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Zeros of the partition function for Ising models with many-body interactions

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Abstract. The location of the zeros of the partition function for Ising models having four-, six-, or eight-body interactions are studied. For quasi-one-dimensional models the zeros are found to lie on intersecting circles in the y plane where $y = \exp(2\beta h)$. These circles are part of a family of circles which includes the unit circle of Lee and Yang. Two, three, and four circles are needed for the four-body, six-body, and eight-body interaction systems, respectively. A counter example is found to show this behaviour does not hold for all such systems.

1. Introduction

Ever since 1952 when Lee and Yang (1952a, b) presented their theory of phase transitions based on the location of the zeros of the partition function, there has been continual interest in determining the location of the zeros for specific systems. Approaches to this problem have varied from proving theorems stating regions of the complex plane where no zeros exist (Dunlop 1977, 1979, Ruelle 1971) to looking at systems which are simple enough to be able to calculate the partition function explicitly and find the exact location of the zeros (Katsura and Ohminami 1972, Katsura *et al* 1972 and, for a general review, Kurtze 1979).

Examples of the latter approach have generally been based on calculations involving one-dimensional Ising-model systems having pair interactions. We continue in this basic approach but with some significant changes. First we consider only systems having many-body interactions (three-, four- or higher-body interactions) along with the single-body interaction between a spin and the external magnetic field. Second, the systems are not strictly one-dimensional but are what might be called quasi-one-dimensional, e.g., the ladder type lattice shown in figure 7. In most of the previous studies, apart from the cases where the Lee–Yang circle theorem is known to be true, it has been found that the location of the zeros is of rather complex form, e.g., see the figures in Katsura and Ohminami (1972). With the systems under consideration here, the location of the zeros is rather simple and this is one reason we feel the results are of interest.

We begin in the next section by considering a single unit or building block of the full quasi-one-dimensional systems considered in § 3. We see that the nature of the location of the zeros is not changed when we go from the single unit to the full system. In the fourth section we look at some small two-dimensional and three-dimensional systems to determine the location of their zeros and, more importantly, to see how much they retain the simple structure that the loci of the zeros have for the quasi-one-dimensional case.

2. Basic cell systems

We begin by looking at single units or basic cells of a lattice because of the simplicity of calculating the zeros for such systems. An equally important factor is that many examples in the past have shown that the general loci of the zeros does not depend on the size or dimensionality of the system, the classic illustration again being the Lee–Yang circle theorem. Therefore, these simple systems hopefully reflect the characteristics of larger systems.

Throughout the paper we will be dealing with spin-$\frac{1}{2}$ systems with S_i indicating the spin variable on the ith site and $S_i = \pm 1$. Each system has a Hamiltonian which is a function of the configuration of the system where {S} denotes a specific configuration. The partition function is

$$Z(\beta, J, h) = \sum_{\{S\}} \exp[-\beta H(\{S\})] \tag{2.1}$$

where $\beta = 1/kT$, k is the Boltzmann constant, and T the temperature.

The first system we consider is the four-spin system shown in figure 1(a). The Hamiltonian for the system is

$$H(\{S\}) = -JS_1\bar{S}_1S_2\bar{S}_2 - h(S_1 + \bar{S}_1 + S_2 + \bar{S}_2). \tag{2.2}$$

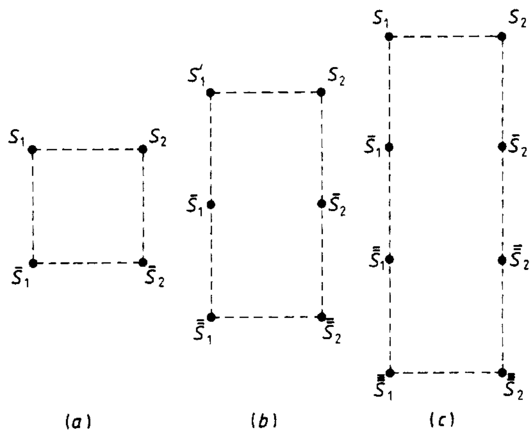

Figure 1. Basic cell systems of four, six, and eight spins in (a), (b) and (c), respectively.

The location of the zeros of the partition function for this system is shown in figure 2. Rather than plot the zeros in the complex h plane they have been plotted in the complex y plane where $y = \exp(2\beta h)$. The location of the zeros is shown for various non-negative values of J ranging from zero to infinity. The value of J is related to the value of x shown in the figure by $x = \exp(\beta J)$. The zeros lie on two circles which intersect each other at the points $y = \pm 1$ and whose centres are at $y = \pm i$.

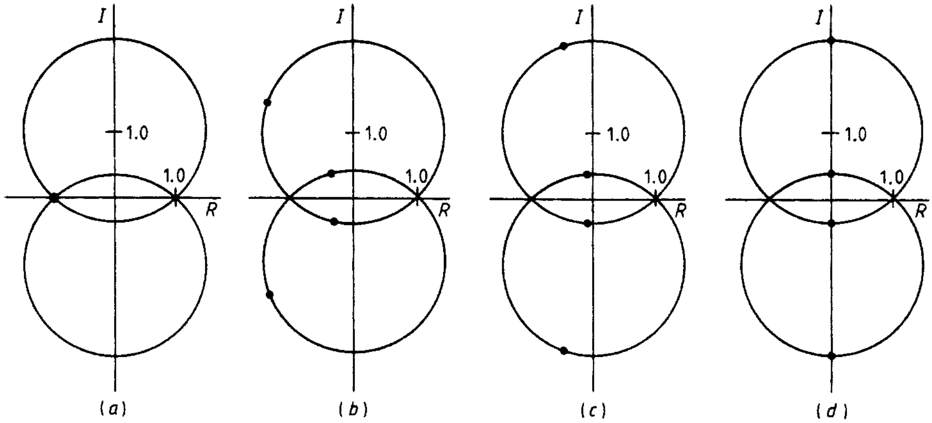

Figure 2. Zeros for the basic cell system of four spins with the zeros plotted in the $y = \exp(2\beta h)$ plane for cases of: (a) $x = 1.0$; (b) $x = 1.1$; (c) $x = 2.0$; and (d) $x = \infty$.

While the location of the zeros is simple in the y plane, if we define

$$w = (y - 1)/(y + 1) = \tanh(\beta h) \tag{2.3}$$

their location in the w plane is perhaps even simpler. The transformation (2.3) takes the two circles into two straight lines through the origin of the w plane, one at 45° and the other at 135°. In fact any circle passing through the points $y = \pm 1$ in the y plane becomes a straight line passing through the origin of the w plane (Ahlfors 1966). The zeros of the four-spin system plotted in the w plane are shown in figure 3. We will see that the entire family of circles are of importance. The location of the zeros for systems with pair interactions, i.e., the unit circle in the y plane, is a member of this family of circles.

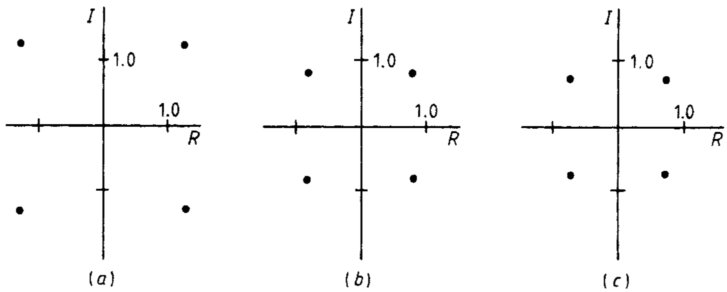

Figure 3. Zeros for the basic cell system of four spins with the zeros plotted in the w plane for cases where: (a) $x = 1.1$; (b) $x = 2.0$; and (c) $x = \infty$. The zeros for $x = 1.0$ are at infinity.

We next want to consider a system of six lattice sites, as shown in figure $1(b)$, with a Hamiltonian

$$H(\{S\}) = -JS_1\bar{S}_1\bar{\bar{S}}_1S_2\bar{S}_2\bar{\bar{S}}_2 - h(S_1 + \bar{S}_1 + \bar{\bar{S}}_1 + S_2 + \bar{S}_2 + \bar{\bar{S}}_2). \tag{2.4}$$

The partition function and its zeros can be easily calculated and the zeros are found to lie along three intersecting circles in the y plane. The location for various values of

J are shown in figure 4. In the w plane the zeros lie along three intersecting straight lines as shown in figure 5. The lines make angles of 30°, 90°, and 150° with the positive, real w axis.

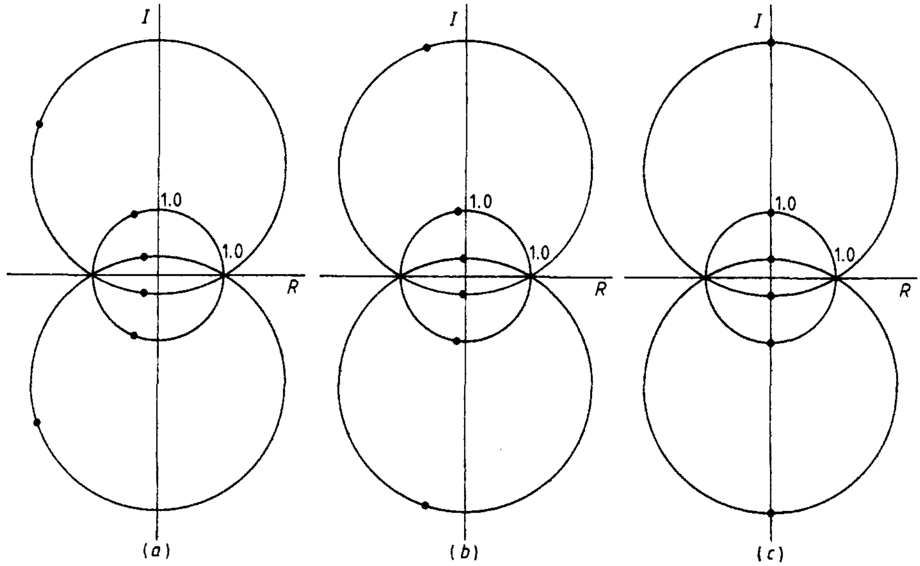

Figure 4. Zeros for the basic cell system of six spins with the zeros plotted in the $y = \exp(2\beta h)$ plane for cases of: (a) $x = 1.1$; (b) $x = 2.0$; and (c) $x = \infty$. The zeros for $x = 1.0$ are all at $y = -1.0$.

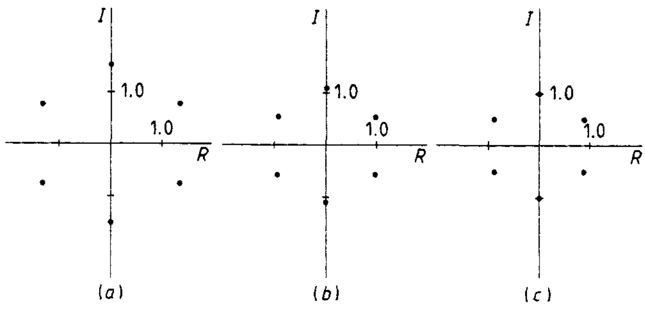

Figure 5. Zeros for the basic cell system of six spins with the zeros plotted in the w plane for cases where: (a) $x = 1.1$; (b) $x = 2.0$; and (c) $x = \infty$. The zeros for $x = 1.0$ are at infinity.

If we consider the next step in this progression of basic cell systems we consider an eight-spin system as shown in figure 1(c) whose Hamiltonian is

$$H(\{S\}) = -JS_1\bar{S}_1\bar{\bar{S}}_1\bar{\bar{\bar{S}}}_1S_2\bar{S}_2\bar{\bar{S}}_2\bar{\bar{\bar{S}}}_2 - h(S_1+\bar{S}_1+\bar{\bar{S}}_1+\bar{\bar{\bar{S}}}_1+S_2+\bar{S}_2+\bar{\bar{S}}_2+\bar{\bar{\bar{S}}}_2). \tag{2.5}$$

Here we see a continuation of the results from the two-, four- and six-spin systems. The zeros lie on four intersecting circles in the y plane or four straight lines through the origin in the w plane as shown in figure 6.

One sees from figures 3, 5 and 6 that in the w plane while the zeros lie on straight lines, they may also be characterised as being on circles whose centre is the origin of

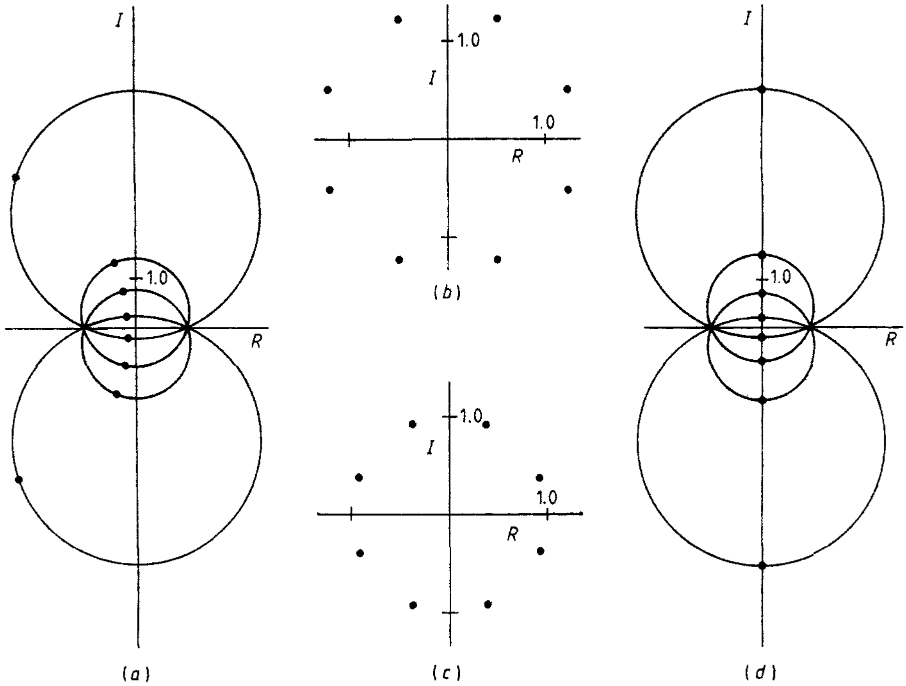

Figure 6. Zeros of the basic cell system of eight spins with the zeros plotted for $x = 2$ in the y plane in (a) and in the w plane in (b). For $x = \infty$ the zeros in the w plane are plotted in (c) and in the y plane in (d).

the w plane. As the interaction strength J is weakened, the radius of the circle on which the zeros are located increases. When J is infinite (x is infinite) the circle is of unit radius. When J becomes zero (x is equal to one) the circle has expanded to infinite radius. For the two extremes J being equal to zero and J being equal to infinity, all three systems have radii for the circle on which the zeros lie as infinity and unity, respectively. But at an intermediate value of J, e.g. the J corresponding to $x = 1.1$, the eight-spin system has a circle associated with its zeros which is the smallest of the three systems and the four-spin system has the largest radii associated with its zeros.

3. Quasi-one-dimensional systems

We now wish to investigate the location of the zeros of the partition for quasi-one-dimensional systems, using as the basic cells or building blocks the systems we have considered in the previous section. The first system we consider consists of $2N$ sites arranged to form the ladder-type lattice shown in figure 7(a). The Hamiltonian for the system is

$$H(\{S\}) = -J \sum_{i=1}^{N} S_i\bar{S}_i S_{i+1}\bar{S}_{i+1} - h \sum_{i=1}^{N} (S_i + \bar{S}_i) \tag{3.1}$$

where we impose periodic boundary conditions by having $S_{N+1} = S_1$. We can calculate the partition function of this model using the usual transfer matrix method (Huang

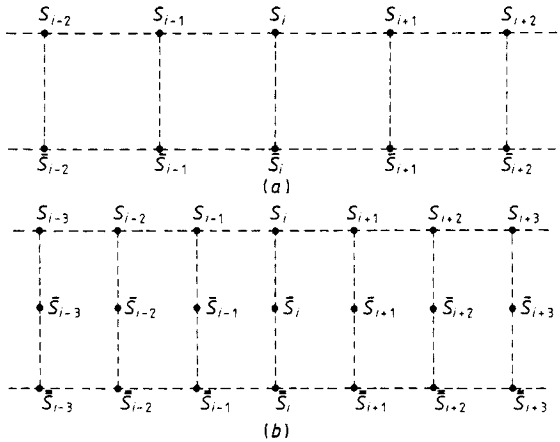

Figure 7. Quasi-one-dimensional systems of four-body interactions in (*a*) and with six-body interactions in (*b*).

1967, Thompson 1972). The transfer matrix is a four-by-four matrix with four eigenvalues. The eigenvalues of the matrix are easy to calculate due to the fact that two of them are zero. The two non-zero eigenvalues are

$$\lambda_\pm = 2x\cosh^2(\beta h) \pm 2[x^2\sinh^4(\beta h) + (1/x^2)\cosh(2\beta h)]^{1/2} \tag{3.2}$$

where again $x = \exp(\beta J)$. The partition function is then simply

$$Z = (\lambda_+)^N + (\lambda_-)^N. \tag{3.3}$$

Since we are after the zeros of the partition function, we rewrite it as

$$Z = \prod_{\gamma=1}^{N} (\lambda_+ - \exp(-\theta_\gamma)\lambda_-) = 0 \tag{3.4}$$

where $\theta_\gamma = (2\gamma - 1)\pi/N$.

With the explicit values of λ_+ and λ_- inserted in (3.4), one can find the zeros of the partition function. If the results of the previous section for the four-spin system carry over to the quasi-one-dimensional system, the zeros of the partition function plotted in the $w[\tanh(\beta h)]$ plane will lie along two straight lines: one at 45° and the other at 135° to the real axis. Even simpler is the fact that for the partition function equal to zero $[\tanh(\beta h)]^4$ takes on negative real values. One finds by explicit calculation using (3.2) and (3.4) that

$$[\tanh(\beta h)]^4 = \frac{-\tan^2(\theta_\gamma/2) - 1/x^4}{1 - 1/x^4}. \tag{3.5}$$

Equation (3.5) holds for arbitrary N and for $x \geqslant 1$, i.e., $J \geqslant 0$, and is a direct proof that the zeros for the full one-dimensional system have the same simple characterisation as the zeros of the four-spin system of section two. A plot of the zeros in the w plane for a system where $N = 10$ is given in figure 8. Two cases are illustrated: one where x is infinite and one where $x = 1.1$, and one sees that the zeros move in toward the origin and along the straight-line segments as x is increased. At $x = 1.0$, i.e. $J = 0$, all zeros are at infinity.

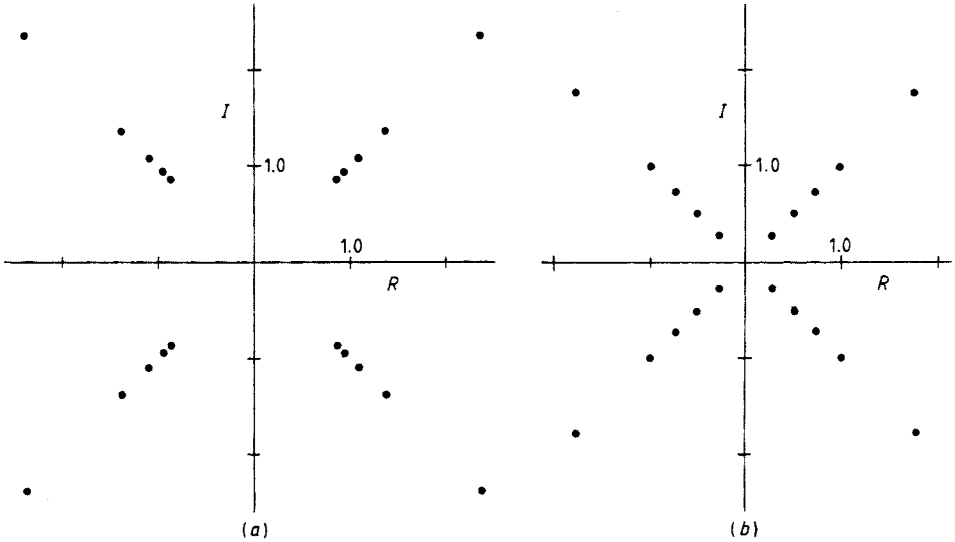

Figure 8. Zeros of the quasi-one-dimensional system with four-body interactions in the w plane with $N = 10$; in case (a) $x = 1.1$ and in case (b), $x = \infty$.

A similar calculation has been done for a lattice consisting of individual six-spin units combined to form the quasi-one-dimensional lattice shown in figure 7(b). The Hamiltonian for the system is

$$H(\{S\}) = -J \sum_{i=1}^{N} S_i \bar{S}_i \bar{\bar{S}}_i S_{i+1} \bar{S}_{i+1} \bar{\bar{S}}_{i+1} - h \sum_{i=1}^{N} (S_i + \bar{S}_i + \bar{\bar{S}}_i). \tag{3.6}$$

Again the transfer matrix method has been used to calculate the partition function. The transfer matrix is eight-by-eight and, therefore, has eight eigenvalues. Again all but two of the eigenvalues are zero. The two non-zero eigenvalues are

$$\lambda_{\pm} = 8x \cosh^3(\beta h) \pm \{64x^2 \cosh^6(\beta h) - 4(x^2 - 1/x^2)[6\cosh(4\beta h) + 10]\}^{1/2}. \tag{3.7}$$

The zeros in terms of $\tanh(\beta h)$ can be calculated in the same manner as with the previous system. However, due to the distribution of the zeros of the simple six-spin system investigated in the previous section, we can conjecture that it is simpler to look at $[\tanh(\beta h)]^6$ which should be negative when the partition is zero. The equation giving the zeros in terms of $[\tanh(\beta h)]^6$ is

$$[\tanh(\beta h)]^6 = \frac{-\tan^2(\theta_\gamma/2) - (1/x^4)}{1 - (1/x^4)}. \tag{3.8}$$

The right-hand side of (3.8) is identical to the right-hand side of (3.5). The zeros for any N then lie along the three line segments of figure 5. The zeros for $N = 10$ and x equal to infinity and 1.1 are plotted in figure 9.

The system consisting of eight-spin interactions which would be the next step in the series of quasi-one-dimensional systems would result in a sixteen-by-sixteen matrix. We have not constructed such a matrix, rather the simple connection between equation (3.5) pertaining to the four-spin interactions and (3.8) pertaining to the six-spin interactions leads to the obvious conjecture that for a system which is a natural extension of the type systems we have considered in this section, but having in general

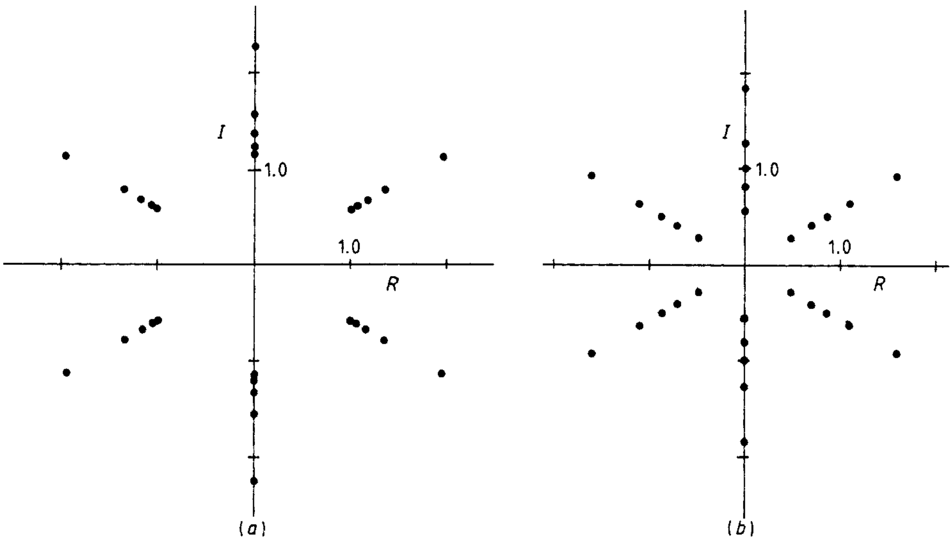

Figure 9. Zeros of the quasi-one-dimensional system with six-body interactions in the w plane with $N = 10$; in case (a) $x = 1.1$ and in case (b) $x = \infty$.

$2N$-spin interactions one has

$$[\tanh(\beta h)]^{2n} = \frac{-\tan^2(\theta_\gamma/2) - (1/x^4)}{1-(1/x^4)}. \tag{3.9}$$

For the case $n = 4$ and $N = 2$ the values of $\tanh(\beta h)$ given by (3.9) check with those calculated for the eight-spin system of § 2 after taking into consideration the periodic boundary conditions imposed in this section. For example, one must be careful not to take $x = 1.1$ in (3.9) if one wants to compare the results to the $x = 1.1$ case for the eight-spin system of § 2. Because of the periodic boundary conditions one should take $x = (1.1)^{1/2}$ in equation (3.9).

4. Higher-dimensional systems

We conclude by finding the zeros of the partition function for a two-dimensional and three-dimensional system. We look at only the simplest examples of each such system having four-body interactions.

The two-dimensional system consists of nine spins each located on a vertex of a three-by-three square lattice. Therefore, the system is merely a two-by-two array of the basic building block of figure 1(a), each building block has a four-body interaction associated with it as in the previous sections. The partition function can be calculated directly and is

$$\begin{aligned} x^4(y^9+1) &+ (4x^2+4+x^{-4})(y^8+y) + (8x^2+14+12x^{-2}+2x^{-4})(y^7+y^2) \\ &+ (6x^4+16x^2+30+28x^{-2}+4x^{-4})(y^6+y^3) \\ &+ (9x^4+36x^2+48+24x^{-2}+9x^{-4})(y^5+y^4) \end{aligned} \tag{4.1}$$

where as before $y = \exp(2\beta h)$ and $x = \exp(\beta J)$. The zeros of the partition function are plotted in figure 10 for various values of x. In this figure the two intersecting circles along which the zeros of the four-body interaction systems of §§2 and 3 are shown. The zeros for this case do not lie along these two intersecting circles. This example thus illustrates that, unlike the pair interaction systems of Lee and Yang where one can have any set of pair-interactions, one cannot have any set of four-body interactions and still have the zeros lying on the two intersecting circles of the previous sections.

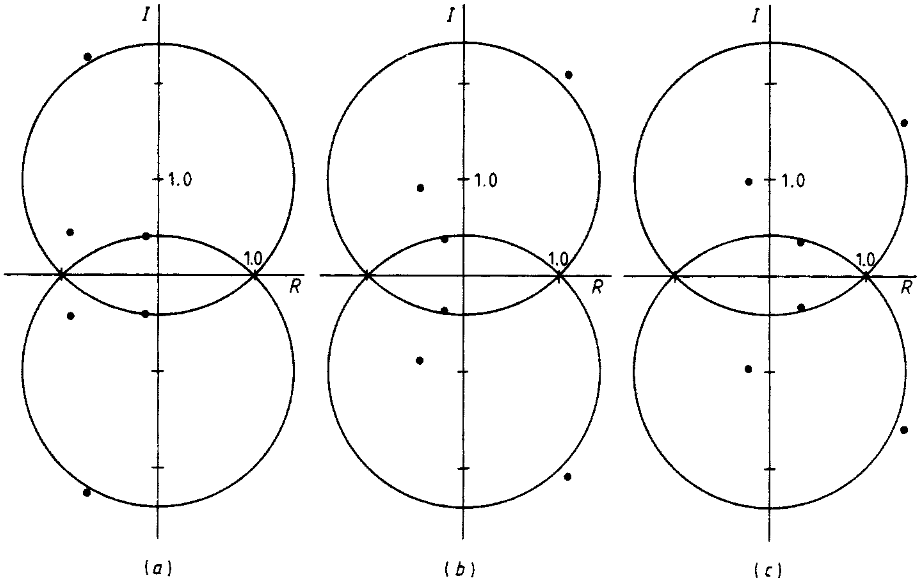

Figure 10. Zeros of the two-dimensional 3×3 square lattice with four-body interactions plotted in the y plane for cases of: (a) $x=1.1$; (b) $x=2.0$; and (c) $x=\infty$.

For the three-dimensional system we consider a system of eight spins located on the corners of a cube. The four spins on the corners of each face interact with one another. Hence we have six, four-body interactions. The partition function for this system is

$$x^6(y^8+1)+8(y^7+y)+(12x^2+12x^{-2}+4x^{-6})(y^6+y^2) \\ +56(y^5+y^3)+(14x^6+24x^2+24x^{-2}+8x^{-6})y^4 \tag{4.2}$$

where again $x=\exp(\beta J)$ and $y=\exp(2\beta h)$. The zeros of (4.2) are plotted in figure 11. In this case the zeros are again on the same two intersecting circles found for the four-body interactions of §§ 2 and 3.

From the two systems studied in this section we have shown that one does not have the possibility of a general theorem restricting the zeros to the two intersecting circles of the previous sections for all four-body interaction systems. The two systems, however, do not rule out the possibility of still having some restricted theorem, especially since the cubic system does have its zeros on these intersecting circles. We plan to discuss this problem in a future publication looking at a set of systems which hopefully will indicate a general property which, if satisfied, would require the zeros to lie on the two intersecting circles.

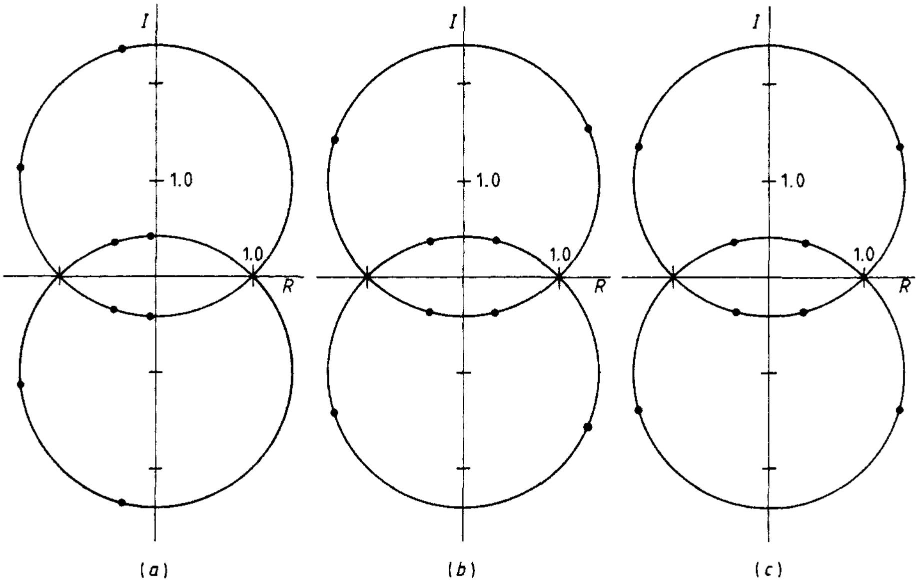

Figure 11. Zeros of the three-dimensional cube with four-body interactions plotted in the y plane for cases of: (a) $x=1.1$; (b) $x=2.0$; and (c) $x=\infty$.

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