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1990 J. Phys. A: Math. Gen. 23 L689

(http://iopscience.iop.org/0305-4470/23/13/010)

J. Phys. A: Math. Gen. 23 (1990) L689-L695. Printed in the UK

LETTER TO THE EDITOR

Absence of phase transitions in self-dual Ising models with multisite interactions and a field

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Received 30 March 1990

Abstract. We investigate Ising spin systems having a single translationally invariant multispin interaction and an external magnetic field. These models are self-dual and for certain intervals of the self-dual line Heringa, Blöte and Hoogland have very recently obtained by Monte Carlo simulations evidence for a first-order phase transition. We find intervals of the self-dual line where one can rigorously prove the absence of a phase transition (these areas do not contradict the Monte Carlo results). We do this by looking at the zeros of the partition function.

In a very recent article Heringa *et al* [1] investigated a number of two- and three-dimensional Ising models with multispin interactions and a field. Using Monte Carlo simulations they established the presence of a first-order phase transition in these models when the field is non-zero. In particular they considered square and cubic lattice systems where on each lattice site there was a spin taking on values ± 1. The spins interacted through multisite couplings and a field, described by the reduced Hamiltonian

$$\frac{\mathcal{H}}{kT} = -K \sum_{\boldsymbol{r}} \prod_{i=0}^{n-1} S_{\boldsymbol{r}+\boldsymbol{a}_i} - H \sum_{\boldsymbol{r}} S_{\boldsymbol{r}} \tag{1}$$

where $\boldsymbol{r}$ and $\boldsymbol{r}+\boldsymbol{a}_i$ denote the position of the spin sites and the n vectors $\boldsymbol{a}_i$ specify the multisite interactions. The models have been shown to be self-dual [2] and the self-dual line is given by

$$\sinh(2K)\sinh(2H) = 1. \tag{2}$$

It is along a portion of this self-dual line that the presence of a first-order phase transition was found.

Heringa *et al* point out that the present author [3] has shown that for sufficiently small K there is no phase transition. These results were part of some work considering the location of the zeros of the partition function for a variety of Ising systems some of which had multisite interactions. Due to the interesting results of [1] we reconsider the problem of the zeros of the partition function for these systems. While in the previous paper for multisite interaction systems we looked only for values of K where for all H there was no phase transition, we now look at the entire positive H-K plane. One outcome of this is that, besides proving that there are sufficiently small K for which no phase transition exists for all H, we prove that there are sufficiently large H for which no phase transition exists for all K. Also we expand the region of the self-dual line where no phase transition occurs. Our results are in agreement with those of [1]

0305-4470/90/130689+07$03.50

in that the region where phase transitions are found by Monte Carlo methods lie outside those regions where we can show rigorously that there is an absence of a phase transition. A more quantative comparison is made in our concluding remarks.

Heringa *et al* consider six specific models. Three of their models involve four-site interaction systems and we present our results only for four-site interaction systems. Similar results, however, can be obtained for other multisite systems, in particular the three- and five-site systems of [1]. As in [3] we will use two theorems of Ruelle which we now state. The theorems are best stated in lattice gas language where a site is occupied (unoccupied) if $S_i = +1$ ($S_i = -1$). Let Λ be a set of sites and P be the partition function for Λ. Define $z_i = \exp(2H_i)$ where H_i is the reduced field at the ith site. Then z_i is the activity of the ith site. The partition function is

$$P(z_1, \ldots, z_N) = \sum_{X \subseteq \Lambda} \exp(-\beta U(X)) \prod_{x \in X} z_x \tag{3}$$

where X is then the set of occupied sites. The main theorem of Ruelle follows.

Theorem 1. Let Λ' and Λ'' be two finite sets of sites and P' and P'' be the partition functions for the two sets of sites. It is assumed there exist closed subsets M'_x of the complex z plane such that $0 \notin M'_x$ and $P' \neq 0$ when

$$z'_x \notin M'_x$$

for all $x \in \Lambda'$. Similar assumptions hold for P''. Define

$$P = \sum_{X \subseteq \Lambda' \cup \Lambda''} \exp(-\beta U(X \cap \Lambda') - \beta U(X \cap \Lambda'')) \prod_{x \in X} z_x. \tag{4}$$

Then $P \neq 0$ when

$$z_x \notin \begin{cases} M'_x & x \in \Lambda' \backslash \Lambda'' \\ M''_x & x \in \Lambda'' \backslash \Lambda' \\ -M'_x M''_x & x \in \Lambda' \cap \Lambda'' \end{cases} \tag{5}$$

where

$$-M'_x M''_x = \{-z'_x z''_x : z'_x \in M'_x \text{ and } z''_x \in M''_x\}. \tag{6}$$

As stated in [3] there are two difficulties concerning the use of this theorem. One is the difficulty of determining $-M'_x M''_x$ and the other is that the z_j are independent of each other, whereas we are usually interested in the case where all z_j are the same since all H_j are the same. The regions M'_x are *much* more difficult to find if the z_j are all independent. The next theorem of Ruelle [4], based on a theorem of Grace, allows one to set all z_j equal to one another in special cases.

Theorem 2. Let $Q(z)$ be a polynomial of degree n with complex coefficients and $P(z_1, \ldots, z_n)$ a polynomial which is symmetric in its arguments, of degree 1 in each, and such that

$$P(z, \ldots, z) = Q(z).$$

If the roots of Q are all contained in a closed circular region M, and $z_1 \notin M, \ldots, z_n \notin M$,

then $P(z_1, \ldots, z_n) \neq 0$. A closed circular region is the inside or outside of a circle or a half-plane.

Thus what one does to find the zeros of the partition function of a system is to start with two small subsystems Λ' and Λ'' for which one has some knowledge of the zeros of $P'(z)$ and $P''(z)$ and then combine the two systems to form a bigger system. Theorem 1 then allows one to say something about the zeros of the new, bigger system. One continues this process eventually building up the full system. Each time two systems are combined to form one we say that the sites in $\Lambda' \cap \Lambda''$ are contracted which means the set product defined by equation (6) must be taken.

If we look at a set of m sites having only an m-site interaction and a field the partition function will have the symmetry required by theorem 2. For example, our four-site system with a distinct field on each site will have the reduced Hamiltonian

$$\mathcal{H}/kT = -KS_1S_2S_3S_4 - H_1S_1 - H_2S_2 - H_3S_3 - H_4S_4 \tag{7}$$

which results in a partition function with the necessary symmetry. Note that our system is indpendent of dimension of the lattice and the position of the sites; hence our results for the four-site interaction system will include all three models of reference [1] and any other spin system with only a four-site translationally invariant interaction. Note

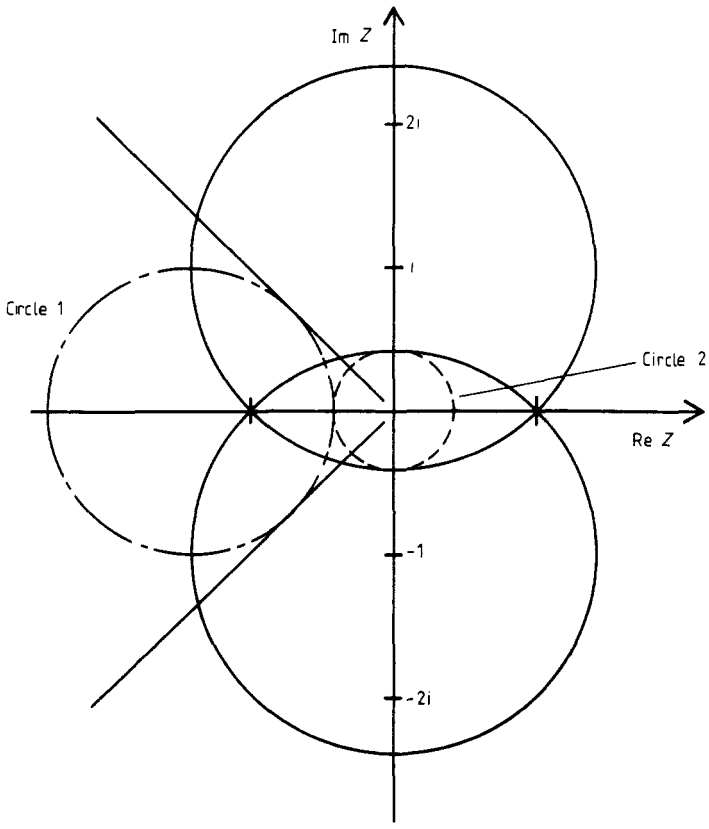

Figure 1. The complex z plane. The two full circles are the circles on which the zeros of the four-site system lie.

also that any system with only an m site translationally invariant interaction will require on each site $(m-1)$ contractions to build up the full system.

We now look explicitly at our four-site interaction system. We take our two initial systems Λ' and Λ'' to be four-site systems each with reduced Hamiltonian (7). In Monroe [5] it is shown that for a four-site system with four-site interaction the zeros lie on two circles each of radius $\sqrt{2}$ and with centres at $\pm i$. When $K=0$ all four zeros are at $z=-1$ and as K is increased the zeros move along the four lines emanating from that point. At $K=\infty$ the zeros are at $\pm(1+\sqrt{2})i$ and $+(\sqrt{2}-1)i$.

We now need to find circular regions M which contain the zeros of $P(z)$. For sufficiently small K the zeros are contained in circle 1 of figure 1. This circle is contained in the angular region defined by $3\pi/4<\phi<5\pi/4$ where ϕ is from the polar coordinate expression for z, i.e. $z=r\,e^{i\phi}$. One set product would extend this angular region to where $\pi/2<\phi<3\pi/2$. To build up our full system we need three contractions on each site and hence three set products for which the angular region is bounded by $0<\phi<2\pi$. Thus the zeros do not lie on the positive z axis and hence in the complex h plane do not lie on the real H axis. Therefore for all H we have no phase transition. This is the approach that was taken in [3] and referred to in [1]. For our four-site interaction system we have no phase transition for

$$0<K<\tfrac{1}{2}\ln\left(\frac{9-6\sqrt{2}}{6\sqrt{2}-8}\right) \tag{8}$$

and *all* H. This eliminates the possibility of a phase transition in one region of the positive H-K plane shown in figure 2.

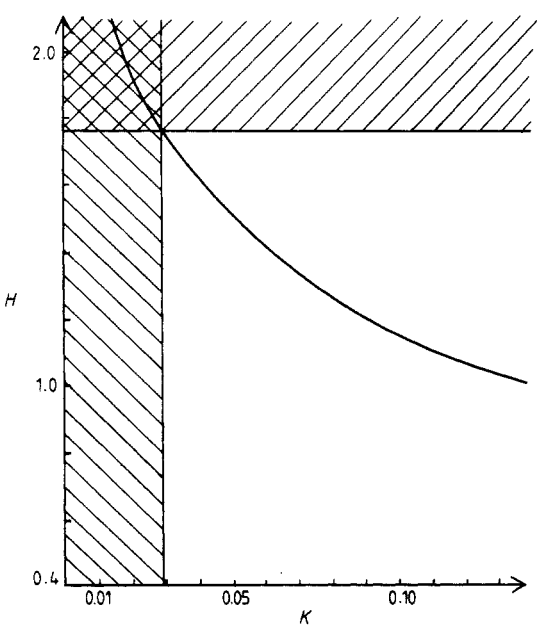

Figure 2. The positive H-K plane where the hatched regions have no phase transition. The region given by $0<K<\frac{1}{2}\ln[(9-6\sqrt{2})/(6\sqrt{2}-8)]$ and all H is shown as the vertical strip with diagonal hatching. The region given by $H>2\ln(\sqrt{2}+1)$ and all K is the horizontal strip with diagonal hatching.

If, however, we look at circle 2 in figure 1 then for *all* K in the region $z<(\sqrt{2}-1)^4$ one has no zeros (again this is after three contractions). In terms of H one has $H<2\ln(\sqrt{2}-1)$. Now by the spin-flip symmetry of the four-site interaction one also has no zeros in the region where $H>2\ln(\sqrt{2}+1)$. This region is also shown in figure 2.

Both approaches can be refined. Rather than simply take circle 1 of figure 1 which just sits within the angular region $3\pi/4<\phi<5\pi/4$ one can find a circle where the four zeros sit on the perimeter of the circle. At $K=0$ this is a circle of radius 0 since all zeros are at $z=-1$ and as K increases the size of the circle increases. For K in the region given by equation (8) one naturally still has the entire real H axis free of zeros but for larger K the circle extends outside the angular region necessary to guarantee this is true (see circle 1 in figure 3). We cannot then say that the entire real H axis is free of zeros; however, we can say that a certain region of the H axis is free of zeros. Because we must make three contractions we want to look at $z_1z_2z_3z_4$ where z_1, z_2, z_3 and z_4 are elements in M. Since we are only concerned about the real H axis or in other words the positive z axis we want $z_1z_2z_3z_4=r_1r_2r_3r_4\exp[i(\phi_1+\phi_2+\phi_3+\phi_4)]$ where $\phi_1+\phi_2+\phi_3+\phi_4=n(2\pi)$, $n=0,1,2,\ldots$. Clearly the points z_0 and z_0' shown in figure 3 when multiplied together meet this condition as would any product of four points on the line at $\phi=3\pi/4$ or $\phi=5\pi/4$. The products cover an interval of the z

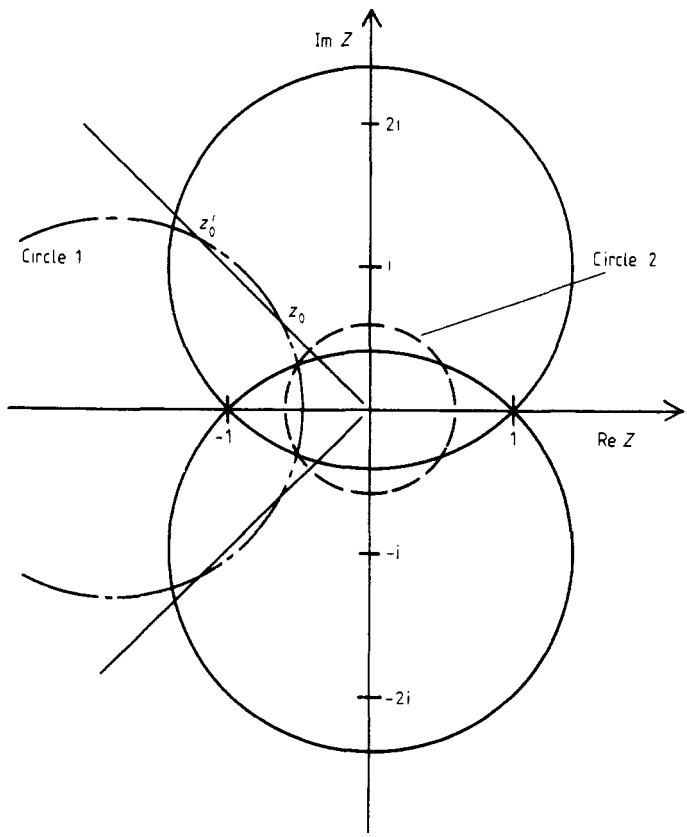

Figure 3. The complex z plane where circle has the four zeros of the partition function on its perimeter. The location of the zeros would be where the full circles intersect circle 1. Circle 2 has the two zeros closest to the origin on its perimeter.

axis with $|z_0|^4$ giving the minimum value of the interval and $|z_0'|^4$ the maximum value. One cannot by a product of four values of z in m find a product where $\phi_1+\phi_2+\phi_3+\phi_4 = n(2\pi)$ which is greater than $|z_0'|^4$. This is because to maximise $r_1r_2r_3r_4$ we might try to move z_1 to a point where $\phi_1 > \frac{3}{4}$ this would allow us to increase r_1 but we must move z_2, z_3 or z_4 to keep the condition $\phi_1+\phi_2+\phi_3+\phi_4 = n(2\pi)$ satisfied. But it is apparent due to the rate of curvature of the circle with respect to the line at $\phi = 3\pi/4$ that we would be able to increase r_1 less than we would be forced to decrease r_2, r_3 or r_4 and therefore we would decrease the value of $|z_1z_2z_3z_4|$. Hence $|z_0'|^4$ is the maximum value one can obtain by our three set products if we require the outcome to fall on the positive z axis. Thus while we do not have the entire x axis free of zeros we do the regions have for which $|z| < |z_0|^4$ and $|z| > |z_0'|^4$ free of zeros. The resulting zero-free region of the positive H-K plane is shown in figure 4.

A similar refinement occurs with circle 2 in figure 1. Rather than take the radius of circle 2 to be $(\sqrt{2}-1)$ as was done in figure 1, we can require circle 2 to be such that the two zeros closest to the origin of the z plane lie on its perimeter. This is the situation shown in figure 3. Thus the radius of the circle is a function of K and, as above, our zero-free region will likewise be a function of K. The resulting zero-free region is shown in figure 4.

By comparing the zero-free region of the positive H-K plane shown in figure 4 with that of the vertical strip of figure 2 we see that we have significantly extended the zero-free region from that of [3]. As stated earlier Heringa *et al* [1] investigated six models, three of which involved four-site interactions. Using their designations these are models 2, 4 and 5 (for specific descriptions, see [1]). To compare our rigorous results, establishing where there is the lack of a phase transition, with the Monte Carlo results, indicating where there is the presence of a phase transition, we note that H_c,

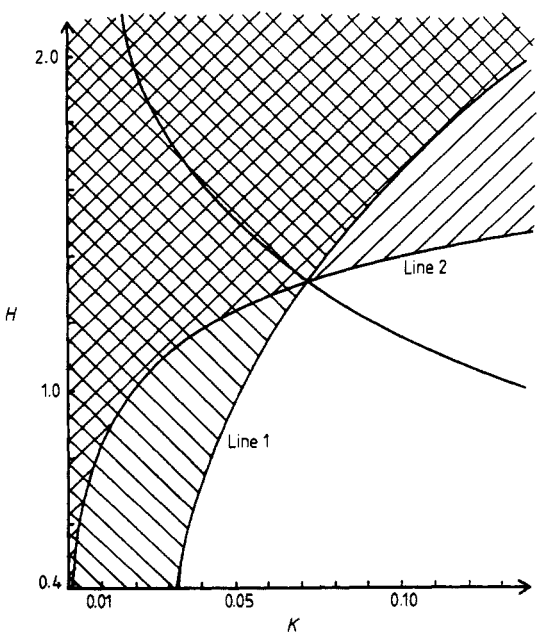

Figure 4. The positive H-K plane. The zero-free region based on circle 1 is the region with diagonal hatching whose boundary is line 1. The zero-free region based on circle 2 is the region with diagonal line whose boundary is line 2.

the largest external magnetic field for which a phase transition is indicated in [1], is equal to 0.295, 0.239 and is less than 0.14 for models 2, 4 and 5 respectively. Hence there is still a wide gap between the two regions.

For completeness we mention that for the case of $H = 0$ this system and similar ones have been considered by a number of authors [6–8]. In particular for a system with a single translationally invariant multisite interaction (the dimension of the lattice is unimportant) it is known that the system can be 'reduced' to a collection of small independent systems [8]. Hence for $H = 0$ no phase transition exists.

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