3+66\rho^4-33\rho^5+11\rho^6)\,(1-\rho+\rho^2)^{\frac{1}{2}}(1-5\rho+5\rho^2)^{\frac{1}{2}}]^{\frac{1}{2}}. \end{aligned} \qquad (12.28)$$

Similar results for the non-physical branches can be written down from (12.28) by changing the signs of the various square roots. A considerable simplification of the formula (12.28) can be achieved by using the transformation (12.27).

The four branches of the algebraic function $z = z(\rho)$ do not all have the same singularity structure in the ρ-plane. However, one finds that at least one of the branches of $z = z(\rho)$ is non-analytic at each of the singular points (12.21). Thus, the function $z = z(\rho)$ has no apparent singular points in the finite ρ-plane. The *physical* branch (12.28) is non-analytic at the singular points ρ_c, $(\frac{1}{5})\,\rho_c^{-1}$, $\exp(\pm\frac{1}{3}i\pi)$, $\rho_0^{\pm}$, $\rho_3^{\pm}$, and *analytic* at the remaining singular points 0, 1, $\rho_1^{\pm}$, $\rho_2^{\pm}$. It follows, therefore, that the physical branch has a Taylor series representation about $\rho = 0$ of the type

$$z = z(\rho) = \sum_{l=1}^{\infty} c_l\,\rho^l, \quad |\rho| < \rho_r \qquad (12.29)$$

where ρ_r denotes the radius of convergence of the series. The closest singularities to the origin $\rho = 0$ are at $\rho = \rho_0^{\pm}$, where $\rho_0^{\pm}$ are defined in (12.26). We see, therefore, that the radius of convergence ρ_r is given by

$$\rho_r = |\rho_0^{\pm}| = \tfrac{1}{10}\sqrt{5}\,[(4\sqrt{10}-5\sqrt{5}+5)-\sqrt{10}(4\sqrt{10}-5\sqrt{5}-4\sqrt{2}+7)^{\frac{1}{2}}]^{\frac{1}{2}}, \tag{12.30}$$

where $\rho_r \approx 0.2414560$ is less than $\rho_c \approx 0.2763932$.

The asymptotic behaviour of the coefficient c_l as $l \to \infty$ is determined by the singular behaviour of (12.28) in the neighbourhood of the two *complex* singularities $\rho_0^{\pm}$ and, as a result, one would expect the coefficients c_l to exhibit an interesting periodic variation in sign. Confirmation of this analysis can be obtained by inspecting the exact values of c_l, which are listed in table 10 for $l \leqslant 24$.

TABLE 10. COEFFICIENTS c_l IN THE EXPANSION (12.29)

l	c_l
1	1
2	7
3	40
4	204
5	966
6	4332
7	18593
8	76805
9	306101
10	1176929
11	4354322
12	15409712
13	51566857
14	159476161
15	432427213
16	868329043
17	11520061
18	−13297007747
19	−102350921811
20	−581153060583
21	−2883976266915
22	−13172644850333
23	−56578139817485
24	−230665040819003

(d) *Virial expansion for* $\Gamma_-(\rho)$

The results obtained for the inverse function $z = z(\rho)$ will now be used to investigate the virial expansion for $\Gamma_-(\rho)$. We first introduce the generating function

$$-\ln[z(\rho)/\rho] = \sum_{l=1}^{\infty} \beta_l \rho^l, \quad |\rho| < \rho_r \tag{12.31}$$

where $z(\rho)$ denotes the *physical* branch (12.28) of the algebraic function $z = z(\rho)$, and the coefficients β_l are the lattice gas analogues of the Mayer irreducible cluster integrals. A list of the integer coefficients $l\beta_l$ is given in table 11 for $l \leqslant 24$.

The required virial expansion is now readily derived from (12.1) and (12.31). We find that

$$pa_0/k_B T = \Gamma_-(\rho) \equiv \ln \Xi_-(\rho) = \sum_{l=1}^{\infty} B_l \rho^l, \quad |\rho| < \rho_r \tag{12.32}$$

where $$B_l = -[(l-1)/l]\,\beta_{l-1}, \quad (l \geqslant 2) \tag{12.33}$$

TABLE 11. COEFFICIENTS β_l IN THE EXPANSION (12.31)

l	$l\beta_l$
1	−7
2	−31
3	−115
4	−391
5	−1237
6	−3529
7	−8155
8	−8311
9	62543
10	612809
11	3759551
12	19472387
13	91607873
14	402535529
15	1671753125
16	6585730265
17	24544637087
18	85671502739
19	273505952615
20	753160139729
21	1456884883535
22	−860351408035
23	−30699547973425
24	−228155349143341

with $B_1 = 1$, and the radius of convergence ρ_r is defined in (12.30). The asymptotic behaviour of the virial coefficient B_l has been determined by analysing the generating function (12.31) in the neighbourhood of the dominant branch-point singularities $\rho_0^{\pm}$. To leading-order the final result is

$$B_l \sim A_0 l^{-\frac{3}{2}} \rho_r^{-l} \cos(l\theta_0 - \phi_0), \tag{12.34}$$

as $l \to \infty$, where

$$\left.\begin{aligned} A_0 &\approx 0.889355, \\ \theta_0 &\approx 0.149118(\tfrac{1}{2}\pi), \\ \phi_0 &\approx 0.408936(\tfrac{1}{2}\pi). \end{aligned}\right\} \tag{12.35}$$

This formula gives a reasonably good approximation for B_l provided that the integer l is not close to one of the values $[(n+\frac{1}{2})\pi+\phi_0]/\theta_0$, where $n = 0, 1, 2, \ldots$. Gaunt & Joyce (1980) have already discussed the significance and importance of the hard-hexagon model series (12.32) in a more general context. The exact values of B_l for $l \leqslant 24$ are also included in this work.

Finally we note that the equation of state can be written in the integral form

$$pa_0/k_B T = \Gamma_-(\rho) = I_3(\rho) + c_3, \tag{12.36}$$

where

$$I_3(\rho) = \int \rho[z'(\rho)/z(\rho)]\, \mathrm{d}\rho, \tag{12.37}$$

$z(\rho)$ denotes the *physical* branch (12.28) of the algebraic function $z = z(\rho)$, and c_3 is a constant of integration. If the algebraic relation (12.10) is differentiated with respect to ρ we see that the integrand in (12.37) can be expressed as a rational function of ρ and z. Hence $I_3(\rho)$ is an abelian integral (see Bliss 1966, p. 93). It is also clear that $I_3(\rho)$ must be an elementary integral of a purely logarithmic type (Davenport 1981), because we know from our previous work that $\Gamma_-(\rho)$ is the logarithm of an algebraic function.

The direct evaluation of the integral $I_3(\rho)$ appears to be a difficult problem. It is fortunate, therefore, that a closed-form expression for $\Gamma_-(\rho)$ can be readily obtained by solving the implicit form of the equation of state given by Richey & Tracy (1987).

13. Concluding remarks

In this paper we have seen that the theory of modular functions, hauptmoduls and modular equations developed by Klein & Fricke plays an important role in the mathematical analysis of the hard-hexagon model. Because many exact solutions in lattice statistics (Baxter 1982) have a similar structure to that of the hard-hexagon model it is reasonable to expect that the Klein & Fricke theory will also give a systematic procedure for investigating and classifying other solvable models.

Evidence for the validity of this conjecture is provided by the exact solution of the Ising model with pure triplet interactions on the triangular lattice (Baxter & Wu 1973, 1974; Baxter 1974). For this model it can be shown from the work of the present author (Joyce 1975*a*, *b*) that the free energy per spin F can be written in the form

$$4F/k_B T = -\ln(4\theta^2) + \ln[-\omega_3^{(1)}(J)], \tag{13.1}$$

where

$$\omega_3^{(1)}(J) = (64J)^{-1}[{}_2F_1(\tfrac{1}{4}, \tfrac{7}{12}; \tfrac{4}{3}; J^{-1})]^4, \tag{13.2}$$

$$J = -(1-\theta^2)^4/[16\theta^2(1+\theta^2)^2], \tag{13.3}$$

$$\theta = \sinh K,$$

with $0 \leqslant \theta < \infty$ and $-\infty < J \leqslant 0$. If this result is compared with (8.6) we see that the underlying mathematical structure of the free energy F is basically the same as that of the reduced potential $\Gamma_+(z')$ for the hard-hexagon model.

I am extremely grateful to Professor R. J. Baxter, Professor D. S. Gaunt and Dr W. J. Harvey for their continued interest and encouragement in this work. I also thank Professor J. H. Davenport, Dr J. L. Martin and Dr M. Punjani for expert assistance and advice on various aspects of computer algebra. Finally, I thank Dr R. Pinch and one of the referees for their helpful comments on the paper.

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