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Restrictions on the Phase Diagrams for a Large Class of Multisite Interaction Spin Systems

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Through the proof of two very general theorems involving Ising spin systems with multisite interactions, specific regions of the complex h plane, where h is the external magnetic field, are shown to be free of zeros of the partition function. Hence in these regions the partition function is analytic and phase transitions are absent. As an example: for systems with ferromagnetic multisite interactions involving even numbers of sites, no phase transition occurs outside of an interval centered on the origin of the real h axis and of the form $(-C(T), C(T))$, where T is the temperature. For $T \to 0$, $C(T) \to 0$ and phase transitions can occur only at $h = 0$.

KEY WORDS: Ising spin model; Lee–Yang zeros; multisite interactions.

Lattice spin systems with multisite interactions, where by multisite interactions we mean interactions involving three or more sites and which hereafter will be denoted as MSIs, have been used to model a wide variety of physical systems, ranging from binary alloys[(1)] to gauge field theories[(2)] to lipid bilayers.[(3)] Such systems have very rich and interesting phase diagrams as well as other interesting properties. Due to the greater complexity of such systems, rigorous results for these systems are rather limited. For example, for ferromagnetic pair-interaction Ising spin models one has the Lee–Yang circle theorem[(4)] for the zeros of the partition function, which guarantees that phase transitions can occur only when the magnetic field is zero. No such analogous results exist for MSI systems. In fact, Monte Carlo results indicate the presence of phase transitions at nonzero values of the magnetic field for a number of MSI system.[(5,6)]

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Hence phase diagrams indicate that zeros of the partition function, are not confined to the unit circle as they are in the Lee–Yang cases. This has been shown for some quasi-one-dimensional systems by direct computation.[7] However, no theorems exist locating the zeros for any general group of such systems. Only very limited results for specific systems exist.

Ruelle[8,9] has presented a theorem setting forth conditions which if met lead to finding regions of the complex magnetic field plane free of zeros, thereby establishing the lack of phase transitions in these regions. While Ruelle applied his theorem to a number of lattice spin models having pair interactions, it can be applied to MSI systems as well. In the past the present author has used the theorem to study some specific MSI systems,[10] but here we wish to present some general results which put some overall restrictions on the structure of the phase diagrams of such systems. The results deal with two very general sets of MSI systems, one having ferromagnetic interactions involving even numbers of sites with the exception of the single-site interactions with the magnetic field, and another set of systems with again ferromagnetic interactions involving an even number of sites and in addition either ferromagnetic or antiferromagnetic interactions involving an odd number of sites. Each site may interact with only a finite number of other sites. The specific type of lattice or even the dimensionality of the lattice does not come into play. Hence the results apply to a very general class of MSI systems.

We denote by Λ a collection of sites and on each site is a spin variable $\sigma_i = \pm 1$, where the subscript i denotes the ith site, $i \in \Lambda$. The spin interactions are given by the Hamiltonian

$$\mathscr{H}(\{\sigma\}) = -\sum_{A \subseteq \Lambda} j_A(\sigma_A + 1) - \sum_{i \in \Lambda} h_i(\sigma_i + 1) \tag{1}$$

where $\sigma_A = \prod_{i \in A} \sigma_i$ and A is any finite set of lattice sites of Λ with $|A| =$ the number of sites in A and $|A| \geqslant 2$. Physically, h_i represents the external magnetic field acting on the ith site. The partition function can be written as

$$P(z_1, z_2, \ldots, z_{|\Lambda|}) = \sum_{X \subseteq \Lambda} e^{-\beta U(X)} \prod_{i \in X} z_i \tag{2}$$

The sum is over all $X \subseteq \Lambda$, where X is the collection of sites with $\sigma = +1$, $U(X)$ the contribution from the first sum in (1) given X, $z_i = \exp(2\beta h_i)$, and $\beta = 1/(kt)$.

Ruelle's theorem uses the idea of "contractions" introduced by Asano,[12] where one takes two separate sets of sites and then contracts these to form one bigger system. This process can be repeated indefinitely to form larger and larger systems. The theorem follows.

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

$$z_i' \notin M_i' \tag{3}$$

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

$$P = \sum_{X \subset \Lambda' \cup \Lambda''} \exp[-\beta U'(X \cap X') - \beta U''(X \cap X'')] \prod_{i \in X} z_i \tag{4}$$

Then $P \neq 0$ when

$$z_i \notin \begin{cases} M_i', & i \in \Lambda' \backslash \Lambda'' \\ M_i'', & i \in \Lambda'' \backslash \Lambda' \\ -M_i' M_i'', & i \in \Lambda' \cap \Lambda'' \end{cases} \tag{5}$$

where

$$-M_i' M_i'' = \{-z_i' z_i'' : z_i' \in M_i' \text{ and } z_i'' \in M_i''\} \tag{6}$$

A great deal of difficulty arises in the use of this theorem because, as stated, all the z_i are independent of each other. Since in general $h_i = h$ for all $i \in \Lambda$, we are interested in the case where all z_i are equal to each other. Ruelle's next theorem allows us to set all z_i equal to one another in special circumstances and then find regions free of zeros.

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

$$P(z, z,..., z) = Q(z) \tag{7}$$

If the roots of Q are all contained in a closed circular region M, and $z_i \notin M,..., z_n \notin M$, then $P(z_1,..., z_n) \neq 0$.

A circular region is the inside or outside of a circle or a half-plane. All the systems considered in the following two sections have the symmetry required by Theorem 2.

We now present our new theorems regarding MSI systems.

Theorem 3. For spin systems with Hamiltonians given by (1) with only ferromagnetic interactions involving an even number of sites, i.e., $J_A \geq 0$, $|A|$ an even number, and no site is involved in more than a finite number of interactions N, then there is in the complex h plane an interval of the real h axis, centered on $h=0$, and of the form $(-C(T), C(T))$ *outside* of which there are no phase transitions. As $T \to 0$, $C(T) \to 0$ and hence the interval shrinks to $h=0$.

Proof. Consider separately each MSI and the set of sites it involves, that is, each MSI determines a system A'. The Hamiltonian for one of these systems consists of the appropriate z_i and a single term $-J_A(\sigma_A+1)$. For such a system the conditions of Theorem 2 are met and we can set all z_i equal. $Q(z)$ has the form

$$Q(z)=Wz^{|A|}+\binom{|A|}{|A|-1}z^{|A|-1}+W\binom{|A|}{|A|-2}z^{|A|-z}+\cdots+W \quad (8)$$

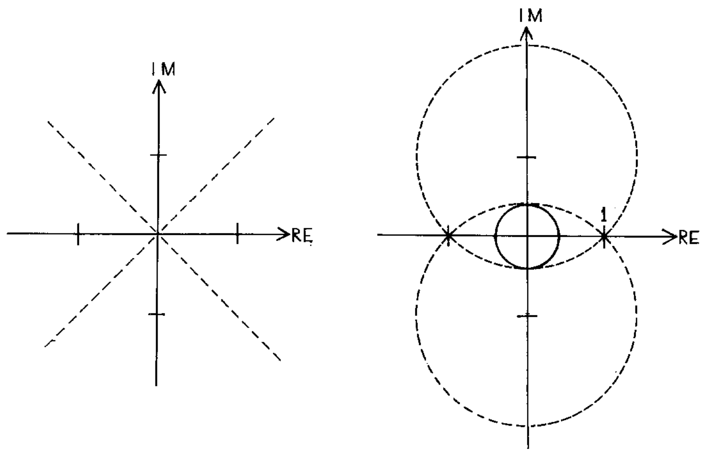
where $W=\exp(2\beta J_A)$. We need to find a closed circular region containing the zeros of $Q(z)$. After some rearrangement the above can be written as

$$Q(z)=z^{|A|/2}2^{|A|-1}\cosh^{|A|}(\beta h)[(W+1)+(W-1)\,\mathrm{th}^{|A|}(\beta h)] \quad (9)$$

Hence for the zeros of $Q(z)$ we have

$$\tanh(\beta h)=\left(\frac{1+W}{1-W}\right)^{1/|A|} \quad (10)$$

Therefore $\tanh(\beta h)$ equals the $|A|$th roots of the negative number $(1+W)/(1-W)$. For the case $|A|=4$ a typical arrangement is shown in Fig. 1a. As W is varied, by varying the temperature T, the solutions to (10)



(a) (b)

Fig. 1. a.) Zeros in the $\tanh(\beta h)$-plane for a four site system with a ferromagnetic four site interaction lie on the two dotted lines shown. b.) Zeros in the z-plane for the system of part 1a lie on the two dotted circles shown. The closed circular region M is the solid-line circle and the region outside the circle.

move along the two dashed lines shown. In general there are $|A|/2$ lines through the origin of the $\tanh(\beta h)$ plane along which the zeros lie, but for $|A|$ an even number, no dashed line lies along the real $\tanh(\beta h)$ axis. We need to find closed circular regions of the z plane containing the zeros of $Q(z)$. The straight lines of the $\tanh(\beta h)$ plane map to circles in the z plane which pass through the points $z = \pm 1$ (see Ahfors[13]). The two circles to which the two dashed lines of Fig. 1a map are shown in Fig. 1b. Hence we have as our closed circular region containing the zeros of $Q(z)$ the outside of a circle centered on the origin of the z plane and with a small enough radius r to lie inside the circles through the points ± 1. The solid circle of Fig. 1b is such a circle for the $|A| = 4$ case. It is important to note that the radius r is independent of T. Hence by Theorem 2 we have closed subset M_i, meeting the requirements of Theorem 1. For a given site each contraction by the rules of the set product, Eq. (5), will produce a new circular region centered on the origin whose new radius is simply a product of the radii of the two circles associated with the precontracted systems. Since each site is involved in a finite number of interactions, then after the full system is built up, each z_i will have a circular region of nonzero radius R, $R > 0$, centered on the origin of the z plane which is free of zeros of the partition function. Thus, for $h < (kT/2)\ln(R) = -C(T)$ one has no phase transition, i.e., the partition function is analytic. Now by symmetry, since $|A|$ is even, one also has the same result for $h > (kT/2)\ln(1/R) = C(T)$, and then as $T \to 0$ one has a phase transition only at $h = 0$. ∎

The above theorem is stated so as to emphasize the general restrictions one can place on the phase diagrams of an extremely wide class of MSI systems. For a specific MSI system one must find the radius r shown in Fig. 1b appropriate for that system. Then the radius R is found based on the number of contractions necessary to construct the full system. As an example we show in Fig. 2 the phase transition-free region in the h–T plane for a system involving four-site interactions where each spin is a part of four such interactions. The models numbered 2, 4, and 5 of Heringa *et al.*[5] all meet these requirements.

For the case where interactions involving both odd and even numbers of sites are present, we do not have the symmetry of the Hamiltonian we had in Theorem 3 and therefore the portion of the real h axis free of phase transitions is more restricted. The theorem for such systems follows.

Theorem 4. For spin systems with Hamiltonians given by (1) with $J_A \geq 0$ if $|A|$ is an even number and $J_A \leq 0$ if $|A|$ is an odd number, and no site is involved in more than a finite number of interactions, there is in the complex h plane an interval of the real h axis of the form $(-\infty, C(T))$

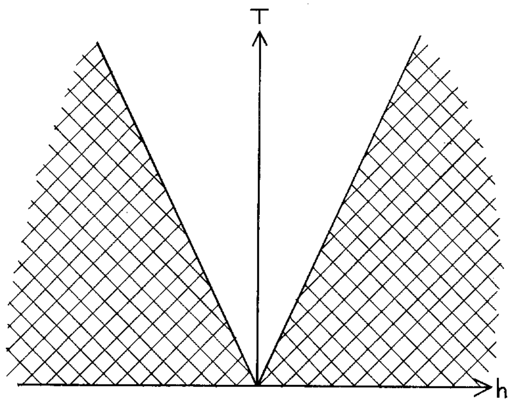


Fig. 2. The cross-hatched region of the $h-T$ plane is free of the zeros of the partition function and therefore is a region where phase transitions can not occur.

with $C(T)<0$ in which no phase transition occurs. As $T \to 0$, $C(T) \to 0$ and therefore along the entire negative, real h axis there are no phase transitions.

Proof. The proof is very similar to that of Theorem 3 and only those areas where differences occur will be presented in detail. For the initial precontracted systems with only a single J_A and $|A|$ even, everything is exactly as before. For the precontracted systems with $|A|$ odd, the zeros in the $\tanh(\beta h)$ plane are still given by (10). However, since $J_A \leqslant 0$, we have the $|A|$th roots of the *positive* number $(1+W)/(1-W)$. In fact, $(1+W)/(1-W)>1$, and hence one zero will be on the positive, real, $\tanh(\beta h)$ axis at some point >1. For $|A|=3$ one has the situation shown in Fig. 3a. The real $\tanh(\beta h)$ axis maps to a circle of infinite radius through the points ± 1 in the z plane, i.e., it maps to the real z axis. We need only be concerned with that part of the real $\tanh(\beta h)$ axis where $\tanh(\beta h)>1$ which maps to the negative, real z axis with $z<-1$. Therefore again one has a circle free of zeros which is centered on the origin of the complex z plane and which has a nonzero radius r independent of the temperature (see Fig. 3b). As in Theorem 3, as each contraction is made, the set product reduces the size of the circular region free of zeros, yet since we have a finite number of contractions of any one site, since each site is involved in only a finite number of interactions, after the complete system is built up there remains a circle of nonzero radius R free of zeros. Hence for $h<(kT/2)\ln(R)=C(T)$ there exist no phase transitions. ■

Due to the presence of J_A with A odd we do not have the symmetry necessary to say anything about the $h>0$ axis. However, by symmetry for the system of Theorem 4 but with $J_A>0$ for $|A|$ odd there is no phase

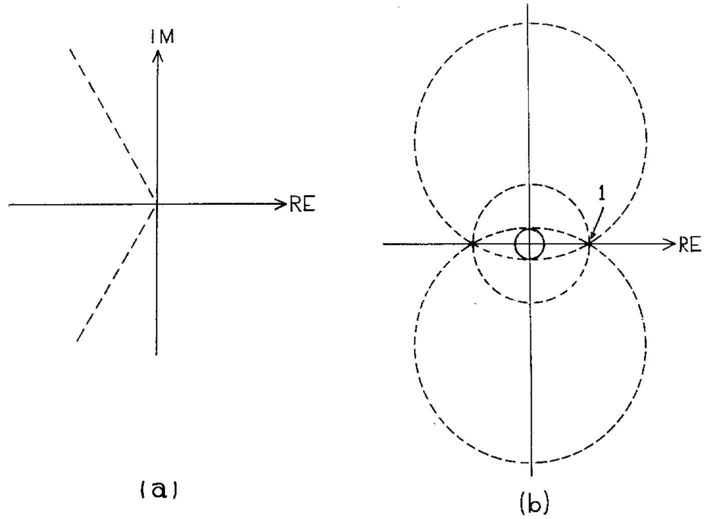


Fig. 3. a.) Zeros in the $\tanh(\beta h)$-plane for a three site system with antiferromagnetic three site interaction lie on the two dotted lines shown along with the positive real axis with $\tanh(\beta h) > 1$ b.) Zeros in the z-plane for the system of part 3a lie on the three dotted circles shown. The closed circular region M is the solid-line circle and the region outside the circle.

transition in the interval of the real h axis given by $(C(T), \infty)$, where $C(T) = (kT/2) \ln(1/R)$. Now when $T \to 0$ there can be no phase transitions on the positive h axis.

We conclude by stating that we have presented two theorems which allow one to find regions of the phase diagram in the z–T or h–T plane where phase transitions do not occur for a very large class of MSI systems. These systems do not have to be on any regular lattice, can be of any dimension, and can include systems with a very complex set of MSIs.

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