

Two-dimensional infinite repulsive systems: the Yang-Lee singularities are isolated branch points

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1984 J. Phys. A: Math. Gen. 17 907

(<http://iopscience.iop.org/0305-4470/17/4/031>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 31/05/2010 at 07:59

Please note that [terms and conditions apply](#).

Two-dimensional infinite repulsive systems: the Yang–Lee singularities are isolated branch points

S Baer

Department of Physical Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

Received 27 September 1983

Abstract. The singularities of the pressure as a function of the activity z are examined by a certain limiting procedure applicable to the solved hard-hexagon model (Baxter 1980) and the tempered hard-square model (Fisher 1963). For hard hexagons the only singularities found in the finite complex z plane are two isolated branch points on the real z axis. For the tempered hard squares, the only singularities found are three isolated branch points on the real z axis. By the same procedure applied to the Ising model, the singularities of the energy as a function of temperature are found to be isolated branch points in the complex temperature plane. Comparison with numerical results shows that the dense distribution of singularities of finite systems disappears in the infinite system limit, save for a few isolated points.

1. Introduction and summary

In 1952 Yang and Lee put forward a theory about the distribution of the zeros of the grand partition function $\Xi(z, V)$ in the complex activity z plane and its relation to the singularities of the pressure $p(z)$ and density $\rho(z)$ in general and to the phase transition points in particular. They have succeeded in proving a celebrated theorem (Lee and Yang 1952) on the distribution of the zeros of $\Xi(z, V)$ on the unit circle for lattice systems with attractive interactions between particles on different lattice sites. Their work has opened up a new line of research on the relation between specific types of intermolecular potentials and the analytic properties, in particular the type and distribution of the singularities of $p(z)$, in the complex z plane. In this connection the Lee–Yang circle theorem was extended to general classes of ferromagnetic Ising and Heisenberg models including many spin interactions (Suzuki and Fisher 1971), showing a change of the distribution of zeros from a circle to a line on the negative real z axis. In the case of continuous one-dimensional systems it was proved (Penrose and Elvey 1968) that for hard-core and finite-range interactions the distribution of zeros always consists of connected arc segments. By a different method Ruelle (1971) has found a way of determining regions in the complex z plane which are free of zeros and this method was applied (Runnels and Hubbard 1972) to find that the monomer–dimer system has no phase transition point, i.e. has the positive real z axis free of singularities.

Systems with pure repulsive interactions are of special interest. Since the cluster integrals, which are the coefficients of the power series expansion of $\beta p(z)$, alternate in sign (Groeneveld 1962), the singularity of $\beta p(z)$ nearest to the origin must be on

the negative real axis and for finite systems the positive real z axis must be free of singularities. Yet numerical analysis (Gaunt and Fisher 1965, Gaunt 1967) and exactly solved systems (Baxter 1980) provide examples of infinite repulsive systems which undergo a phase transition at high densities. Therefore, these systems possess a singular point z_c on the positive real z axis which is the transition point from a fluid to an ordered state. However, nothing is known about the neighbourhood of this point in the complex z plane and how, according to the Yang-Lee theory (1952), the singularities 'close in' on z_c in the limit of the infinite system. Baram (1982) has studied numerically several repulsive systems and has found that their cluster expansions, as far as one can go, are well represented by certain continued fractions. He examined their associated tridiagonal matrices and found that the elements in each diagonal of the matrix tend to a certain constant and hence he approximated the matrix, from a certain point onward, by a constant tridiagonal (a Toeplitz) tail. The resulting expression for $\beta p(z)$ ($\rho(z)$) possesses two isolated square-root branch points: $z_c > 0$ and $z_0 < 0$, $|z_0| \ll z_c$. The two points can be taken as representing, respectively, the phase transition point and the singularity nearest to the origin determining the radius of convergence of the power series expansion of $\beta p(z)$.

This form of the approximate $\beta p(z)$, resulting in two isolated branch points, cannot by itself indicate the general pattern of behaviour. However, examination of the singularities in exactly solved model systems supports these results. In the following we examine two two-dimensional systems. One is the hard-hexagon system solved by Baxter (1980). The second is a system of hard squares with added special attractive interactions (tempered hard squares) which was solved by Fisher (1963) for a special isotherm, apparently above the critical point.

The method used for finding the singular points in the complex z plane is based on the fact that for both systems the dependence of the pressure p on the activity z is represented parametrically by giving p and z as analytic functions of a parameter τ . In both cases $z(\tau)$ and $p(\tau)$ are related to certain elliptic functions of the complex parameter. They are defined for all $\text{Im } \tau > 0$ and have the real τ axis as their natural boundary. Hence all singular values of z must be obtained as limiting values of $z(\tau)$ on the real τ axis. These limiting values are found by making use of the representation of elliptic functions as ratios of theta functions. The latter are powerful computational tools for this purpose since the actual limiting process $\text{Im } \tau \rightarrow 0^+$ is easily applied to the theta functions. More precisely, limiting values can be obtained directly only for the rational points on the real τ axis. In the case of the tempered hard squares $z(\tau)$ could be evaluated explicitly for all rational τ 's and it was found that all limiting values of $z(\tau)$ were only one of the three values: $-\frac{1}{2}$, z_0 , z_c . In the case of the hard hexagons the actual evaluation of the limiting values of $z(\tau)$ could be done only numerically for a representative set of a thousand points. All limiting values thus obtained were only one of the 4 values: z_0 , 0 , z_c , ∞ . Ignoring the infinity and noting that the $z = 0$ is actually a regular point of $p(z)$ (although not of the free energy density), we are left with the two finite singularities z_0 and z_c .

These results support the conjecture that for repulsive systems $p(z)$ has only two isolated singularities, z_0 and z_c , on the real z axis, where $z_c > 0$ determines the fluid-solid phase transition point and $z_0 < 0$, $|z_0| < z_c$, determines the radius of convergence of the expansion of $p(z)$. Thus the approximate continued fraction representation of $p(z)$, leading to corresponding two square-root branch points, can serve as a reasonable representation of the behaviour of thermodynamic functions when extended to the

complex z plane. As mentioned (Baram 1982) it fails to reproduce correctly the critical exponents in the neighbourhood of the transition point z_c .

The forementioned method for finding singularities is also applied to find the singular points of the (free) energy of the Ising model in the complex temperature plane. Comparison with numerical results for finite systems shows that a dense distribution of singular points on the two circles

$$y = \pm 1 + \sqrt{2} e^{i\phi}, \quad y = e^{-2\beta J} \quad (1.1)$$

actually disappears in the thermodynamic limit save for the four isolated points $\pm 1 \pm \sqrt{2}$.

2. Theta functions: definitions and transformation formulae

We shall use the following definition and notation of general theta functions of a complex variable u , depending on a complex parameter τ ($\text{Im } \tau > 0$) and having a characteristic defined by a pair of real numbers $0 \leq \alpha, \beta < 1$ (Krazer 1903)

$$\theta \begin{bmatrix} \alpha \\ \beta \end{bmatrix} (u, \tau) = \sum_{n=-\infty}^{\infty} \exp[i\pi\tau(n+\alpha)^2 + 2\pi i(n+\alpha)(u+\beta)]. \quad (2.1)$$

The four special theta functions of Jacobi (see, e.g. Magnus *et al* 1966, ch X and references therein) will then be written as

$$\theta_0(u, \tau) \equiv \theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix} (u, \tau) \quad \theta_1(u, \tau) \equiv -\theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} (u, \tau) \quad (2.2a, b)$$

$$\theta_2(u, \tau) \equiv \theta \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} (u, \tau) \quad \theta_3(u, \tau) \equiv \theta \begin{bmatrix} 0 \\ 0 \end{bmatrix} (u, \tau). \quad (2.2c, d)$$

We shall make use of the following transformation formulae (Krazer 1970, ch II § 5). When the parameter τ is changed by an additive rational constant

$$\tau' = \tau + w, \quad w = k/l, \quad k, l \text{ integers}, \quad (2.3)$$

we have

$$\theta \begin{bmatrix} \alpha \\ \beta \end{bmatrix} (u, \tau') = \sum_{\mu=0}^{l-1} C_{\mu} \theta \begin{bmatrix} \alpha \\ \beta' \end{bmatrix} (u, \tau), \quad \beta' = \beta - \frac{1}{2}k + \alpha k/l + \mu/l \quad (2.4)$$

where

$$C_{\mu} = \exp \left\{ -\pi i \left[\alpha^2 \frac{k}{l} + \alpha \left(\frac{2\mu}{l} - k \right) \right] \right\} \left(\frac{1}{l} \right) \sum_{\lambda=0}^{l-1} \exp \pi i \left[\frac{k}{l} \lambda^2 + \left(k - \frac{2\mu}{l} \right) \lambda \right]. \quad (2.5)$$

The Poisson sum formula applied to (2.1) gives (see Krazer 1903, ch III, Magnus *et al* 1966):

$$\theta \begin{bmatrix} \alpha \\ \beta \end{bmatrix} (u, \tau) = (-i\tau)^{-1/2} \sum_{n=-\infty}^{\infty} \exp \left(-\pi i \frac{(u+\beta+n)^2}{\tau} - 2\pi i \alpha n \right) \quad (2.6)$$

which can be written as another transformation formula:

$$\theta \begin{bmatrix} \alpha \\ \beta \end{bmatrix} (u, \tau) = (-i\tau)^{-1/2} \exp \left(-\frac{\pi i u^2}{\tau} + 2\pi i \alpha \beta \right) \theta \begin{bmatrix} -\beta \\ \alpha \end{bmatrix} \left(\frac{u}{\tau}, -\frac{1}{\tau} \right). \quad (2.7)$$

Applying (2.4) and (2.6) in succession we have the transformation formula

$$\theta \begin{bmatrix} \alpha \\ \beta \end{bmatrix} (u, \tau') = (-i\tau)^{-1/2} \sum_{\mu=0}^{l-1} C_{\mu} \sum_{n=-\infty}^{\infty} \exp\left(-\pi i \frac{(u + \beta' + n)^2}{\tau} - 2\pi i \alpha n\right),$$

$$\beta' = \beta - \frac{1}{2}k + \alpha k/l + \mu/l \tag{2.8}$$

with the C_{μ} given by (2.5) and τ' related to τ by (2.3).

Finally, we shall make use of the Jacobi infinite product representation of the four theta functions.

$$\theta_{0,3}(u, \tau) = Q_0(\tau) \prod_{n=1}^{\infty} [1 \mp q^{2n-1} \exp(2\pi i u)][1 \mp q^{2n-1} \exp(-2\pi i u)] \tag{2.9}$$

$$\theta_{1,2}(u, \tau) = \frac{\sin \pi u}{\cos \pi u} \left\{ 2Q_0(\tau)q^{1/4} \prod_{n=1}^{\infty} [1 \mp q^{2n} \exp(2\pi i u)][1 \mp q^{2n} \exp(-2\pi i u)] \right\} \tag{2.10}$$

where $q = \exp(i\pi\tau)$ and

$$Q_0(\tau) = \prod_{n=1}^{\infty} (1 - q^{2n}). \tag{2.11}$$

Going to the limit $u \rightarrow 0$ in the first of the pair of equations (2.10) we have also

$$\theta'_1(0, \tau) = 2\pi q^{1/4} [Q_0(\tau)]^3 \tag{2.12}$$

where the prime denotes a derivative with respect to the variable u .

3. Singularities of the hard-hexagon system

The hard-hexagon model is a two-dimensional model of particles on a triangular lattice with nearest-neighbour exclusion interactions. It was solved by Baxter in 1980 and seems to be the only example of a solved non-trivial repulsive system. Baxter gives the following parametric representation of the activity z and the partition function κ per lattice site.

$$z = -x[g(x)]^5, \quad \kappa = [g(x)]^2 g_1(x) h_0(x) h_1(x) \tag{3.1}, (3.2)$$

when $0 > x > -1$, and

$$z^{-1} = x[g(x)]^5, \quad \kappa = x^{-1/3} [g(x)]^{-3} g_1(x) k_1(x) \tag{3.3}, (3.4)$$

when $1 > x > 0$. The functions $g(x)$, $g_1(x)$, $h_0(x)$, $h_1(x)$, $k_1(x)$ are defined respectively by

$$g(x) = \prod_{n=1}^{\infty} \frac{(1 - x^{5n-4})(1 - x^{5n-1})}{(1 - x^{5n-3})(1 - x^{5n-2})} \tag{3.5}$$

$$g_1(x) = \prod_{n=1}^{\infty} \frac{(1 - x^{5n})^2}{(1 - x^{5n-3})(1 - x^{5n-2})} \tag{3.6}$$

$$h_0(x) = \prod_{n=1}^{\infty} \frac{(1 - x^{6n-3})^2}{(1 - x^{6n-1})(1 - x^{6n-5})} \tag{3.7}$$

$$h_1(x) = \prod_{n=1}^{\infty} \frac{(1-x^{6n-4})(1-x^{6n-2})}{(1-x^{6n})^2} \tag{3.8}$$

$$k_1(x) = \prod_{n=1}^{\infty} \frac{(1-x^{3n-2})(1-x^{3n-1})}{(1-x^{3n})^2}. \tag{3.9}$$

All five functions are regular functions of x for $|x| < 1$ and the circle $|x| = 1$ is their natural boundary. Hence, all points on this circle must correspond to singular points in the complex z plane, i.e., points for which $\kappa = \kappa(z)$ is singular. To find out the singular values of z and κ for limiting points on the unit circle, we make use of the remarkable analytic properties of theta functions which make them a most efficient tool for computations involving elliptic functions. We rewrite (3.5)–(3.9) as ratios of theta functions by utilising (2.9)–(2.12). Putting $x = \exp(i\pi\sigma)$, we have

$$g(x) = \theta_0(\frac{3}{4}\sigma, \frac{5}{2}\sigma) / \theta_0(\frac{1}{4}\sigma, \frac{5}{2}\sigma) \tag{3.5'}$$

$$g_1(x) = (1/2\pi)[\theta'_1(0, \frac{5}{2}\sigma) / \theta_0(\frac{1}{4}\sigma, \frac{5}{2}\sigma)] \exp(-\pi i \frac{5}{8}\sigma) \tag{3.6'}$$

$$h_0(x) = \theta_0(0, 3\sigma) / \theta_0(\sigma, 3\sigma) \tag{3.7'}$$

$$h_1(x) = 2\pi[\theta_0(\frac{1}{2}\sigma, 3\sigma) / \theta'_1(0, 3\sigma)] \exp \pi i \frac{3}{4}\sigma \tag{3.8'}$$

$$k_1(x) = 2\pi[\theta_0(\frac{1}{4}\sigma, \frac{3}{2}\sigma) / \theta'_1(0, \frac{3}{2}\sigma)] \exp \pi i \frac{3}{8}\sigma. \tag{3.9'}$$

Now, we can easily obtain the limiting values of these functions on the unit circle $x = \exp(i\pi\nu)$, ν real, if we restrict ourselves to rational ν . For in this case we can apply (2.8) to each of the theta functions in the foregoing formulae. In particular, to find the limiting values of $g(x)$ we put

$$\sigma = i\delta + \nu, \quad \nu = s/r, \quad s, r \text{ integers, } \delta > 0 \tag{3.10}$$

and substitute in (2.8)

$$\begin{aligned} \tau' = \frac{5}{2}\sigma = \tau + w, & \quad \tau = \frac{5}{2}i\delta, \\ w = \frac{5}{2}\nu = k/l, & \quad k = 5s, \quad l = 2r \end{aligned} \tag{3.11}$$

and

$$u = \frac{3}{4}\sigma \text{ for the numerator,} \quad u = \frac{1}{4}\sigma \text{ for the denominator} \tag{3.12}$$

of (3.5'). Thus $g(x)$ is obtained as a ratio of two series of exponentials, as given by (2.8), and in the limit $\delta \rightarrow 0$, i.e. $\tau \rightarrow 0$, we see immediately that only the terms whose exponents have the smallest negative real part contribute to the limit. Noting (2.2a) we obtain the limiting value

$$g(\exp i\pi\nu) = \frac{C_{\mu_1} \exp(-3i\theta) + C_{\mu_2} \exp(3i\theta)}{C'_{\mu'_1} \exp(-i\theta) + C'_{\mu'_2} \exp(i\theta)} \tag{3.13}$$

where

$$C_{\mu_1, \mu_2} = \frac{1}{2r} \sum_{\lambda=0}^{2r-1} \exp \left\{ \pi i \left[\frac{5s}{2r} \lambda^2 + \left(\frac{3s \mp \varepsilon}{2r} + 1 \right) \lambda \right] \right\}, \tag{3.14}$$

$$C'_{\mu'_1, \mu'_2} = \frac{1}{2r} \sum_{\lambda=0}^{2r-1} \exp \left\{ \pi i \left[\frac{5s}{2r} \lambda^2 + \left(\frac{s \mp \varepsilon}{2r} + 1 \right) \lambda \right] \right\} \tag{3.15}$$

and where

$$\begin{aligned} \theta &= \pi/20r, \quad \varepsilon = 1 && \text{when } s \text{ odd,} \\ \theta &= \pi/10r, \quad \varepsilon = 2 && \text{when } s \text{ even.} \end{aligned} \tag{3.16}$$

The sums in (3.14) and (3.15) are related to the Gaussian sums (Krazer 1903, Hasse 1950) which contain only pure quadratic terms in the exponents and whose values are numbers out of a quadratic field. The former sums are more complicated and have been evaluated explicitly only for small r . In particular for $\nu = 1$, i.e. $r = 1$, $s = 1$, $x = -1$, we have from (3.13) (Baxter 1980),

$$g(-1) = 2 \cos \frac{1}{3}\pi \tag{3.17}$$

and the corresponding activity

$$z(-1) \equiv z_c = 11.090\ 17 \dots \tag{3.18}$$

which is the critical activity of the transition point of the hard hexagons from a fluid to a solid phase. Furthermore, for $\nu = 0$, i.e. $r = 1$, $s = 0$, $x = 1$, we have (Baram 1982)

$$g(1) = [2 \cos \frac{1}{3}\pi]^{-1} = [g(-1)]^{-1} \tag{3.19}$$

and the corresponding activity

$$z(1) \equiv z_0 = -1/z_c = -0.090\ 169 \dots \tag{3.20}$$

which is the singular point of $\kappa(z)$ determining its radius of convergence. Incidentally we see from (3.19) that (3.1) and (3.3) are both valid for $x = 1$ and $x = -1$.

As mentioned above, it was not possible to obtain an explicit analytic expression for (3.13) for general ν , but numerical evaluation of (3.13) was carried out for one thousand reduced fractions $\nu = s/r$, $1 \leq r \leq 57$, $0 \leq s \leq r$, $x = \exp(i\pi\nu)$. The corresponding evaluation of z from (3.1) for these numbers invariably gave one of the four values z_0 , 0 , z_c , ∞ , and this in a totally discontinuous manner, the actual values depending only on the number-theoretic properties of r and s . We leave open the question of the limiting values of z for irrational ν which possibly might be non-existent, the values of z fluctuating between 0 and ∞ in the neighbourhood of the limit point. Thus from the above numerical evidence on the limiting values of z for rational ν we conclude that the points z_0 , 0 , z_c , all of them on the real axis, are the only singular points of $\kappa(z)$ in the finite complex z plane.

The corresponding limiting values of κ were obtained via an expression for $\kappa(x)$ similar to (3.13), with $x = \exp i\pi\nu$ and ν rational, and its numerical evaluation for the above specified set of ν 's. All the limiting values of $\kappa(x)$ thus obtained were distributed on a finite set of concentric circles centred at the origin of the complex κ plane. This limited range of values of κ implies that the singularities of $\kappa(z)$ cannot be essential singularities and hence must be branch points.

4. Singularities of the tempered hard squares

Fisher (1963) devised a two-dimensional model of particles on a square lattice with nearest-neighbour exclusion and with additional attractive interactions between particles on a certain subset of next-nearest-neighbour sites. The attractive interaction was chosen in such a way that, for a particular temperature, the partition function of the

model was reducible to that of the two-dimensional Ising model in zero field. The resulting formulae relate the pressure and density of the system to the activity z via a parameter K' given by

$$e^{4K'} = 1 + 4z. \tag{4.1}$$

The pressure and density are given by

$$\beta p(z) = K' + \int_0^{K'} \omega_1(K) dK \tag{4.2}$$

and

$$\rho(z) = \frac{1}{4}(1 - e^{-4K'})[1 + \omega_1(K')] \tag{4.3}$$

where $\omega_1(K)$ (the reduced energy) is given by

$$\omega_1(K) = \frac{1}{2} \coth 2K[1 + (2/\pi)k'_1 K_1(k_1)]. \tag{4.4}$$

Here, $K_1(k_1)$ is the complete elliptic integral of the first kind. Its modulus k_1 is related parametrically to z by

$$k_1 = 2(\tanh 2K'/\cosh 2K') \tag{4.5}$$

and the complementary modulus k'_1 is given by

$$k'_1 = (1 - k_1^2)^{1/2} = 2 \tanh^2 2K' - 1. \tag{4.6}$$

Explicitly it is related to z by

$$z = \frac{1}{2}[1 + k'_1 \pm \sqrt{2(1 + k'_1)^{1/2}}]/(1 - k'_1). \tag{4.7}$$

Writing $K_1 \equiv K_1(k_1)$, $K'_1 \equiv K_1(k'_1)$ and $\tau = iK'_1/K_1$ we have the relations (see e.g. Magnus *et al* 1966):

$$k_1 = [\theta_2(0, \tau)/\theta_3(0, \tau)]^2 \quad k'_1 = [\theta_0(0, \tau)/\theta_3(0, \tau)]^2. \tag{4.8a, b}$$

Substituting (4.8) into (4.7) and (4.4) we obtain a representation of the activity z and the density ρ as functions of the parameter τ . As in § 3, this provides a convenient representation for the purpose of finding the singularities of $\rho(z)$. Indeed both $z = z(\tau)$ and $\rho = \rho(\tau)$ have the real τ axis as their natural boundary and the limiting values of $z(\tau)$ on the real τ axis constitute the set of singular points of $\rho(z)$ in the complex z plane. By (4.7) these correspond to the limiting values of the moduli k_1 and k'_1 on the real τ axis. With the aid of (2.8) the latter values can be found from (4.8) for all the rational numbers on the real τ axis. We put

$$\tau' = \tau + \nu, \quad \tau = i\delta, \quad \nu = s/r, \quad s, r \text{ integers}, \tag{4.9}$$

and substitute into (2.8), with $u = 0$. Noting (2.2a) and (2.2d), we obtain respectively:

$$\begin{aligned} \theta_m(0, \tau') &= (-i\tau)^{1/2} \sum_{\mu=0}^{r-1} C_\mu \sum_{n=-\infty}^{\infty} \exp[-\pi i(\beta + n)^2/\tau] \\ \beta &= \begin{cases} \mu/r - s/2 + \frac{1}{2}, & m = 0, \\ \mu/r - s/2, & m = 3, \end{cases} \end{aligned} \tag{4.10}$$

where

$$C_\mu = \frac{1}{r} \sum_{\lambda=0}^{r-1} \exp \left\{ \pi i \left[\frac{s}{r} \lambda^2 + \left(s - \frac{2\mu}{r} \right) \lambda \right] \right\}. \tag{4.11}$$

Thus when $\delta \rightarrow 0 (\tau \rightarrow 0)$ the dominant terms in the sums of (4.10) are easily picked up and we find in this limit

$$k'_1 = \left(\frac{\theta_0(0, \tau + \nu)}{\theta_3(0, \tau + \nu)} \right)^2 = \begin{cases} \infty, & s \text{ odd,} \\ 0, & s \text{ even.} \end{cases} \tag{4.12}$$

By (4.7) the $k'_1 = \infty$ limit corresponds to $z = -\frac{1}{2}$ and the $k'_1 = 0$ limit corresponds to either of the values

$$z_0 \equiv \frac{1}{2}(1 - \sqrt{2}) = -0.2071 \dots \tag{4.13}$$

or

$$z_c \equiv \frac{1}{2}(1 + \sqrt{2}) = 1.2071 \dots \tag{4.14}$$

As in the case of the hard hexagons, z_c is the activity at a phase transition point and z_0 is the singularity of $\rho(z)$ nearest to the origin. However, we have here a third singularity at $z = -0.5 < z_0$. Note in this connection the findings of Suzuki and Fisher (1971) of a whole line of singularities on the negative real z axis for generalised Ising systems.

5. Singularities in the complex temperature plane for the two-dimensional Ising model

The results of the previous section can be applied at once to find the singularities of the (free) energy of the two-dimensional Ising model, viewed as a function of $y = e^{2K}$, where $K = \beta J$. Indeed the energy of the Ising model is given by (4.4) and together with (4.5) or (4.6) constitutes a parametric representation of the energy ω_1 as a function of y via the parameter $k'_1 (k_1)$ in the same way as these equations (with the additional relation (4.1)) constituted a parametric representation of the energy ω_1 as a function of z in the tempered hard-squares system.

Fisher (1965, see p 58) conjectured that the singularities of $\omega_1(y)$ are distributed on the two circles

$$y = \pm 1 + \sqrt{2} e^{i\phi} \tag{5.1}$$

in the complex y plane. Now, if we write in place of (4.6)

$$y^2 = \{3 + k_1 \pm 2[2(1 + k_1)]^{1/2}\} / (1 - k'_1) \tag{5.2}$$

we get in the limit (4.12), corresponding to the limiting values of $y = y(\tau)$ on the real τ axis, i.e., on the natural boundary of $y(\tau)$ and $\omega_1(\tau)$,

$$y = \pm i \text{ when } k'_1 = \infty, \quad y = \pm(1 \pm \sqrt{2}) \text{ when } k'_1 = 0. \tag{5.3}$$

Thus we have altogether six singular points in the complex y plane. Four of these are just the real points of the circles (5.1) and the two additional points are situated outside these circles at $y = \pm i$.

Abe and Katsura (1970) have checked Fisher's conjecture by numerical evaluation of the zeros of the partition function for finite systems (up to $N = 10 \times 10$ lattice points). Their results indicate a distribution of points close to the circles (5.1) increasing in density with increasing N . How can one reconcile these results with our findings of just a few isolated branch points for the infinite systems? One could claim that we have failed to find all the singularities by neglecting the irrational points on the natural

boundary of $y(\tau)$. We doubt this claim and believe that the irrational points give no determinate values of $y(\tau)$. But it remains an open question which presently we are unable to answer.

However, one should keep in mind that the trend of an increasingly dense distribution of points with increasing N does not ensure a continuous distribution in the $N \rightarrow \infty$ limit. This can be visualised by the following example of the truncated geometric series $f_N(z) = 1 + z + \dots + z^N$. It has a uniform distribution of N zeros on the unit circle, becoming increasingly dense with increasing N , yet in the $N \rightarrow \infty$ limit it gives $f(z) = (1 - z)^{-1}$ which has just one singularity at $z = 1$.

Acknowledgment

I am indebted to Dr A Baram for introducing me to his work on repulsive systems and for bringing to my attention the unique exact solution by Baxter of the hard hexagons as well as the exact solution of the tempered hard squares by M Fisher. I wish to thank also Professor L Ehrenpreis for useful remarks concerning properties of theta functions.

References

- Abe Y and Katsura S 1970 *Prog. Theor. Phys.* **43** 1402-4
 Baram A 1982 *J. Phys. A: Math. Gen.* **26** L19-25
 Baxter R J 1980 *J. Phys. A: Math. Gen.* **13** L61-70
 Fisher M E 1963 *J. Math. Phys.* **4** 278-86
 — 1965 *Boulder Lectures in Theoretical Physics* 1964 (Boulder) **7c** 1-159
 Gaunt D S 1967 *J. Chem. Phys.* **46** 3237-59
 Gaunt D S and Fisher M E 1965 *J. Chem. Phys.* **43** 2840-63
 Groeneveld J 1962 *Phys. Lett.* **3** 50-1
 Hasse H 1950 *Vorlesungen über Zahlentheorie* (Berlin: Springer-Verlag)
 Krazer A 1903 *Lehrbuch der Thetafunktionen* (Leipzig, reprinted 1970, New York: Chelsea)
 Lee T D and Yang C N 1952 *Phys. Rev.* **87** 410-9
 Magnus W, Oberhettinger F and Soni R P 1966 *Formulas and Theorems for the Special Functions of Mathematical Physics* (Berlin: Springer-Verlag)
 Penrose O and Elvey J S N 1968 *J. Phys. A: Math. Gen.* **1** 661-74
 Ruelle D 1971 *Phys. Rev. Lett.* **26** 303-4
 Runnels L K and Hubbard J B 1972 *J. Stat. Phys.* **6** 1-20
 Suzuki M and Fisher M E 1971 *J. Math. Phys.* **12** 235-46
 Yang C N and Lee T D 1952 *Phys. Rev.* **87** 404-9