A new method for the $S = \frac{1}{2}$ antiferromagnetic Ising model’s properties at any temperature and any magnetic field on the infinite square lattice

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Abstract

Since the introduction of the $S = \frac{1}{2}$ Ising model on the square lattice, many hundreds of articles have dealt with several properties of the ferromagnetic Ising model, but very few articles had included the antiferromagnetic Ising model. We have known that the Ising antiferromagnetism on a bipartite lattice is not zero in a considerable area of the magnetic field, $H$, and temperature, $T$. Now we present the dimensionless specific heat, $C$, and susceptibility, $\chi$, per vertex using a new method to obtain the data in about 10,000 points in the interesting $(T, H)$ area. Our last four figures show the contours and the smooth hills and valleys of $C$ and of $\chi$.

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1. Introduction

The Ising model [1] was introduced in 1925, yet there are still some properties that can be improved or even discovered. An early example by Peirls [2] found that the $S = \frac{1}{2}$, two-dimensional Ising model has a spontaneous magnetization at low temperature and zero magnetic field, and so it is a ferromagnet. Five years later Kramers and Wannier [3] discovered a method to obtain the exact critical point, $T_c$, in the temperature of the $S = \frac{1}{2}$ ferromagnetic Ising model on the square lattice. In 1944 on the same lattice Onsager derived the precise nature of the specific heat singularity [4]. Later Kaufman...
and Onsager simplified the method and obtained correlations [5]. Yang obtained on the square lattice the spontaneous magnetization exactly [6]. A very important theorem of the zeros of the grand partition function of the Ising model was published by Yang and Lee [7].

Several more papers were published up to 1960 on a variety of properties of the $S = \frac{1}{2}$ ferromagnetic Ising model on the various two dimensional lattices. In particular, Domb published two quarterly supplements in 1960 “On the Theory of Cooperative Phenomena in Crystals” [8]. These two quarterlies totalled 213 pages, and they were primarily on the ferromagnetic Ising models in two and three dimensions. Nevertheless, Domb did provide something about the antiferromagnetic Ising model in two dimensions. In his Fig. 39 he demonstrated that there is a curve separating from the area to the left and below as an antiferromagnetic long-range order from the area to the right and above for which there is no antiferromagnetic long-range order.

At present we are much more interested in the antiferromagnet than the ferromagnet on the $S = \frac{1}{2}$ Ising model on the square lattice. Two papers by Fisher in 1959 and 1960 started to show the properties of the $S = \frac{1}{2}$ antiferromagnetic Ising model on the square lattice [9,10]. He stated that in the square lattice Ising model “no exact expressions have yet been found for the properties of the model in a finite magnetic field, $H$, and the susceptibility, $\chi(T)$, is unknown even in the limit of zero field”. (A few months before, Fisher published a much larger paper on the $S = \frac{1}{2}$ antiferromagnetic Ising model on a slightly different square lattice.) The susceptibility of the ferromagnet on the $S = \frac{1}{2}$ Ising model on any two-dimensional lattice becomes infinite as the temperature, $T \rightarrow T_c$, and the magnetic field, $H = 0$. On the other hand, on the antiferromagnet Ising model in two dimensions, the susceptibility, $\chi$, remains finite for $0 \leq T < \infty$ and $H = 0$. (However, the derivative, $d\chi/dT$, becomes infinite as $T \rightarrow T_c$.) Near the critical point, the susceptibility, as obtained by Wu [11], is

$$\chi(T,H) = \chi(T,0) - DH^2 \ln|T - T_c| + \cdots.$$  \hspace{1cm} (1)

Shortly after Domb’s two large quarterlies Baker introduced the now well-known Padé approximant method to obtain much more precise coefficients [12]. We end the introduction section by examining what Domb has written in Chapter 6 in Vol. 3 of Phase Transitions and Critical Phenomena. He explained almost everything we knew about the Ising model up to 1974.

2. The $S = \frac{1}{2}$ antiferromagnetic Ising model on the square lattice

The $S = \frac{1}{2}$ ferromagnetic Ising model in two dimensions was studied as early as 1936 [2]. By 1960 many more articles were published on the ferromagnetic $S = \frac{1}{2}$ Ising model at the zero magnetic field on various two- and three-dimensional lattices. Many hundreds of more articles on the ferromagnetic Ising model have been published up to the present. On the other hand, almost nothing was known about antiferromagnetic Ising models up to 1970.

On Domb’s page 363 in Vol. 3 of Phase Transitions and Critical Phenomena [13] he showed a rough curve of singularities for an antiferromagnetic $S = \frac{1}{2}$ Ising model...
in two and three dimensions. Long-range order was to be in the area within what he believed to be a parabola in the \( T \) and \( H \) area. Later Rapaport and Domb [14] devised a parabola of singularities at small \( H \),

\[
T_c(H) = T_c[1 - 0.012(\frac{mH}{J})^2 + O(H^4)].
\]

Next, Müller-Hartmann and Zittartz [15] started with large \( H \) and small \( T \), the opposite end of the curve of singularities. They devised

\[
H = H_c - T_c \ln 2 + O(T_c).
\]

Next Kaufman [16] displayed the critical line near \( H = 0 \) as

\[
T_c(H) = T_c^0(1 - 0.038023259H^2).
\]

and the leading contribution to the susceptibility

\[
\chi = 0.014718006H^2 \ln(1/t).
\]

This reduced temperature used is \( t = T/T_c \). At present, we display the dimensionless data of \( H \) as a function of \( T \) over the whole range of the critical line for the \( S = \frac{1}{2} \) Ising antiferromagnet on the square lattice. We do so on Table 1 by reducing slightly the table produced very recently by Monroe [17]. All seven \( H(T) \) lines are very similar.

Using these data in Table 1 we can obtain the curve in Fig. 1. The temperature, \( T \), and the magnetic field, \( H \) are dimensionless. The ends of the \( (T,H) \) curve are \((2.269,0)\) and \((0,4)\). Note that \( T = H = 1.924 \). The \( (T,H) \) area for the left and below the curve, for which the antiferromagnetism is not zero, is shaded grey. The other part of the area is white.

Now we turn to the chapter by Privman et al. [24] for experimental results for several \( S = \frac{1}{2} \) antiferromagnetic Ising models on a square lattice. Table 2 has been obtained from part of their Table 7.8. The experimental results of amplitudes of specific heats were obtained by Hatta and Ikeda [25].

In Table 2 we see that the ratios, \( A/A' \), are close to 1 in each of the six antiferromagnetic compounds. The theoretical ratio, \( A/A' \), is exactly 1. Thus we believe that each of the six compounds in Table 2 have the magnetic system of the antiferromagnetic \( S = \frac{1}{2} \) Ising model in two dimensions. The correlation length, \( \xi(t,H) \) or \( \kappa(t,H) \), is

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
\hline
0 & 4 & 4 & 4 & 4 & 4 & 4 & 4 \\
0.25 & 3.933 & 3.837 & 3.827 & 3.833 & 3.833 & 3.836 & 3.888 \\
0.5 & 3.655 & 3.673 & 3.653 & 3.666 & 3.666 & 3.676 & 3.726 \\
1.5 & 2.732 & 2.749 & 2.704 & 2.731 & 2.732 & 2.751 & 2.701 \\
1.924 & 1.926 & 1.942 & 1.902 & 1.924 & 1.924 & 1.927 & 1.932 \\
2.0 & 1.716 & 1.731 & 1.695 & 1.715 & 1.715 & 1.715 & 1.739 \\
2.269 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
\end{tabular}
\caption{The temperature spans the curved critical line from \( T = 0 \) to \( T_c \) derived in seven methods from seven articles. This table is a smaller, revised table from one by Monroe [17].}
\end{table}
Fig. 1. In the antiferromagnet on the square lattice the curve from \((T = 0, H = 4)\) to \((T = 2.269, H = 0)\) divides finite magnetization below the curve and zero magnetization above the curve.

Table 2
Properties of six antiferromagnets on \(S = \frac{1}{2}\) Ising model on a square lattice and their experimental amplitudes of the specific heats

<table>
<thead>
<tr>
<th>Antiferromagnets</th>
<th>(A/A') ratio</th>
<th>K(_2)CoF(_4)</th>
<th>Rb(_2)CoF(_4)</th>
<th>Ba(_2)NiF(_6)</th>
<th>Rb(_2)NiF(_4)</th>
<th>K(_2)MnF(_4)</th>
<th>K(_2)NiF(_4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A/A') ratio</td>
<td>0.96</td>
<td>0.97</td>
<td>0.94</td>
<td>1.10</td>
<td>1.06</td>
<td>0.96</td>
<td></td>
</tr>
</tbody>
</table>

Amplitude \(A\), just above \(T_c\) and amplitude \(A'\), just below \(T_c\), are used to obtain the ratio \(A/A'\).

regarded theoretically as \(A/A' = 2\) very close to the critical point. Cowley et al. [26] found that K\(_2\)CoF\(_4\) experimentally yields \(A/A' = 1.85 \pm 0.22\).

At the end of this section we have found something about the curve of singularities of the two-dimensional \(S = \frac{1}{2}\) Ising antiferromagnets. We also learned about real 2D Ising system experiments.

3. Finite bipartite lattices useful at all temperatures and magnetic fields

The method of exact diagonalization on finite two-dimensional lattices on the ground state was invented by Oitmaa and Betts [27]. Extension of these data by the use of a scaling equation obtained physical properties on infinite spin models at zero temperature. Soon thereafter Lin developed sophisticated computing on larger finite lattices [28]. Further improvement was made by Betts et al. by introducing, on the infinite square lattice, new finite lattices based on parallelogram tiles [29].
Bernu et al. introduced an extensive set of low-lying levels by using the ground state for each total spin on each finite lattice [30]. This Paris group also introduced finite lattices on the infinite triangular lattice. It is quite useful to read a very recent article by Lhuillier, et al. for presenting other articles using the triangular lattice [31]. The finite lattice method has been expanded within large review articles by Manousakis [32] and Dagotto [33].

We authors decided that the better finite bipartite square lattices of vertices $16 < N < 34$ should be used to obtain the properties of the $S = \frac{1}{2}$ Ising antiferromagnet at any temperature and any magnetic field. We have used the range of dimensionless temperature, $T$, from 0 to 10—more than four times the critical temperature $T_c = 2.269$ at $H = 0$. Furthermore, we also used the dimensionless magnetic field, $H$, from 0 to 10—nearly three times the critical magnetic field. $H = 4$ at $T = 0$.

From previous experience we believe that any good bipartite finite lattice must have at least $N = 18$ vertices. In Fig. 2 there are two ways to display one good finite lattice—18a. On the other hand we were not able to work on bipartite lattices of $N > 32$ vertices because of the very large amount of time on our computer. You see that the number of states on each lattice is $2^N$. That means $2^{34} = 8.6$ billion states! Thus Table 3 has a total of 10 useful finite bipartite lattices from $N = 18$ to 32.

There is more than one type of finite lattices for each number $N$. Therefore we label a lower case letter beside the $N$. For example lattices 18a and 18c are both very good. Each finite lattice is derived from a parallelogram tile with two edges, $L$ and $l$, and two diagonals, $D$ and $d$. In squared order, $D \geq d \geq L \geq l$. Each lattice is completely defined by $(d^2, L^2, l^2)$. $I_g$ and $I_f$ are the geometric and topological imperfections, respectively. $S$ denotes the reflection and rotational symmetry.

A computer using the C programming language was used for all large calculations. A program was developed to run through all of the possible spin combinations for each of the finite lattices. Each spin combination corresponded to one energy state of the system. For each energy state, interaction energies and the corresponding sum of the spins (each spin being $\pm \frac{1}{2}$) were calculated. The energies of the states and their multiplicities were then calculated and used to produce a partition function for each lattice. From the partition functions, the computer calculated the specific heat and the magnetic susceptibility and substituted in particular values of $T$ and $H$ to give numerical values for these quantities. For each $T$–$H$ combination, the numerical values of the specific heat for the infinite lattice were approximated by taking the least squares regression of the values of each of the chosen lattices. This regression was linear with respect to $N^{-3/2}$, where $N$ is the number of vertices. In the regression it was only necessary to calculate the intercept with the specific heat axis. This intercept was the extrapolated value for $N \rightarrow \infty$.

Notice that the points of 18a and 18c, in Fig. 3, are almost identical on each of the two lines used. The same case is seen for 32a and 32b. This process was repeated for the susceptibility but with $N^{1/2}$ points on the horizontal numbers.

We cannot print copies of exact specific heat nor exact susceptibility of any one of the finite lattices that are large enough to be useful. Such equations remain in the computing system’s memory. However, we can display one equation for a small bipartite lattice of $N = 8$ vertices. That equation is the canonical partition
Fig. 2. This figure displays the finite square lattice 18a in two ways: (i) the numerical arrangement of the vertices, and (ii) the lines that can be used as tiles.
Table 3
Below is the description of the 10 best bipartite square lattices with vertices from \(N = 18\) to 32 inclusive

<table>
<thead>
<tr>
<th>(N\alpha)</th>
<th>((d^2, L^2, l^2))</th>
<th>(I_g)</th>
<th>(I_f)</th>
<th>(S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>18a</td>
<td>(26,20,18)</td>
<td>0</td>
<td>0</td>
<td>(C_2)</td>
</tr>
<tr>
<td>18c</td>
<td>(36,18,18)</td>
<td>2</td>
<td>0</td>
<td>(D_4)</td>
</tr>
<tr>
<td>20d</td>
<td>(40,20,20)</td>
<td>3</td>
<td>1</td>
<td>(C_4)</td>
</tr>
<tr>
<td>22a</td>
<td>(34,26,20)</td>
<td>1</td>
<td>2</td>
<td>(C_2)</td>
</tr>
<tr>
<td>24a</td>
<td>(32,26,26)</td>
<td>0</td>
<td>3</td>
<td>(D_2)</td>
</tr>
<tr>
<td>26c</td>
<td>(52,26,26)</td>
<td>2</td>
<td>5</td>
<td>(C_4)</td>
</tr>
<tr>
<td>28b</td>
<td>(40,34,26)</td>
<td>1</td>
<td>2</td>
<td>(C_2)</td>
</tr>
<tr>
<td>30a</td>
<td>(36,34,34)</td>
<td>1</td>
<td>1</td>
<td>(D_2)</td>
</tr>
<tr>
<td>32a</td>
<td>(40,40,32)</td>
<td>2</td>
<td>0</td>
<td>(D_2)</td>
</tr>
<tr>
<td>32b</td>
<td>(50,34,32)</td>
<td>2</td>
<td>0</td>
<td>(C_2)</td>
</tr>
</tbody>
</table>

Fig. 3. The horizontal line displays eight integers, \(N\), in accordance of length \(N^{−3/2}\) from infinity at the origin. The vertical line of two pieces is the specific heat. Each of the two slanted regression lines is fitted by its respective 10 circular points.

The specific heat and susceptibility equations are each too long to show here even for \(N\) as small as 8. Therefore equations of the specific heat, \(C(T,H)\), and the susceptibility, \(\chi(T,H)\), on the antiferromagnetic Ising model are tremendous for \(N > 16\).
4. Properties of the $S = \frac{1}{2}$ antiferromagnetic Ising model throughout the most interesting area of $T$ and $H$

For several decades it was not well known where the $(T, H)$ curve in the $S = \frac{1}{2}$ antiferromagnetic Ising model on the infinite square lattice. It was known that to the left and below the curve of singularities in the dimensional $T$–$H$ field, antiferromagnetism was finite, while to the right and above the curve that antiferromagnetism was zero. In Section 2 we now know the curve precisely. However, we do not know whether the properties of the $S = \frac{1}{2}$ antiferromagnet Ising model crosses the curve smoothly or drops suddenly to zero.

Using a very good system in our computers, we have obtained $S = \frac{1}{2}$ antiferromagnetic Ising properties such as specific heat, $C$, and susceptibility, $\chi$, at a very large number of points on the $(T, H)$ area. We chose the $(T, H)$ area as a square, $0 \leq T \leq 10$ and $0 \leq H \leq 10$. Within that square we used all points $(0.1m, 0.1n)$, where $m$ and $n$ are integers. From the heights of any property at each point used we obtained contours on the square area.

First we show the specific heat above the $(T, H)$ area. A contour of $\chi$ is made at several levels: 0.12, 0.24, 0.36, etc.

Notice that there seems to be a peak at about $T = 2.3$ and $H = 0$. Also see that there is a small pit in the area near $T = 0$ and $H = 4$ (Fig. 4).

Next, we show the contours of susceptibility drawn in the same way.

Fig. 4. In the area of dimensionless magnetization, $H$, and temperature, $T$, are several specific heat, $C$, contours of the antiferromagnet. These contours show a high peak near $T = 2.3$ and $H = 0$. The contours near $T = 0$ and $H = 4$ indicate a zero.
Fig. 5. Here in the $T-H$ area are contours of the magnetic susceptibility of the antiferromagnet. The contours indicate a high peak near $T = 0$ and $H = 4$.

The susceptibility contours seem to show that there is a peak near $T = 0.2$ and $H = 3.9$ (Fig. 5).

Then we decided that we needed to obtain figures in appearance of three dimensions—the $(T,H,X)$ box. The $X$ could be the specific heat, $C$, the susceptibility, $\chi$, or some other property of the $S = \frac{1}{2}$ antiferromagnetic Ising model on the square lattice. We start with $(T,H,C)$.

There we discovered three-dimensional hills and valleys. Most obvious is the specific heat mound at $T = 2.23$ and $H = 0.0$. The height of this mound, $C_m = 1.14$. The second most interesting item is the pit at $T = 0$ and $H = 4$ with a very small floor at $C = 0$. The third item is a straight ridge. It seems to start very close to the pit, and it slowly increases the height of the ridge as it moves farther away from $T = 0 = H$.

From Fig. 6 we can see the top of the ridge most clearly where $H = 10$. Here is a little rough table (Table 4) using $C$ as a function of $T$ at $H = 10$. Our last figure in this article is Fig. 7. The susceptibility, $\chi$, is also in a box—$(T,H,\chi)$.

It is obvious that the susceptibility surface in the box is much smoother than the specific heat box’s surface. Indeed the only interest on the surface is a very sharp, high pinnacle going through the $\chi = 1.5$ “roof” of the box. At the roof, the pinnacle has a small semi-ellipse centred about $H = 4.0 \pm 0.1$ and $T = 0.0 \pm 0.1$. Clearly in our second article, we will consider further the pinnacle of $\chi$ near $T = 0$ and $H = 4$. 
Fig. 6. Here is our first three-dimensional surface; the specific heat of the antiferromagnet. Notice a finite peak on the surface at \( H = 0 \) and \( T = 2.23 \) and a zero point of the surface at \( H = 4 \) and \( T = 0 \).

Table 4
The rough study of \( C \) as a function of \( T \) and \( H = 10 \)

<table>
<thead>
<tr>
<th>( T )</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C )</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>2.9</td>
<td>3.8</td>
<td>3.7</td>
<td>3.4</td>
<td>3.2</td>
<td>2.8</td>
<td>2.6</td>
<td>2.4</td>
</tr>
</tbody>
</table>

5. Summary and outlook

We are pleased that we tried a new method for the properties of the \( S = \frac{1}{2} \) antiferromagnetic Ising model on the square lattice, and it worked well! Indeed, we have been able to obtain several properties of the antiferromagnetic Ising model at any point on the area of \((T,H)\). Of course, we had to work long and hard on modern computers. At the end the most important events are shown in Figs. 6 and 7. Look particularly at the valleys and the high pinnacles.

In the future we or others will use finite bipartite square lattices including \( N = 34 \) and perhaps \( N = 36 \) for use in the \((T,H)\) area or otherwise. Again we or others may use squares smaller than \( 0.1\delta T \times 0.1\delta H \). The squares may be \( 0.05 \times 0.05 \) or even smaller. Indeed one may look most carefully around the antiferromagnetic susceptibility pinnacle to see its greater height and more precise place of centre via still smaller squares in that area.

One cannot use finite triangular lattices for antiferromagnetic properties of any kind.
Fig. 7. The second three-dimensional surface of the antiferromagnet is of the magnetic susceptibility. The very high, perhaps infinite, peak near $T = 0$ and $H = 4$ is the most interesting part of the surface.

However, one can study the $S = \frac{1}{2}$ antiferromagnet Ising model on the honeycomb lattice using similar finite bipartite lattices over a different $(T, H)$ area. More likely we or colleagues will try to study properties of antimagnetization on three-dimensional lattices. Simple cubic and bcc lattices can be used but fcc lattices can not be used. We would use all the best finite bipartite lattices for properties such as specific heat, susceptibility and other properties on all useful areas of $T$ and $H$.

References