Exact solution and high-temperature series expansion study of the one-fifth-depleted square-lattice Ising model

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Phys. Rev. E **87**, 062143 — Published 28 June 2013

DOI: 10.1103/PhysRevE.87.062143

Exact solution and high temperature series expansion study of the 1/5-th depleted square lattice Ising model

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The critical behavior of the 1/5-th depleted square lattice Ising model with nearest neighbor ferromagnetic interaction has been investigated by means of both an exact solution and a high-temperature series expansion study of the zero-field susceptibility. For the exact solution we employ a decoration transformation followed by a mapping to a staggered 8-vertex model. This yields a quartic equation for the critical coupling giving $K_c(\equiv \beta J_c) = 0.695$. The series expansion for the susceptibility, to $\mathcal{O}(K^{18})$, when analyzed via standard Padé approximant methods gives an estimate of K_c, consistent with the exact solution result to at least four significant figures. The series expansion is also analyzed for the leading amplitude and subdominant terms.

PACS numbers: 05.50.+q, 75.10.Hk, 05.70.Jk, 64.60.fd

I. INTRODUCTION

Exact solutions of lattice models play an important role in the study of phase transition and critical phenomena. In his seminal work, Onsager solved the two dimensional (2D) square lattice Ising model (2D-Ising) exactly [1]. Solutions have been obtained for other regular 2D lattices [2]. A number of complex configurations such as the Union Jack, the bathroom tile (or 4-8), the 4-6, and the $1/9^{th}$ depleted lattice models have also been investigated [3–10]. The 1/5-th depleted antiferromagnetic S=1/2 Heisenberg model has been an earlier topic of investigation [11]. In this article we obtain the critical point of a 1/5-th depleted Ising model on a square lattice using both an exact solution by mapping to a staggered 8-vertex model and a high-temperature series expansion (HTSE). The vacancies form a $\sqrt{5}\times\sqrt{5}$ lattice. The Ising model Hamiltonian is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i, \qquad (1)$$

where s_i is the classical dimensionless Ising variable at site i taking the values $\pm$ 1. $J > 0$ (ferromagnetic interaction) and h (magnetic field) denote constant parameters with dimensions of energy. The structure of the depleted lattice with every 5^{th} missing site is shown in Fig. 1.

In principle all planar Ising models (i.e. with non-crossing bonds) are solvable by the Pfaffian method [2]. The method has been utilized to solve a variety of lattice models including the 8-vertex model. The 8-vertex model has been investigated both for translationally invariant and staggered vertex weight [12, 13]. In the staggered model the vertex weights are allowed to vary taking different values on the staggered plaquettes of the square lattice. The relevance of the staggered model lies in its relationship to a number of important models in statistical mechanics - the percolation model [14], the Potts model [15], and the Ashkin-Teller model [16, 17].

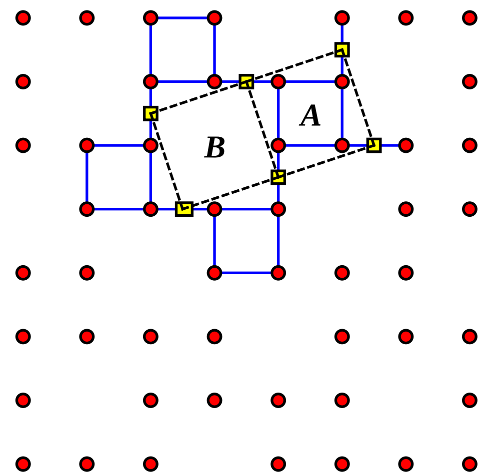

FIG. 1. (Color online) 1/5-th depleted lattice Ising model. Filled red circles denote points on the original lattice. Yellow squares denote points on the decorated lattice. Solid blue lines denote bonds on the original lattice. Dashed black lines denote bonds on the decorated lattice. *A* and *B* represent the two types of plaquettes created after the decoration transformation. The transformed lattice has a staggered configuration of *A* and *B* plaquettes.

We compute the partition sum to obtain the critical point of the 1/5-th depleted Ising model with two methods. First, we carry out an exact solution by using a decoration transformation [18] followed by a mapping to a staggered 8-vertex model [12, 13]. Second, we obtain the HTSE for the zero-field susceptibility upto $\mathcal{O}(K^{18})$ where $K = \beta J$ ($\beta = 1/k_B T$). T is the temperature and k_B the Boltzmann constant. Using Padé approximants (PA) we analyze the series for its leading amplitude and subdominant terms.

This paper is organized as follows. In Section I we introduce the 1/5-th depleted lattice Ising model. In Sec-

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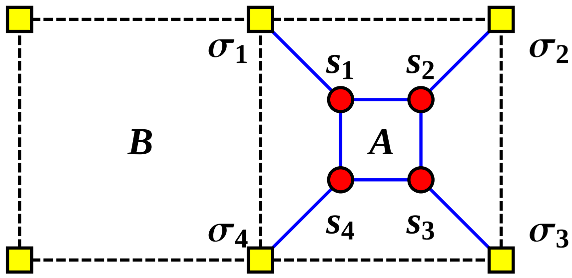

FIG. 2. (Color online) Ising spins on the original lattice are denoted by s_i, i=1,2,3,4 (filled red circles). Spins on the transformed decorated lattice are given by σ_i, i=1,2,3,4 (yellow squares). Interactions between s-spins is given by K. Interactions between s and σ-spins is given by $K^{'}$.

tion II we obtain the exact solution. In Section III we compute the HTSE for the zero-field susceptibility and display the series coefficient results. In Section IV we analyze the leading and subleading amplitudes of our series expansion result. Finally in Section V we summarize and conclude the main results of the paper.

II. EXACT SOLUTION

We carry out a two step procedure to obtain the exact solution. In the first step a decoration transformation is performed. A new spin σ (filled yellow squares in Fig. 1) is introduced in the original lattice placed at the midpoint of bonds which do not lie in the small square (see Fig. 1). The interactions on these bonds are replaced by new interactions with the σ spins to obtain the relation between the spins (s) in the original lattice and the decorated lattice (σ) [18, 19]. The scaled interactions K and $K^{'}$ are defined by,

$$e^{Ks_1s_2} = A\sum_{\{\sigma\}} e^{K^{'}\sigma s_1} e^{K^{'}\sigma s_2}, \tag{2}$$

where A is a yet undetermined overall constant. Carrying out the summation we obtain

$$e^{Ks_1s_2} = 2A\cosh K^{'}(s_1+s_2). \tag{3}$$

Utilizing the fact that s_1 or s_2 spins can take on a value of ± 1, we obtain an expression for A and eventually the following relation between K and $K^{'}$

$$e^{2K} = \cosh(2K^{'}). \tag{4}$$

We map this configuration to a staggered 8-vertex model. This transforms the 1/5-th depleted Ising model to a square lattice with more complex interactions with nearest neighbour coupling $\tilde{K}$, a diagonal next-nearest-neighbour coupling $\tilde{L}$, and a four-spin coupling $\tilde{M}$ [20]. The decoration process introduces two different types of plaquettes A and B as shown in Fig. 2. The transformed Z is

$$Z(\sigma_1,\sigma_2,\sigma_3,\sigma_4) = \sum_{\{s\}} \exp[K^{'}(s_1\sigma_1+s_2\sigma_2+s_3\sigma_3+s_4\sigma_4)] \times \exp[K(s_1s_2+s_2s_3+s_3s_4+s_4s_1)]. \tag{5}$$

Enumerating the summation over the original lattice spins, s_i (i=1,2,3,4), we can write

$$Z(\sigma_1,\sigma_2,\sigma_3,\sigma_4) = \Lambda(K)\exp[\tilde{K}(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_1\sigma_4)] \times \exp[\tilde{L}(\sigma_1\sigma_3+\sigma_2\sigma_4)]\exp[\tilde{M}(\sigma_1\sigma_2\sigma_3\sigma_4)], \tag{6}$$

with

$$\Lambda e^{4\tilde{K}+2\tilde{L}+\tilde{M}} = 4e^{-2K^{'}} + 4e^{2K^{'}} + e^{4K-4K^{'}} + e^{4K^{'}+4K} + 2e^{-4K} + 4 = P_1(K), \tag{7}$$

$$\Lambda e^{-4\tilde{K}+2\tilde{L}+\tilde{M}} = 4e^{-2K^{'}} + 4e^{2K^{'}} + e^{-4K^{'}-4K} + e^{4K^{'}-4K} + 2e^{4K} + 4 = P_2(K), \tag{8}$$

$$\Lambda e^{-2\tilde{L}+\tilde{M}} = e^{-4K^{'}} + 4e^{-2K^{'}} + 4e^{2K^{'}} + e^{4K^{'}} + 2e^{-4K} + 2e^{4K} + 2 = P_3(K), \tag{9}$$

$$\Lambda e^{-\tilde{M}} = e^{-4K^{'}} + 2e^{-2K^{'}} + 2e^{2K^{'}} + e^{4K^{'}} + e^{-2K^{'}-4K} + e^{4K-2K^{'}} + e^{2K^{'}-4K} + e^{2K^{'}+4K} + 6 = P_4(K). \tag{10}$$

The vertex weights satisfy the free fermion condition [13]. Using Eqs. 13 and 21 from Ref. 13 the condition for the critical point for our model is

$$P_1(K) + P_2(K) - 2P_3(K) - 4P_4(K) = 0. \tag{11}$$

The above equation can be written in terms of the variable $x = e^{2K}$ as

$$x^4 - 4x^3 - 1 = 0. \tag{12}$$

We obtain the exact solution of the physical root as,

$$x_c = 1 + \frac{1}{\sqrt{2}} + \sqrt{\frac{1}{2}(5+4\sqrt{2})}. \tag{13}$$

Numerically $x_c = 4.015445$, yielding a critical coupling value of $K_c = 0.695074$. In terms of the variable $v = \tanh(K)$ Eq. 12 takes the form

$$v^4 + 4v^3 - 1 = 0, \tag{14}$$

giving v_c=0.601232 as the solution of the critical point.

III. HIGH TEMPERATURE SERIES

The HTSE technique is one of the most effective approaches to study critical phenomena [21]. Much work has been devoted to the HTSE of the Ising model [22–24]. Thermodynamic properties are derivable from the partition function

$$\mathcal{Z} = \sum_s \exp(-\beta\mathcal{H}), \tag{15}$$

$$= \sum_s \exp(K\sum_{\langle i,j\rangle} s_i s_j + \beta h \sum_i s_i), \tag{16}$$

The zero field susceptibility, χ, is given by

$$\chi(v) = \beta^{-1} \lim_{h\to 0} \frac{\partial^2}{\partial h^2}\left(\frac{1}{N}\ln\mathcal{Z}\right). \tag{17}$$

Using the identity below for both the regular and the field term

$$\exp(Ks_i s_j) = \cosh K(1 + v s_i s_j), \tag{18}$$

we can construct a graphical expansion. Each bond carries a factor of $v s_i s_j$ and, in addition, each site has a factor of either 1 or τs_k. Only those graphs with precisely two factors of τs_k contribute to the above equations. As a result the graphs which contribute are those with precisely two vertices of odd degree, those to be compenstated by the two τs_k factors. We then obtain the following result

$$\frac{\mathcal{Z}}{(\cosh K)^{2N}(\cosh\beta h)^N} = \sum_{\{s\}}\prod_{\langle ij\rangle}(1 + v s_i s_j)\prod_k (1 + \tau s_k), \tag{19}$$

TABLE I. High-temperature series expansion coefficients, a_r, of the zero-field susceptibility for the 1/5-th depleted Ising model. The expansion parameter is $v = \tanh(\beta J)$.

Order	Coefficient
1	0.300000000000D+01
2	0.600000000000D+01
3	0.120000000000D+02
4	0.220000000000D+02
5	0.400000000000D+02
6	0.740000000000D+02
7	0.136000000000D+03
8	0.246000000000D+03
9	0.444000000000D+03
10	0.782000000000D+03
11	0.137200000000D+04
12	0.240600000000D+04
13	0.420800000000D+04
14	0.738600000000D+04
15	0.129240000000D+05
16	0.223940000000D+05
17	0.387280000000D+05
18	0.667820000000D+05

TABLE II. Pade approximation analysis of the high-temperature series expansion coefficients of the zero field susceptibility for the 1/5 depleted Ising model. The critical coupling constant and the leading amplitude is listed below.

(N,D)	v_c	A_0	A_1
(10,8)	0.601461	0.686077	0.707575
(9,9)	0.601405	0.686598	0.707919
(8,10)	0.601437	0.686265	0.707625
(9,8)	0.601554	0.686771	0.707614
(8,9)	0.600934	0.686810	0.707385

where $v = \tanh\beta J$ and $\tau = \tanh\beta h$. The high temperature susceptibility can be expanded in the form

$$\beta^{-1}\chi(v) = 1 + \sum_{r=1}^{\infty} a_r v^r. \tag{20}$$

The coefficients a_r can be related to the graph counting problem and evaluated exactly [21]. The computed series expansion coefficients for the zero-field susceptibility of the 1/5-th depleted Ising model are listed in Table I.

IV. SUSCEPTIBILITY ANALYSIS

The universality hypothesis in critical phenomena implies that thermodynamic quantities are not sensitive to the microscopic details of a system near a critical point [25, 26]. It is known from earlier work that near the transition point the high temperature susceptibility, $\chi(v)$, of the 2D-Ising model on all 2D lattices has an asymptotic form. For our model we can express the susceptibility as

$$\chi(v) = A_o\left(1 - \frac{v}{v_c}\right)^{-7/4} + A_1\left(1 - \frac{v}{v_c}\right)^{-3/4} + \cdots, \tag{21}$$

with v_c=0.601232. To analyze the $\chi(v)$ series for its pole and its leading and subleading amplitude we first consider constructing the series

$$f_1(v) = [\chi(v)]^{4/7} \sim A_o^{4/7}(1 - v/v_c)^{-1} + \cdots. \tag{22}$$

Direct PA's to $f_1(v)$ give a consistent pole at $v_c \sim 0.6015 \pm 0.0002$. This result is close to the exact solution value of v_c=0.601232. The residues, which are estimates of $A_o^{4/7} v_c$ are all in the range 0.486 - 0.490. Considering the value to be 0.488 we obtain $A_o \sim 0.694$. A more consistent set of results can be obtained by constructing the series

$$f_2(v) = (1 - v/v_c)^{7/4}\chi(v), \quad \sim A_o + \text{terms which vanish at } v_c, \tag{23}$$

and forming PA's to $f_2(v)$. Evaluating these at v_c=0.601232 gives $A_o \sim 0.687 \pm 0.001$. To obtain the subdominant contribution we analyze the function

$$f_3(v) = (1 - v/v_c)^{3/4}[\chi(v) - 0.686(1 - v/v_c)^{-7/4}], \quad \sim A_1 + \text{terms which vanish at } v_c. \tag{24}$$

PA's of $f_3(v)$ computed at v_c=0.601232 provide a consistent set of estimates for $A_1 \sim 0.708 \pm 0.001$.

The above analysis can be repeated with the HTSE χ series expressed in the K variable

$$\chi(K) = C_o \left(1 - \frac{K}{K_c}\right)^{-7/4} + C_1 \left(1 - \frac{K}{K_c}\right)^{-3/4} + \cdots . \tag{25}$$

To obtain a consistent set of critical coupling value, K_c , we perform the PA analysis on a $\chi^{4/7}$ series. The leading amplitude, C_o, can be computed by investigating the PA analysis of $(1 - K/K_c)^{7/4}\,\chi$. However, such an analysis does not lead to a consistent set of values for C_1. We therefore obtain both C_0 and C_1 from A_0 and A_1. To do so we expand the $\chi(v)$ series in a Taylor series in 1-K/K_c up to 2nd order to obtain the following

$$K_c = 0.695 \pm 0.001, \tag{26}$$

$$C_0 = 1.167 \pm 0.001, C_1 = 0.036 \pm 0.001. \tag{27}$$

The agreement of the series estimate of K_c with our result from Eq. 12 provides confirmation that our analysis in Section II is correct.

V. CONCLUSION

We have obtained the critical point exactly, and the estimated values of the leading two amplitudes of the asymptotic form of the zero-field susceptibility for the Ising model on an unusual lattice obtained by regularly removing 1/5-th of the sites of a square lattice. It is worth noting, however, that the familiar honeycomb and kagome lattices result from particular 1/3-rd and 1/4-th depletions of the triangular lattice. The 1/5-th depleted square lattice, considered here, is in fact realized in the material CaV_4O_9, but not as an Ising system.

To obtain the critical point, we relate partition function of the model to that of a staggered eight-vertex model and use established results for that model. The vertex weights satisfy a 'free fermion' condition, confirming that the model lies in the normal Ising universality class. We note that in the 1/5-th depleted lattice there are two classes of nearest-neighbor bonds. While we have only considered the case of equal strengths, our transformation method applies equally well to the more general case of different couplings J, J'. After we had completed this work it was pointed to us [27] that the 1/5-th depleted lattice considered here is, in fact, topologically equivalent to the "bathroom tile" lattice, and indeed our result for the critical point is identical to that obtained previously. However, our method is new.

We have also derived an 18-term high temperature series for the zero-field susceptibility. Because of the low coordination number and open structure of the lattice, the number of graphs that contribute at a given order is much reduced. As a consequence, the series is not as well behaved as that of the parent square lattice. However, using standard PA methods, we obtain an estimate of the critical temperature in good agreement with the exact value. As explained in Section IV we obtain rather precise estimate of the leading two amplitudes in the asymptotic form of $\chi(v)$ near the critical point and, rather less precise, estimates of the amplitudes in the K-representation.

For the square lattice exact expressions of the spin-spin correlation functions allow these amplitudes to be obtained, essentially exactly, from the solution of a Painlevé equation III [28]. In addition an exact result relating the coefficients C_0, C_1, viz., $C_1/C_0 = \sqrt{2}K_c/8$, has been proven. It is not clear whether a similar calculation could be done for the depleted lattice. However, the ratio C_1/C_0, in this case, does not appear to satisfy a simple relationship of the above type.

Finally, we remark that depletion of any regular lattice will reduce the average coordination number and this leads to a *less rigid* structure. Hence the ordered state will be less robust to thermal fluctuations, and the critical temperature will be lowered. This is seen in our study, with $k_B T_c/J$ being reduced by some 36%, from 2.2692... to 1.4387....

ACKNOWLEDGMENTS

Simeon Hanks acknowledges financial support from the Savannah River Scholars Program (NSF-DUE Grant # 0966195). T.D. acknowledges Cottrell Research Corporation Grant # 20073 and Georgia Regents University College of Sciences and Mathematics for funding support.

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