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Distribution of zeros of the partition function for the one dimensional Ising models

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Abstract. The loci of zeros of the partition functions of the following one dimensional Ising models are obtained. (i) Those of $S = \frac{1}{2}$ and with the nearest (J) and the next nearest (J') neighbour interactions. The loci of zeros are classified in several patterns according to a combination of J and J'. In particular when $J < 0$ and $J' > 0$, the existence of two nearly concentric circular arcs whose heads approach points on the positive real axis of z corresponding to the critical field at zero temperature is confirmed. This suggests that the locus of the two and three dimensional Ising antiferromagnet ($J < 0$, $J' > 0$) will be closed two concentric circles below the Néel temperature. (ii) Those of $S = 1$ and of $S = \frac{3}{2}$ with the nearest neighbour (J) interaction. The locus shrinks to $2S$ points ($\theta = 2\pi j/(2S+1)$, $j = 1, 2, \ldots, 2S$) on the unit circle at $T = \infty$. It extends along the unit circle for $J > 0$ and along a nearly radial direction for $J < 0$ when the temperature decreases.

1. Introduction

When we discuss phase transitions, one useful method is to investigate the distribution of zeros of the partition function. If we can find the locus and the distribution function on it, physical quantities are determined. We denote the locus of zeros in the complex fugacity plane by C. The locus and the distribution on it are expressed by $z(s)$ and $g(s)$ in the parametric representation. Then the thermodynamic potential $\chi(z)$ and its derivative are given by

$$\chi(z) \equiv \lim \frac{1}{N} Z_N(z) = \int_{\mathrm{C}} \mathrm{d}s\, g(s) \ln\left(1 - \frac{z}{s}\right) \tag{1}$$

$$\chi'(z) = \int_{\mathrm{C}} \mathrm{d}s \frac{g(s)}{z-s} \tag{2}$$

where $Z_N(s)$ is the partition function of an N particle system. Phase transitions occur when C cuts the positive real axis of z (at z_{c}) and $\int_{\Delta} \mathrm{d}s g(s)$ is finite, where Δ is a part of C in the neighbourhood of z_{c} (Yang and Lee 1952). The phase transition is of first or higher order, when $g(0)$ is finite or zero, respectively. The critical behaviour of the system is determined by the nature of $g(s)$ near z_{c} (Abe 1967, Suzuki 1967).

Lee and Yang (1952) proved that the zeros of the partition function of the Ising model of $S = \frac{1}{2}$ made of any connected graph, each bond of which may have a different interaction strength, lie on the unit circle in the complex fugacity plane, provided that all interactions are ferromagnetic (circle theorem).

The review of the investigations of the distribution of zeros is given in the introduction of Katsura *et al* (1971, to be referred to as KAY). Recently Asano (1970a, 1970b) proved the circle theorem for the Heisenberg model with ferromagnetic interaction. Suzuki and Fisher (1971) discussed generalizations of the circle theorem for the Ising model with many-spin interactions and for the Heisenberg model with a general anisotropic case.

In the case of antiferromagnetic interaction, however, the situation which corresponds to the circle theorem is not yet clear. Zeros of the one dimensional Ising model for $J < 0$ lie on the negative real axis (Yang 1952)†. There are some systems which are shown to have only negative real zeros. The Husimi–Temperley model (complete cluster) with the antiferromagnetic interaction is one of the examples (Heilmann 1971, preprint).

Our purpose is to clarify the nature of the antiferromagnetic phase transitions from the viewpoint of the distribution of zeros. Suzuki *et al* (1970) found that some complex zeros appear besides most of the negative real zeros for the finite (4×4 and 4×6) Ising models with the nearest neighbour interaction. KAY investigated the finite (4×4 and 4×6) Ising models of $S=\frac{1}{2}$ with the nearest (J) and the next nearest (J') neighbour interactions‡, and found some typical patterns corresponding to combinations of signs and values of J and J'. In particular, they found that when $J<0$, $J'>0$, the zeros are nearly on two concentric circles which cut the positive real axis of z at z_c ($=\exp(\pm g\mu H_c/kT)$) corresponding to the critical magnetic field.

The locus in that paper, however, was the one estimated by a set of finite points, and in a few cases a unique connection of the points was not clear. In the present paper the loci of zeros of the one dimensional Ising model of $S=\frac{1}{2}$ with the nearest and the next nearest neighbour interactions, and those of higher spins ($S=1$ and $\frac{3}{2}$) with the nearest neighbour interaction are obtained. Though these systems do not show phase transitions, the continuous loci§ of the models can be obtained from the eigenvalues of the transfer matrices by the method of Nilsen and Hemmer (1967). The pattern thus obtained resembles the results of numerical experiments of the 4×6 system (KAY) above the critical temperature and makes a prediction below it possible.

2. One dimensional Ising model with the nearest and next nearest neighbour interactions (spin 1/2)

We consider the one dimensional Ising model with the nearest and the next nearest neighbour interactions. The Hamiltonian of this system is written as

$$\mathscr{H} = -2J\sum_i S_iS_{i+1} - 2J'\sum_i S_iS_{i+2} - g\mu H\sum_i S_i \tag{3}$$

where J is the exchange energy of the nearest neighbour interaction, and J' that of the next nearest neighbour interaction. For the case where the magnetic field is zero, Montroll (1942) obtained the partition function and Stephenson (1970) discussed the correlation function of this system, where the transfer matrices can be reduced to the second order.

Oguchi (1965) obtained the eigenvalue equation of the transfer matrix in the presence of a magnetic field and showed that four kinds of ground states exist at zero temperature.

† The distribution function of zeros of the one dimensional Ising antiferromagnet can be shown to be $g(s) = (\frac{1}{2}\pi)\cosh(s/2)\{x^2-\cosh^2(s/2)\}^{-1/2}$ for $x > \cosh(s/2)$ and equals zero otherwise, where $z = -e^{-s}$, $x \equiv e^{-2K}$ ($K < 0$).

‡ Similar calculations were carried out by Karaki (1971).

§ Noncircular loci for continuous systems (van der Waals gas etc) were given by Hauge and Hemmer (1963), Hemmer and Hauge (1964) and Niemeijer and Weijland (1970).

The partition function Z in the presence of the magnetic field is written, by the use of a transfer matrix

$$Z = \mathrm{Tr}\, V^N$$

$$V = \begin{pmatrix} e^{K+K'+C} & e^{-K-K'-C} & 0 & 0 \\ 0 & 0 & e^{-K+K'+C} & e^{K-K'-C} \\ e^{K-K'+C} & e^{-K+K'-C} & 0 & 0 \\ 0 & 0 & e^{-K-K'+C} & e^{K+K'-C} \end{pmatrix} \quad (4)$$

where $K = J/2kT$, $K' = J'/2kT$, $C = g\mu H/2kT$. We define the fugacity $z \equiv e^{-2C}$. The secular equation of this matrix is

$$F(\lambda) \equiv \lambda^4 - e^{K+K'}(e^C + e^{-C})\lambda^3 + e^{2K'}(e^{2K} - e^{-2K})\lambda^2$$
$$+ e^{-K+K'}(e^{2K'} - e^{-2K'})(e^C + e^{-C})\lambda - (e^{2K'} - e^{-2K'})^2 = 0. \quad (5)$$

Physical quantities are given by the maximum eigenvalue of this equation. When the phase transition exists, the branch which gives the largest eigenvalue should exchange somewhere in the magnetic field. It is known that in one dimensional systems phase transitions do not exist. However, when we consider the magnetic field as a complex variable, the branch which gives the largest absolute value exchanges somewhere in the complex magnetic field. The locus where the exchange occurs is the place where zeros of the partition function exist.

In the special case when $K' \gg 0$, the term $e^{-K'}$ can be neglected and equation (5) is factorized, the four eigenvalues being given by

$$\lambda_1 = \exp(K + K' + C)$$
$$\lambda_2 = \exp(K + K' - C)$$
$$\lambda_3 = \exp(-K + K')$$
$$\lambda_4 = \exp(-K + K'). \quad (6)$$

When $K > 0$, the eigenvalue which gives the largest absolute value is λ_1 for $|z| < 1$ and λ_2 for $|z| > 1$. When $K < 0$, it is λ_1 for $|z| < e^{+4K}$, λ_3 for $e^{+4K} < |z| < e^{-4K}$, and λ_2 for $e^{-4K} < |z|$, respectively. The branch exchanges at the point where $|z| = 1$ for $K > 0$ and $|z| = e^{\pm 4K}$ for $K < 0$†. This means that in the Ising model with nearest and next nearest neighbour interactions, zeros distribute on the unit circle when $J > 0$, $J' > 0$ and on the two concentric circles when $J < 0, J' > 0$. The approximate reason for this has already been given in KAY. In this paper we have explained it from the viewpoint of the eigenvalues of the transfer matrix. Of course, equation (6) holds only at low temperature. At finite temperature, we need to solve equation (5) explicitly.

We can obtain the equation of the locus, where the two absolute values of the eigenvalues λ_k and λ_l become equal, by eliminating ψ from $F(\lambda) = 0$ and $F(\lambda \exp(i\psi)) = 0$, where we put $\lambda_k = \lambda_l \exp(i\psi)$. The equation thus obtained is a fourth order algebraic equation. We did not employ this method but adopted the direct numerical method, since the coefficients are complicated and further selection of the loci where the largest (absolute value) and the second largest eigenvalues coincide is required.

† Saitō and Oonuki (1970) pointed out that a phase transition occurs in the one dimensional antiferromagnet when an infinitely strong ferromagnetic next neighbour interaction is introduced.

Figures 1 and 2 show the loci of zeros thus obtained. In the region where $J > 0$, $J' > 0$, the locus is a circular arc (a part of a unit circle) as proved by the Lee–Yang theorem. As the temperature decreases, the opening of the circle becomes narrower and the heads of the locus approach the point $z = 1$. This means that the one dimensional Ising model tends to have a phase transition at $H = 0$ as $T \to 0$.

In the region $J > 0$, $J' < 0$, the locus consists of a circular arc and four branches coming out at the end of the arc. When J increases, part of a unit circle extends, and the heads of branches reach into the right half plane, and when J increases further, the branches vanish. On the other hand when $|J'|$ increases, part of the arc shrinks and the branches become close to the real axis.

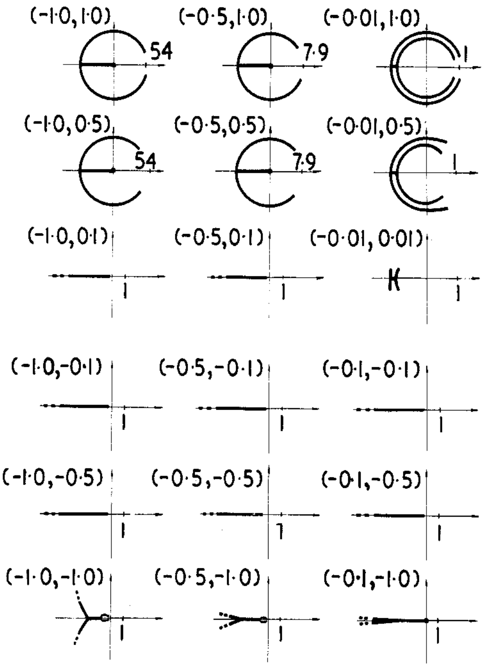

Figure 1. The locus of zeros of the one dimensional Ising model for $S = \frac{1}{2}$, $J < 0$, $J' \gtrless 0$. The first and the second numbers denote J/kT and J'/kT, respectively. The scales are different from subfigure to subfigure, and are denoted by numbers on the positive real axis. The inner circles are denoted by points at the centres in the upper left four subfigures.

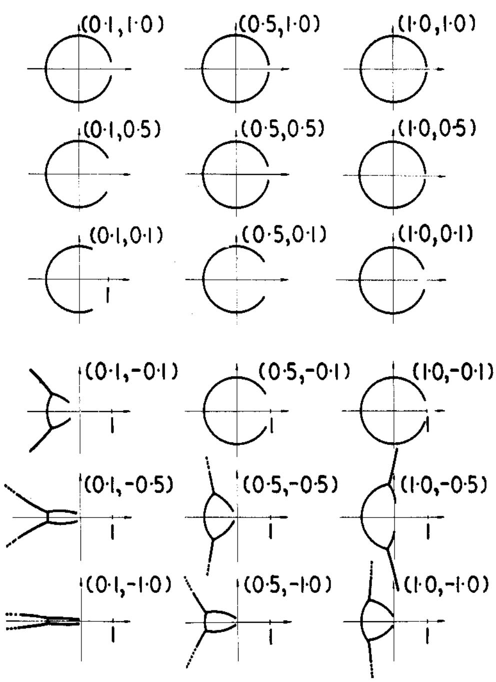

Figure 2. The locus of zeros of the one dimensional Ising model for $S = \frac{1}{2}$, $J > 0$, $J' \gtrless 0$. The first and the second number in parentheses denote J/kT and J'/kT, respectively. The scales are the same for all subfigures. The dotted section means that the locus extends outside the written region.

In the region $J < 0$ and $J' > 0$, where these interactions make the occurrence of the antiferromagnetic state easy, the locus consists of two nearly concentric circles and a segment of a line connecting them. The radii of the circles are given by $|z| = \exp(\pm g\mu H_c/kT)$, where H_c is a critical field, and $H_c = \pm 2J$ at $T = 0$.

In the region $J < 0$ and $J' < 0$, the locus consists of a segment of the negative real axis and four branches coming out from the ends of the segment. When $|J'|$ decreases, the branches do not appear, and when $|J'|$ increases, the branches become dominant.

3. Discussions to the results in § 2

The ground states of the one dimensional Ising model with the nearest and the next nearest neighbour interactions are classified into four types according to the combination of J, J' and H. They are: ferromagnetic state (F, $++++++++$), antiferromagnetic state (AF, $+-+-+-+-$), superantiferromagnetic state (s1, $++--++--$), and the state where spins arrange in the form $++-++-++-$ (Oguchi 1965). We call the last state the s2 state. The energies of them are given by

$$-\frac{E_{\mathrm{F}}}{N} = J+J'+H \tag{7}$$

$$-\frac{E_{\mathrm{AF}}}{N} = -J+J' \tag{8}$$

$$-\frac{E_{\mathrm{S1}}}{N} = -J' \tag{9}$$

$$-\frac{E_{\mathrm{S2}}}{N} = -\frac{J}{3}-\frac{J'}{3}+\frac{H}{3}. \tag{10}$$

The ground state is given by F for $J > 0$, and $J+2J' > 0$ (irrespective of H). For $J < 0$, $J' > 0$, it changes from AF to F at the critical field $H_{c1} = -2J$. For $J > 0$, $J' < 0$ and $J+2J' < 0$, it changes from s1 to F at the critical field $H_{c2} = -J-2J'$. For $J < 0$, $J' < 0$, $-J+2J' > 0$, it changes from AF to s2 and from s2 to F at $H_{c3} = -2J+4J'$, and $H_{c4} = -2J-2J'$, respectively. For $J < 0, J' < 0$, $-J+2J' < 0$, it changes from s1 to s2 and s2 to F at the critical field $H_{c5} = J-2J'$, and $H_{c4} = -2J-2J'$, respectively. The situation is shown in figure 3.

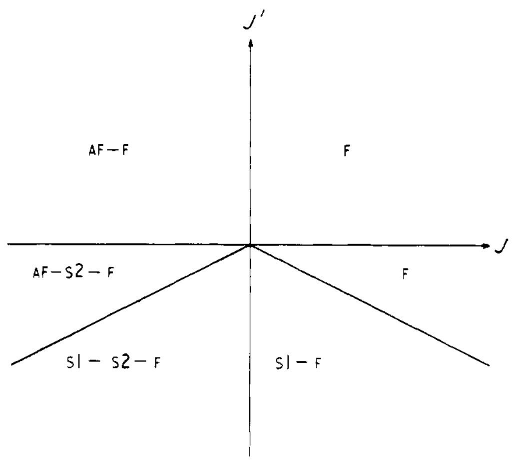

Figure 3. The transition pattern of the one dimensional Ising model with the nearest (J) and the next nearest (J') neighbour interactions. The state written left-most in each region is the ground state at the zero magnetic field and the states written right show the ground state when the magnetic field increases. F, $+++++++++$ ferromagnetic state; AF, $+-+-+-+-+$ antiferromagnetic state; s1, $++--++--+$ superantiferromagnetic state; s2, $++-++-++-$ s2 state.

When these states are sufficiently stable, the existence of the critical fields should be reflected in the locus of the zeros, and hence the two or four heads of branches of the locus should approach points in the positive real axis of z, though these transitions exist only at $T = 0$. Such a situation, however, could not be found in our results. This seems to be similar to the result that zeros distribute on the negative real axis in the case $J < 0$, $J' = 0$, where the critical fields $H_{c1} = \pm 2J$ exist at $T = 0$. In that case two concentric circles corresponding to the critical fields appear by the introduction of the next nearest neighbour ferromagnetic interaction which makes the occurrence of the antiferromagnetic state easy. Hence we expect that the locus of zeros will show the existence of the s1 and s2 states, when the fourth neighbour and third neighbour ferromagnetic interactions, respectively, are introduced.

4. One dimensional Ising model with higher spin

Asano (1968), Suzuki (1968), and Griffiths (1969) proved that the zeros of the partition function of the Ising model of higher spin distribute on the unit circle when the interaction is ferromagnetic. Kawabata and Suzuki (1969) investigated the finite spin systems (4×4, $S = 1$) with antiferromagnetic interaction.

In the present section we consider the distribution of the zeros of the partition function in the one dimensional case. The thermodynamic quantities of the one dimensional Ising models of higher spins are given by Katsura and Tsujiyama (1966) and by Suzuki *et al* (1967) using the transfer matrix method and by Obokata and Oguchi (1968) using the Bethe 'approximation'. We consider the system given by equation (3) where $J' = 0$. In the case of spin 1, the transfer matrix is

$$V = \begin{pmatrix} e^{4K+C} & e^{C/2} & e^{-4K} \\ e^{C/2} & 1 & e^{-C/2} \\ e^{-4K} & e^{-C/2} & e^{4K-C} \end{pmatrix} \tag{11}$$

and the secular equation of this matrix is given by

$$\lambda^3 - \{e^{4K}(e^C + e^{-C}) + 1\}\lambda^2 + \{(e^{4K} - 1)(e^C + e^{-C}) + (e^{8K} - e^{-8K})\}\lambda - e^{-8K}(e^{4K} - 1)^3(e^{4K} + 1) = 0. \tag{12}$$

The locus of the zeros has been obtained by the same method as in § 2.

At infinitely high temperature, the partition function is written as

$$Z = (e^C + 1 + e^{-C})^N. \tag{13}$$

Hence, in the case of spin 1, all zeros accumulate at $\theta = 2\pi/3$, and $4\pi/3$ on the unit circle. When the temperature decreases, the locus extends from these two points along the unit circle when the interaction is ferromagnetic, and it becomes nearly perpendicular to the unit circle when the interaction is antiferromagnetic (figure 4).

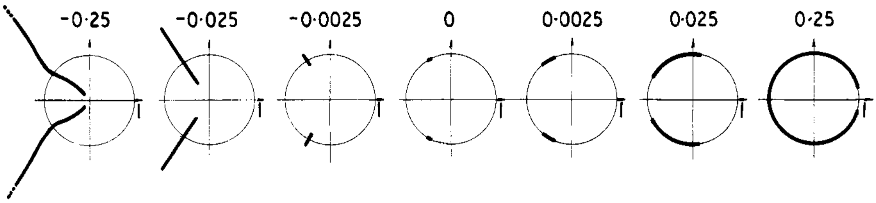

Figure 4. The locus of the one dimensional Ising model for $S = 1$. The number denotes J/kT. The interactions are ferromagnetic in the right three and are antiferromagnetic in the left three.

Similarly in the case of spin 3/2, the transfer matrix is given by

$$V = \begin{pmatrix} e^{9K+3L} & e^{3K+2L} & e^{-3K+L} & e^{-9K} \\ e^{3K+2L} & e^{K+L} & e^{-K} & e^{-3K-L} \\ e^{-3K+L} & e^{-K} & e^{K-L} & e^{3K-2L} \\ e^{-9K} & e^{-3K-L} & e^{3K-2L} & e^{9K-3L} \end{pmatrix} \tag{14}$$

where $L = g\mu H/2kT = C/2$, and the locus of the zeros of the partition function is shown in figure 5. When the temperature becomes infinitely high, zeros converge to $\theta = \pi/2$, π, $3\pi/2$ on the unit circle.

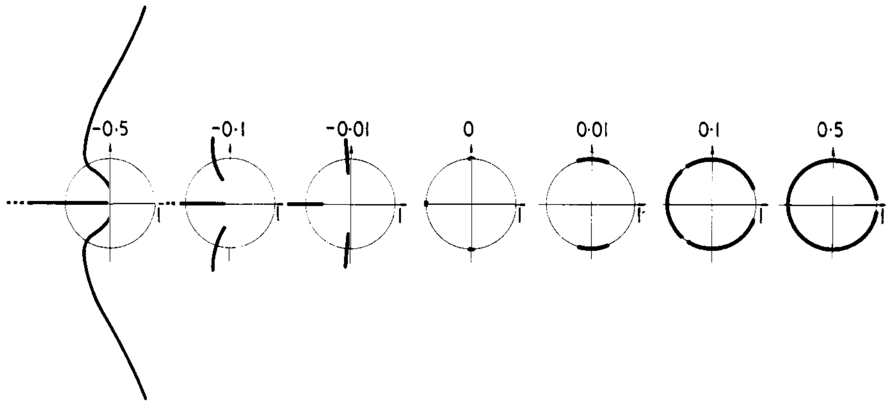

Figure 5. The locus of the one dimensional Ising model for $S = \frac{3}{2}$. The number denotes J/kT. The interactions are ferromagnetic in the right three and are antiferromagnetic in the left three.

In general, when the magnitude of spin is S, zeros at infinitely high temperature degenerate at $z^{2S+1} = 1$ excluding $z = 1$, and the locus extends along the unit circle in the case of ferromagnetic interaction; it extends nearly perpendicularly to the unit circle in the case of the antiferromagnetic interaction, when the temperature decreases.

5. Conclusions

We have obtained the loci of the zeros of the partition function for the one dimensional Ising model with the nearest (J) and the next nearest (J') neighbour interactions (spin 1/2), and those of the zeros of the partition function for the one dimensional Ising model of higher spin with the nearest neighbour interaction.

In the former, the locus of zeros is composed of a circular arc (part of a unit circle) when $J > 0$ and $J' > 0$, two nearly concentric circles and a segment of the negative real axis which connects them when $J < 0$ and $J' > 0$, part of a unit circle and branches which come out from the ends of the arc when $J > 0$ and $J' < 0$, and a segment of the negative real axis and the branches which come out from both ends of it when $J < 0$ and $J' < 0$. Such patterns describe well the distribution of zeros of the numerical experiments by KAY for the finite Ising system (4×6) above the transition point T_c.

The radii of the concentric circles are given approximately by $z_c = e^{\pm 4K}$, which correspond to the critical fields when the temperature is zero. Though the heads of the locus do not approach the points on the real axis in the case of only the nearest neighbour antiferromagnetic interaction, the introduction of the next nearest neighbour ferromagnetic interaction makes the occurrence of the antiferromagnetic state easy, and the distribution of zeros reflects these situations.

The existence of the superantiferromagnetic state and the s2 state were not found to be reflected in the distribution of zeros. They may be found by introducing the fourth and the third neighbour ferromagnetic interactions, respectively.

From the results of KAY and of the present paper, it is expected that below the Néel temperature the locus of the two and three dimensional Ising antiferromagnet will be the two closed, approximately concentric, circles which cut the positive real axis at $z_c = \exp(\pm g\mu H_c/kT)$, where H_c is the critical field at that temperature.

In the higher spin systems, the zeros degenerate at the $2S$ points of the unit circle where $\theta = 2\pi j/(2S+1)$ $(j = 1, 2, 3, \ldots, 2S)$ at $T \to \infty$. When the temperature decreases, the locus extends along the unit circle in the case where the interaction is ferromagnetic, and it extends nearly along the radial direction in the case where the interaction is antiferromagnetic.

Acknowledgments

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Note added in proof. In the third subfigure from the right in figure 5, an arc in the left part is missing.

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