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-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 \( O(K^{18}) \), 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.

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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 [3–8]. The 1/5-th depleted antiferromagnetic S=1/2 Heisenberg model has been an earlier topic of investigation [9]. In this article we predict the critical point of a previously unexplored 1/5-th depleted Ising model on a square lattice. The Ising model Hamiltonian is given by

\[ \mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i, \]  

where \( s_i \) is the classical dimensionless Ising variable at site \( i \), \( J > 0 \) (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 [10, 11]. 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 [12], the Potts model [13], and the Ashkin-Teller model [14, 15].

The partition sum of the 2D-Ising model has been evaluated using a variety of techniques [REF]. 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 followed by a mapping to a staggered 8-vertex model [10, 11]. Second, we obtain the high temperature series expansion (HTSE) for the zero-field susceptibility upto \( O(K^{18}) \) 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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Solving the above equation we obtain a physical root at $\sigma_0 = 1$. The above equation can be written in terms of the variable $s_{i=1,2,3,4}$.

The vertex weights satisfy the free fermion condition \cite{11}. Using Eqs. 13 and 21 from Ref. \cite{11} the condition for the critical point for our model is

$$P_1(K) + P_2(K) - 2P_3(K) - 4P_4(K) = 0.$$  

(10)

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

$$x^4 - 4x^3 - 1 = 0.$$  

(11)

Solving the above equation we obtain a physical root at $x = 4.015445$, yielding a critical coupling value of $K_c = 0.695074$. In terms of the variable $v = \tanh(K)$ Eq. (11) takes the form

$$v^4 + 4v^3 - 1 = 0,$$  

(12)

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

\section{High Temperature Series}

The HTSE technique is one of the most effective approaches to study critical phenomena \cite{13}. Much work has been devoted to the HTSE of the Ising model \cite{19, 21}. Thermodynamic properties are derivable from the
TABLE I. High-temperature series expansion coefficients, \(a_r\), of the zero-field susceptibility for the 1/5 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 |

The zero field susceptibility, \(\chi\), can be expanded in the form
\[
\chi = \frac{\beta^2}{(\cosh K)^2} \left( \frac{1}{N} \ln Z \right).
\]

Using the identity below for both the regular and the field term
\[\exp(Ks_is_j) = \cosh K(1 + vs_is_j),\]
we can construct a graphical expansion. Each bond carries a factor of \(vs_is_j\) and, in addition, each site has a factor of either 1 or \(\tau s_k\). Only those graphs with precisely two factors of \(\tau s_k\) contribute to the above equations. As a result the graphs which contribute are those with precisely two vertices of odd degree, those to be compensated by the two \(\tau s_k\) factors. We then obtain the following result
\[
\frac{Z}{(\cosh K)^{2N}(\cosh \beta h)^N} = \sum_{\{s\}} \prod_{\langle ij \rangle} (1 + vs_is_j) \prod_k (1 + \tau s_k),
\]
where \(v = \tanh \beta J\) and \(\tau = \tanh \beta h\). The high temperature susceptibility can be expanded in the form
\[
\beta^{-1} \chi(v) = 1 + \sum_{r=1}^{\infty} a_r v^r.
\]

The coefficients \(a_r\) can be related to the graph counting problem and evaluated exactly [18]. 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. 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
\[
\chi(v) = A_0 \left( 1 - \frac{v}{v_c} \right)^{-7/4} + A_1 \left( 1 - \frac{v}{v_c} \right)^{-3/4} + \cdots
\]
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
\[
f_1(v) = [\chi(v)]^{4/7} \sim A_0^{4/7}(1 - v/v_c)^{-1} + \cdots
\]
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 \(A_0^{4/7}/v_c\) are all in the range 0.486 - 0.490. Considering the value to be 0.488 we obtain \(A_v \sim 0.694\). A more consistent set of results can be obtained by constructing the series
\[
f_2(v) = (1 - v/v_c)^{7/4} \chi(v)
\]
\(~A_0 + \text{terms which vanish at } v_c\)
and forming PA’s to \(f_2(v)\). Evaluating these at \(v_c = 0.601232\) gives \(A_0 \sim 0.687 \pm 0.001\). To obtain the subdominant contribution we analyze the function
\[
f_3(v) = (1 - v/v_c)^{3/4} \chi(v)f_2(v)
\]
\(~A_1 + \text{terms which vanish at } v_c,\)
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 \(\chi\) series expressed in the K variable,
\[
\chi(K) = C_0 \left( 1 - \frac{K}{K_c} \right)^{-7/4} + C_1 \left( 1 - \frac{K}{K_c} \right)^{-3/4} + \cdots
\]

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 |
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, $C_0$, 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

$$K_c = 0.695 \pm 0.001$$
$$C_0 = 1.167 \pm 0.001, C_1 = 0.036 \pm 0.001.$$  

The agreement of the series estimate of $K_c$ with our result from Eq. [11] provides confirmation that our analysis in Section I 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 the 1/5-th of the sites of a square lattice. There has not been to our knowledge, any systematic study of Ising models on depleted lattices. 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$_4$O$_9$, 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 $J, J'$.

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 precisely, 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 [24]. In addition an exact result relating the coefficients $C_0, C_1$, viz., $C_1/C_0 = \sqrt{2K_c}/8$, 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 $k_BT_c/J$ being reduced by some 36%, from 2.2692... to 1.4387...

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[21] M. Hellmund and W. Janke, Phys. Rev. B 74, 144201 (2006).

[22] W. P. Orrick, B. G. Nickel, A. J. Guttmann, and J. H. H. Perk, Phys. Rev. Lett. 86, 4120 (2001).

[23] S. Gartenhaus and W. S. McCullough, Phys. Rev. B 38, 11688 (1988).

[24] E. Barouch, B. M. McCoy, and T. T. Wu, Phys. Rev. Lett. 31, 1409 (1973).