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The phase diagram of the baxter-Wu model in the magnetic field and temperature plane

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Abstract

Using the Fisher zeros of the partition function of a finite sized cluster with 'spherical' boundary conditions an approximate phase diagram in the magnetic field—temperature plane is obtained for the Baxter-Wu model. The phase diagram compares favourably with previous approximations as well as the known exact results when the magnetic field is zero. The accuracy of the approximated phase diagram, especially for small values of the magnetic field, is dependent on the fact, as shown previously, that for zero magnetic field the Fisher zeros for this cluster lie on loci giving the exact zero field critical temperature.

1. Introduction

The Baxter-Wu model [1–3] is one of a very small number of exactly solved lattice spin models. Like the most famous of these models, the nearest-neighbour (hereafter n.n.), square lattice, Ising model, first solved by Onsager [4], the solution only covers the case where the magnetic field, h, is zero. For the case of $h \neq 0$ one must rely on approximation methods to determine the phase diagram in the h-T (T being the temperature) plane. Approximations of the phase diagram began with the mean-field approach [5]. This was followed shortly by an approximation based on the interface method [6]. These approaches were followed with variational approximations [7], Monte Carlo approximations [8], entropic sampling methods [9–11] and most recently using the Wang-Landau entropic sampling algorithm [12].

Very recently [13], for the $h = 0$ case, the Fisher zeros for this model where examined. In particular the locations of the Fisher zeros for the Baxter-Wu model in the special case of $h = 0$ were presented for two series of finite clusters of spins with what were called spherical boundary conditions. The location of these zeros for these two series of clusters was shown to be particularly simple and give the exact critical temperature found by Baxter and Wu for the $h = 0$ case.

In this paper I look at the Fisher zeros of the Baxter-Wu model using one of the finite site clusters studied in [13] but now for the case of h ≠ 0. From the location of these zeros, I am able to approximate the phase diagram for this system in the h-T plane and by comparison with previous approximations and known exact results one sees the approximated phase diagram is quite accurate. Therefore, this is a new example of the usefulness of partition function zeros for a system with multi-site interactions rather than pair interactions, and one that lacks the up-down symmetry of the n.n., Ising model. It is also another example emphasizing the fact that boundary conditions can play a simplifying role when dealing with finite clusters of sites. This is akin to the results of Brascamp and Kunz [14] who showed for the n.n., square lattice, Ising model that some special boundary conditions, which they specified, give simplified results for the location of the Fisher zeros of that system.

The Baxter-Wu model, notation, and a quick introduction to Fisher zeros are presented in the following section. In section 3 a presentation of the procedure used to obtain the Fisher zeros as well as a couple of examples of the location are given. Section 4 contains the approximation of the phase diagram of the Baxter-Wu model based on the Fisher zeros along with comparisons to several previous approximations. In section 5 are some concluding remarks.

2. Baxter-Wu model, notation, and zeros of the partition function.

The Baxter-Wu model is an Ising model on the triangle lattice with Hamiltonian

$$\mathcal{H}(\sigma) = -J_3 \sum_{\Delta} \sigma_i \sigma_j \sigma_k - h \sum_i \sigma_i \tag{1}$$

where J_3 is the interaction strength of the three-site interactions involving Ising spins σ_i, σ_j, and σ_k, and h is the magnetic field. By Ising spins is meant that the spins take on only the values ± 1. The first sum, indicated by a sum over Δ, is over all elementary triangles forming the lattice and the second is over all sites of the lattice.

The partition function is given by

$$Z(\beta, h) = \sum_{\{\sigma\}} e^{-\beta \mathcal{H}(\sigma)} \tag{2}$$

where $\beta = 1/kT$, k is Boltzmann's constant, and T is the temperature. The sum is over all configurations denoted by $\{\sigma\}$. The partition function can be written as a generalized polynomial in terms of $a = \exp[\beta h]$ and $c = \exp[\beta J_3]$.

With the restriction that $h = 0$, as stated above, this lattice spin system is one of a rather small number of lattice spin systems which have been solved exactly. In particular Baxter and Wu [1–3] showed the critical temperature to be exactly the same as that of the n.n., square lattice, Ising system solved by Onsager [4]. The critical temperature for both models is $2/\mathrm{Log}[1+\sqrt{2}]$. Besides the critical temperature, the value of several critical exponents were found for the Baxter-Wu model at $h = 0$.

In 1952 T D Lee and C N Yang in two seminal papers [15, 16] showed the importance of the zeros of the partition function in terms of the study of phase transitions. Based on properties of the partition function, the zeros for a finite system will not lie on the real axis of the complex plane of some physical value such as the magnetic field. However, in the limit of an infinite system they pinch in on the real axis and thereby cause the non-analytic behaviour of various functions, such as the magnetization, just as expected. The two authors fixed their attention on the complex $\exp[2\beta h]$-plane and show that for any Ising model with ferromagnetic, pair interactions, J_2, the zeros in this complex plane lie on the unit circle, meaning in the complex h-plane they lie on the imaginary axis and they pinch in on the origin. This limits the phase transition in such a model to occurring only when $h = 0$. Because of this history zeros of the partition function involving the magnetic field are known as Lee-Yang (or sometimes Yang-Lee) zeros.

Not long after Lee and Yang's analysis of the zeros in the complex h-plane or some related plane such as the complex $\exp[2\beta h]$-plane, M E Fisher [17] examined the zeros in the complex $\exp[2\beta J_2]$-plane but limiting his analysis to the situation of an Ising model with n.n. interactions on the square lattice. Fisher conjectured that the zeros lie on two intersecting circles with centres at ± 1 and radii $1+\sqrt{2}$. Zeros connected with the complex temperature and related complex-planes are known as Fisher zeros. Later Brascamp and Kunz [14] explicitly showed for two series of clusters given some special boundary conditions that the zeros lie on these two circles for all clusters in their series.

3. Use of the fisher zeros for a given value of h to determine T_c

As stated earlier, looking only at the case of $h = 0$ for the Baxter-Wu model, it was shown [13], that for two series, denoted Series A and B, of smaller finite clusters with 'spherical' boundary conditions the Fisher zeros lie on the same two intersecting circles in the complex $\exp[2\beta J_3]$-plane as occurs for the n.n. interaction model on the square lattice. Hence one conjectures this holds true for all clusters in these two series regardless of size and then, in the infinite limit the Fisher zeros give the exact value of the critical temperature found by Baxter and Wu.

Series B of [13] consisted of clusters, one of which is shown in figure 1. As described in [13] for the system with 'spherical' boundary conditions one considers the set of sites shown in figure 1 as draped over the upper half of a sphere with a similar set on the lower half, making those sites on the boundary of figure 1 sites lying on the equator of the sphere. This produces a 98-site cluster. 'Spherical' boundary conditions for other lattice spin models have been considered, see for example [18], and [19].

While for $h = 0$ the Fisher series for the small cluster sizes examined in [13] regardless of cluster size lie on the two intersecting circles in the complex $\exp[2\beta J_3]$-plane. When $h \neq 0$ the zeros do not all lie on such a simple set of curves, and a loci which does not vary in shape depending on the size of the cluster. This is the normal case when examining the zeros of clusters of a finite number of sites for lattice spin systems. In such cases the larger the cluster size the nearer the distribution that would be found in the thermodynamic limit is obtained. Therefore, in this analysis only the distribution of zeros based on the largest cluster, a 98-site cluster from Series B, the one who's upper hemisphere is shown in figure 1 is used. For this cluster of sites an exact expression for the partition function in terms of $a = \exp[\beta h]$ and $c = \exp[\beta J_3]$, has been obtained and used to approximate the

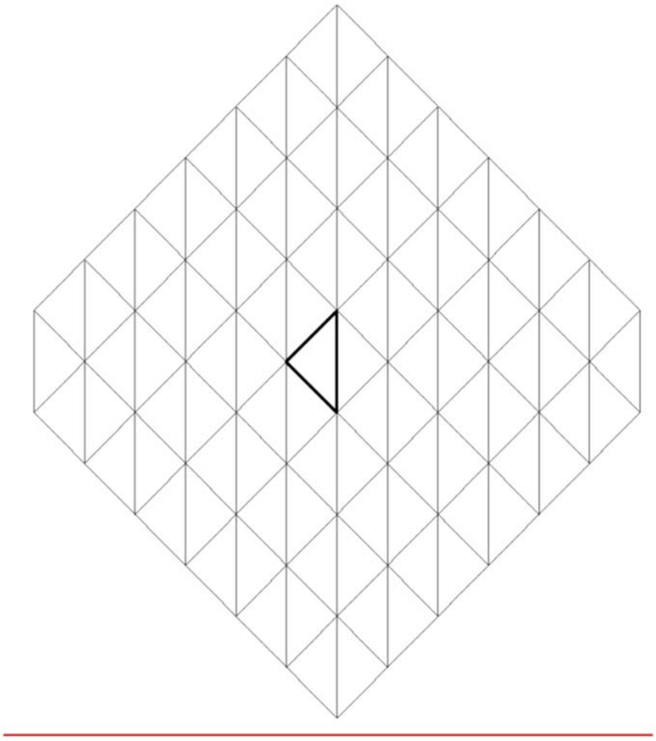

Figure 1. The upper half of the 98-site cluster with one of the elementary triangles in bold.

phase diagram. This is the largest cluster for which an exact expression for the partition function in terms of a and c has been obtained.

For figures showing the location of the Fisher zeros of such a system with $h = 0$ see [13]. Two examples when $h \neq 0$ are shown in figures 2 and 3. In figure 2, h $= -0.10$ and the location of the zeros in the $\exp[2\beta J_3]$-plane is seen in figure 2(a).

The zeros are not far from the two intersecting circles one has in the $h = 0$ case. Beside showing a plot of the Fisher zeros in the $\exp[2\beta J_3]$-plane they have also been plotted, in figure 2(b), in the complex T-plane. Figure 2(b) shows that there is a subset of the total set of zeros that indicates an arc crossing the positive, real T-axis at very approximately $T = 2.25$. It is these zeros, those forming a smooth curve in the complex T-plane, which will be used to estimate the temperature for various values of h at which a phase transition occurs.

In figure 3 the magnetic field has been increased in negative value to $h = -0.50$. In figure 3(a) the zeros are now seen to have considerably moved away from the two intersecting circles one has for $h = 0$. In figure 3(b) are plotted the zeros in the complex T-plane and as in figure 2(b) there are again a subset of the total number of zeros which when interpolated form an arc crossing the real, positive T-axis and again it is these zeros that are used to estimate the temperature at which the phase transition occurs.

The case of $h = 0$ will be considered in terms of giving a detailed procedure for what has been done to estimate the temperature at which the phase transition occurs for a given value of h. For this case one knows the value of the critical temperature. Hence, one can obtain an idea of the best procedure and a best level of accuracy.

The distribution for the case of $h = -0.10$ is graphically close enough to the $h = 0$ case that figure 2(b) is useful as a guide. A subset of the Fisher zeros consisting of those seeming to form an arc in the complex T-plane that crosses the positive T axis are selected. As a final step this arc is to be approximated by an n-th degree polynomial and so one does not want to take all zeros going back to the $T = 0$ axis. Rather one focuses on those zeros with the smallest argument. Figure 2(b) shows 22 zeros or less should be chosen. To approximate this arc by a polynomial expression these zeros are rotated counter-clockwise ninety-degrees by multiplying each value by i. This takes the zeros from forming something close to a vertical semi-circle to something close to a horizontal semi-circle. Next the real and imaginary part of each zero is taken as simply x and y values in an x-y plane. Then using Mathematica and its Fit[] command an approximation using a n-th degree polynomial is made to the curve of zeros. Since one sees that, after the above rotation, the equation for the arc must be an even function in x only even powers of x are used in the polynomial approximation. With 22 zeros one might well consider it best to approximate this with a polynomial having 22 coefficients and hence a 42-degree polynomial. This results in an estimated value for T_c of 2.268822. A reasonably accurate estimate. However, approximating what is almost a semi-circle with a polynomial may not be the best approach. There is no reason to believe using

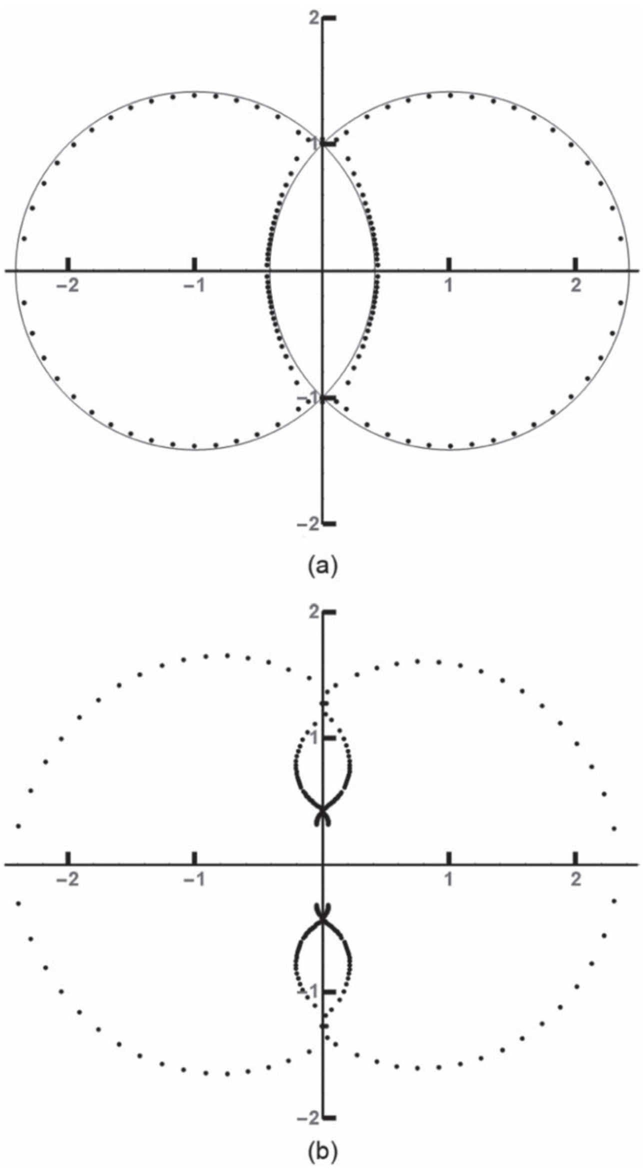

Figure 2. The Fisher zeros for the case of $h = -0.1$ In figure 2(a) are shown the zeros in the exp[$2\beta J_3$]-plane, while 2b shows the zeros in the T-plane.

the maximum number of zeros is the best approach as then a number of zeros rather far from the positive T-axis come into play. If in fact one goes through the same procedure but using only 16 zeros and a 30-degree polynomial one obtains as an estimate of T_c a value of 2.269184844 differing from the exact value, given to the same number of decimal places as 2.269185314 hence differing from the exact result by 0.00002%, an extremely accurate estimate. Further reduction in the number of zeros used does not result in more accurate estimates.

As one decreases the value of h fewer and fewer of the zeros lie on the arc crossing the real, positive T axis. For all h > -2.5 16 Fisher zeros were used. With $h = -2.5$ 14 Fisher zeros were used, with $h = -3.0$, -3.5, and -4.0 12 Fisher zeros were used and finally for $h = -4.5$ only 10 zeros were used. It is for this reason that using Fisher zeros for magnetic fields less than -4.5 likely give fairly inaccurate values compared to the results of [12] and therefore the most negative value for h examined here is -4.5.

4. Phase diagram for the Baxter-Wu model

Results for a series of h values along with comparisons with estimates using other methods are given in table 1. Specifically, results based on the present procedure along with, for comparison, results based on the interface method [6], the variational approximation [7] and results based on the Wang-Landau entropic sampling method using either the specific heat or the isothermal magnetic susceptibility [12] are given. The results found using the Fisher zeros and the results obtained in [12] are clearly the most accurate estimates of the phase

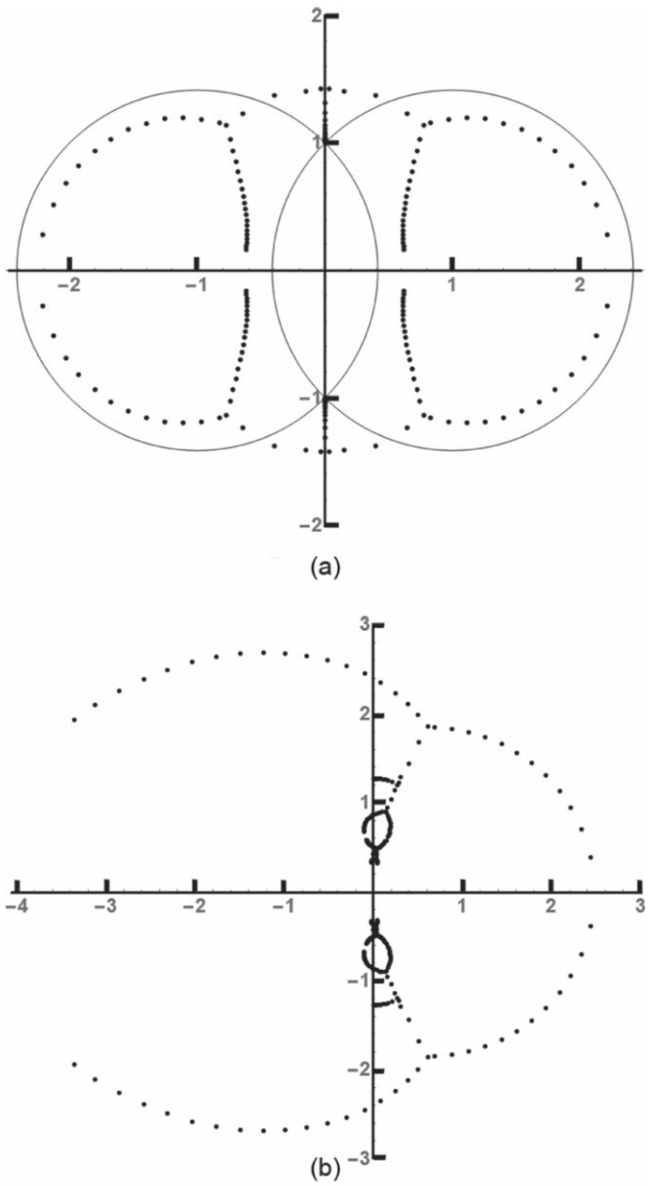

Figure 3. The Fisher zeros for the case of $h = -0.5$ In figure 3(a) are shown the zeros in the $\exp[2\beta J_3]$-plane, while 3b shows the zeros in the T-plane.

diagram. For the region $-1.0 \leqslant h \leqslant 0$ a graphical comparison of the results based on the Fisher zeros and the entropic Monte Carlo sampling results are shown in figure 4.

The error involved in these estimates is difficult to determine. Clearly with the present method errors for small values of h should be rather small, and as already stated, for $h = 0$ case, the method of using 16 Fisher zeros and a 30-degree approximating polynomial results in an error of only 0.00002%. Therefore, for small values of h one might expect very accurate results. As h becomes more negative it is expected that the accuracy drops. However, as figure 4 shows in the region $-1.0 \leqslant h \leqslant 0$ the estimates using the Fisher zeros are generally very close and often fall between the two estimates, one based on the specific heat and one based on the susceptibility, using the Wang-Landau entropic sampling algorithm approach [12]. As table 1 shows for values of $h < -2.0$ the Fisher zero approximations give a critical temperature consistently above that given in [12] with a growing difference between the two approximations as h is decreased in value.

Another approach to gauge the accuracy of these estimates is to consider a cluster of sites from Series A of reference [13]. In particular I look at two results based on the 98-site cluster of Series A. Series A in [13] consists of hexagonal clusters with spherical boundary conditions and as with the 98-site cluster of Series B which is the one being used up until now, the zeros for $h = 0$ lie on two intersecting circles in the complex $\exp[2\beta J_3]$-plane. I have been unable to calculate the partition function in terms of variables a and c for the 98-site Series A cluster as was done for the 98-site cluster of Series B. Here I have only been able to compute the cluster for a pre-determined value of a. This was all that was needed in [13] as only the $h = 0$ case was considered and the partition

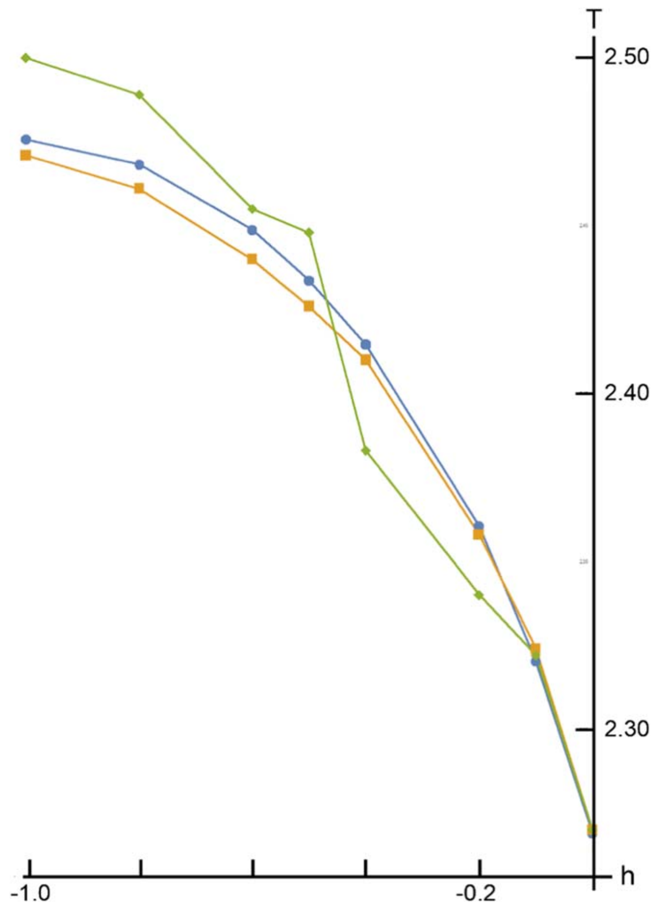

Figure 4. Comparison of results based on the Fisher zeros, indicated by circles, and the results based on Wang-Landau entropic sampling using the specific heat, indicated by diamonds, and using the susceptibility, indicated by squares. Lines connecting the estimates are only a guide to the eye.

Table 1. Estimates of T_c for various h.

h	Series B 98-site system.	Inter-face Mthd.	Varia- tional Ap-prox	Entropic Samp-ling (Sp. Heat)	Entropic Samp-ling (Suscept.)
0.0	2.2692	3.037	2.278	2.270	2.270
−0.02	2.2746				
−0.05	2.2919				
−0.1	2.3198	3.037		2.334	2.322
−0.2	2.3596	3.035		2.358	2.340
−0.4	2.4126	3.027		2.410	2.383
−0.5	2.4315	3.021	2.321	2.426	2.448
−0.6	2.4465			2.440	2.455
−0.8	2.4668			2.461	2.489
−1.0	2.4757	2.973	2.280	2.471	2.500
−1.5	2.4589		2.203	2.457	2.470
−2.0	2.3922	2.770	2.099	2.389	2.380
−2.5	2.2854		1.970	2.275	2.279
−3.0	2.1295	2.405	1.815	2.111	2.112
−3.5	1.9177		1.631	1.883	1.883
−4.0	1.6449	1.819	1.412	1.591	1.588
−4.5	1.3013			1.230	1.230

function for $a = 1$ was obtained. For $a = 19/20$ using the 98-site system in Series A one gets $h = -0.11933$ and $T = 2.3264$ while for the 98-site cluster in Series B at the same value of h one gets $T = 2.3288$ a difference of 0.0024. Velonakis and Martinos [12] do not present results for this value of h but their closest value is −0.10 and the difference between their specific heat and susceptibility results is 0.012. Going out to $h = -0.3902$ Series A gives $T = 2.3905$ while Series B gives $T = 2.3940$, an increase in the difference between the two but only of 0.0035 while the difference in [12] at $h = -0.40$ is 0.027 as seen in table 1.

5. Concluding remarks

As stated in their review of the Yang-Lee approach to phase transitions emphasizing the zeros of the partition function, both Fisher and Lee-Yang zeros, Bena, Droz, and Lipowski [20] state that simple loci of Fisher zeros are rare. The fact that not only are the Fisher zeros for systems presented in [13] simple but lie on loci which for $h = 0$ in the Baxter-Wu model give the exact critical temperature allows one to get an accurate estimate for the critical temperatures, using these zeros, when $h \neq 0$. These estimates compare favourably with recent estimates of Velonakis and Martinos [12] using Monte Carlo methods and are the most accurate available at this time, at least for $-2 < h \leqslant 0$.

As with any approximation method the accuracy of the approximation go hand in hand with the difficulty of obtaining the approximation. All work here in terms of computing partition functions, their zeros, etc was done on a personal computer. The two computations using Series A clusters took considerable time to run and were restricted to a single value of a whereas the partition function for the 98-site cluster in Series B was found symbolically in terms of variables a and c meaning the Fisher zeros or Lee-Yang zeros can be found for any value of a or c and one does not have to repeatedly compute the partition function for a specific value of a or c.

Finally, the results show: first, that the Fisher zeros can be used to obtain accurate phase diagrams even when multi-site interactions and systems without the up-down symmetry of pair interactions systems usually investigated, and second, in parallel with Brascamp and Kunz [14] boundary conditions can play a major role in simplifying matters regarding the locations of partition function zeros.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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