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SIMULATION AND ANALYSIS OF THE
TRIANGULAR ISING MODEL

DISSERTATION

Presented in Partial Fulfillment of the Requirements for
the Degree Doctor of Philosophy in the Graduate
School of The Ohio State University

by

Bruce Dale Metcalf, B.S., M.S.

*******

The Ohio State University
1974

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# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I.</td>
<td>INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>II.</td>
<td>SIMULATION OF THE MODEL</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.1 Generation of the Ensemble</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>2.2 Limitations of Finite Size and Finite Ensemble</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>2.3 Efficiency Considerations</td>
<td>15</td>
</tr>
<tr>
<td>III.</td>
<td>INVESTIGATION OF THE SPIN FLIPPING DECISION</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.1 The Two Criteria</td>
<td>19</td>
</tr>
<tr>
<td></td>
<td>3.2 The Zero Temperature Limit</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>3.3 Occurrence of i-Mate Degeneracy</td>
<td>21</td>
</tr>
<tr>
<td></td>
<td>3.4 The Nonergodicity of Method II at B=B₀ and T=0</td>
<td>22</td>
</tr>
<tr>
<td></td>
<td>3.5 Comparison of the Two Methods</td>
<td>26</td>
</tr>
<tr>
<td></td>
<td>3.6 Unreliable Areas of Study Using Method II</td>
<td>34</td>
</tr>
<tr>
<td>IV.</td>
<td>THE NEAREST NEIGHBOR TRIANGULAR ANTIFERROMAGNET</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.1 The Triangular Lattice</td>
<td>36</td>
</tr>
<tr>
<td></td>
<td>4.2 Exact Solution in Zero Field</td>
<td>40</td>
</tr>
<tr>
<td></td>
<td>4.3 Approximation Methods in Nonzero Field</td>
<td>42</td>
</tr>
<tr>
<td></td>
<td>4.4 Application of the Monte Carlo Method to the Problem</td>
<td>44</td>
</tr>
<tr>
<td></td>
<td>4.5 Discussion of Results</td>
<td>63</td>
</tr>
</tbody>
</table>
# TABLE OF CONTENTS (CONTINUED)

<table>
<thead>
<tr>
<th>Chapter</th>
<th>TRIANGULAR ISING MODEL WITH THE NEAREST AND NEXT NEAREST NEIGHBOR INTERACTIONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>V.</td>
<td>5.1 The Ground State.................................................................................. 72</td>
</tr>
<tr>
<td></td>
<td>5.2 Detecting the Ground State Configuration........................................ 74</td>
</tr>
<tr>
<td></td>
<td>5.3 Results of the Polar J/B - J'/B Plane Scan...................................... 78</td>
</tr>
<tr>
<td></td>
<td>5.4 Discussion of the Ground State.................................................... 80</td>
</tr>
<tr>
<td></td>
<td>5.5 Results for Finite Temperature Behavior......................................... 86</td>
</tr>
<tr>
<td></td>
<td>5.6 Discussion of Finite Temperature Behavior....................................... 92</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Chapter</th>
<th>ANALYSIS OF THE CRITICAL FIELD GROUND STATE FOR THE ANTI-FERROMAGNETIC NEAREST NEIGHBOR ISING MODEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>VI.</td>
<td>6.1 Statement of the Problem.......................................................................................... 96</td>
</tr>
<tr>
<td></td>
<td>6.2 Ground State Degeneracy in the Critical Field - General........................................ 97</td>
</tr>
<tr>
<td></td>
<td>6.3 The One-dimensional Model..................................................................................... 100</td>
</tr>
<tr>
<td></td>
<td>6.4 Extension to Two and Three Dimensions.................................................................... 105</td>
</tr>
</tbody>
</table>

<p>| BIBLIOGRAPHY | .................................................. 117 |</p>
<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Monte Carlo Results for Magnetization per Spin</td>
<td>28</td>
</tr>
<tr>
<td>2.</td>
<td>Summary of Thermodynamic Behavior of Nearest Neighbor Triangular Anti-ferromagnet in a Magnetic Field</td>
<td>70</td>
</tr>
<tr>
<td>3.</td>
<td>Characteristic Ratios of the Five Ground State Phases</td>
<td>79</td>
</tr>
<tr>
<td>4.</td>
<td>Zero Field Variation of the Critical Temperature with $\propto &lt; 0 (J &lt; 0, J' &gt; 0)$</td>
<td>90</td>
</tr>
<tr>
<td>5.</td>
<td>Average Magnetization per Spin for the Triangular Lattice Critical Field Ground State with Lattice Width $m=6$ and Length $n$.</td>
<td>108</td>
</tr>
<tr>
<td>6.</td>
<td>Average Magnetization per Spin for Increasing Width $m$.</td>
<td>108</td>
</tr>
<tr>
<td>7.</td>
<td>Results of Linear Data Fit for $\ln$ Trace $A_m^n$ vs. $n$.</td>
<td>113</td>
</tr>
<tr>
<td>8.</td>
<td>Summarized Results for Various Anti-ferromagnetic Ising Models. Ground State in the Critical Magnetic Field $B_c = \gamma</td>
<td>J</td>
</tr>
</tbody>
</table>
# List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Comparison of Monte Carlo Simulation with Exact Solution for a 16x16 Periodic Square Lattice</td>
<td>11</td>
</tr>
<tr>
<td>2.</td>
<td>Approach to the Thermodynamic Limit</td>
<td>13</td>
</tr>
<tr>
<td>3.</td>
<td>Convergence of the Two Monte Carlo Methods</td>
<td>29</td>
</tr>
<tr>
<td>4.</td>
<td>Magnetization per Spin vs. ( kT/</td>
<td>J</td>
</tr>
<tr>
<td>5.</td>
<td>Topology of the Triangular Lattice</td>
<td>37</td>
</tr>
<tr>
<td>6.</td>
<td>Comparison of Monte Carlo Data with Exact Result for Zero Magnetic Field.</td>
<td>45</td>
</tr>
<tr>
<td>7.</td>
<td>Antiferromagnetic Order Parameter ( \xi ) vs. ( kT/</td>
<td>J</td>
</tr>
<tr>
<td>8.</td>
<td>Specific Heat at Constant Field ( B^* ) vs. ( kT/</td>
<td>J</td>
</tr>
<tr>
<td>9.</td>
<td>Reduced &quot;Staggered&quot; Susceptibility vs. ( kT/</td>
<td>J</td>
</tr>
<tr>
<td>10.</td>
<td>Ordinary Magnetic Susceptibility per Spin vs. ( kT/</td>
<td>J</td>
</tr>
<tr>
<td>11.</td>
<td>Specific Heat Isotherm at ( kT/</td>
<td>J</td>
</tr>
<tr>
<td>12.</td>
<td>Isothermal Ordering</td>
<td>61</td>
</tr>
<tr>
<td>13.</td>
<td>Phase Diagram of the Nearest Neighbor Triangular Ising Antiferromagnet.</td>
<td>64</td>
</tr>
<tr>
<td>14.</td>
<td>Partition of ((J/B,J'/B)) Space for the Ground State of the Triangular Ising Model with (nn) and (nnn) Interactions.</td>
<td>81</td>
</tr>
<tr>
<td>15.</td>
<td>Ground State Spin Arrangements on the Triangular Lattice.</td>
<td>83</td>
</tr>
<tr>
<td>16.</td>
<td>Zero Field Magnetic Susceptibility per Spin and Spontaneous Magnetization per Spin for ( \alpha = -0.2 ) ((J &lt; 0, J' &gt; 0)).</td>
<td>88</td>
</tr>
</tbody>
</table>

vii
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>17.</td>
<td>Phase Diagram of Nearest and Next Nearest Neighbor Triangular Ising Model with $\alpha = -0.2$ ($J &lt; 0, J' &gt; 0$)</td>
<td>93</td>
</tr>
<tr>
<td>18.</td>
<td>ln Trace $A_m^n$ vs. $n$</td>
<td>111</td>
</tr>
</tbody>
</table>
CHAPTER I
INTRODUCTION

The theory of cooperative phenomenon is concerned with the macroscopic behavior resulting from microscopic interactions in a system composed of many particles. Of particular interest is the theory of phase transitions. One of the simplest systems that displays a phase transition is the two-dimensional Ising model. In an attempt to theoretically describe ferromagnetism Ising\(^1\), in 1925, solved the one-dimensional model and found no ferromagnetic phase transition. Further work on the Ising system came in the mid 1930's by Bragg and Williams\(^2\), Bethe\(^3\) and Peierls\(^4\) who formulated approximation methods on the model. Major advances occurred in the forties with the exact location of the ferromagnetic transition temperature for the two-dimensional model in zero magnetic field by Kramers and Wannier\(^5\) followed by the complete solution in the brilliant work of Onsager\(^6\). Since then a tremendous amount of study has gone into this model.

The statistical mechanical formulation of the nearest neighbor Ising model in the presence of a magnetic field B
is as follows. Consider a system of \( N \) lattice sites. At each site \( i \) we assign a scalar spin variable \( \sigma_i = \pm 1 \). The plus will be referred to as the "spin up" state and the minus as the "spin down" state. Each spin is assumed to interact only with its nearest neighbors through the exchange integral \( J \) and with the external magnetic field through a magnetic moment \( m \). The model may then be viewed as a system of tiny interacting bar magnets arranged on a lattice structure. The energy \( E \) of a particular microconfiguration of the set of spins \( \{ \sigma_i \}_{i=1}^N \) is given by

\[
E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - m B \sum_{i=1}^N \sigma_i .
\]

The first sum is over all nearest neighbor pairs of spins \( \langle i,j \rangle \) on the lattice. If \( J > 0 \) the system is referred to as ferromagnetic, since the nearest neighbors tend to align with each other through their interaction. If \( J < 0 \) it is called antiferromagnetic with the nearest neighbor tending to antialign. The thermodynamic behavior of the system is found from the canonical partition function \( Z_N \).

\[
Z_N = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} e^{-\beta E(\sigma_1, \ldots, \sigma_N)} = e^{-\beta F_N} ,
\]

where \( \beta = \frac{1}{kT} \), \( T \) is the temperature, \( k \) is Boltzmann's constant and \( F_N = -kT \ln Z_N \) is the Helmholtz free energy. The thermodynamic functions (entropy \( S \), internal energy \( \langle E \rangle \), average magnetization \( \langle M \rangle \) ) are given by partial differentiation of \( F_N \) as
The magnetic moment \( m \) has been set equal to unity for convenience. The heat capacity at constant magnetic field \( C_B \) is related to the thermal fluctuation in energy by

\[
C_B = \left( \frac{\partial \langle E \rangle}{\partial T} \right)_B = \frac{\langle E^2 \rangle - \langle E \rangle^2}{kT^2},
\]

with a relation of similar form holding for the isothermal magnetic susceptibility \( \chi \) in terms of the fluctuation of the magnetization

\[
\chi = \left( \frac{\partial \langle M \rangle}{\partial B} \right)_T = \frac{\langle M^2 \rangle - \langle M \rangle^2}{kT}.
\]

The two-dimensional ferromagnetic square lattice exhibits the phenomenon of spontaneous magnetization, i.e. a non-zero magnetization in the limit of zero external field for temperatures below the Curie temperature \( T_C \). The specific heat exhibits a logarithmic singularity at \( T_C \). The antiferromagnetic square Ising lattice thermodynamically behaves exactly as the ferromagnetic case. The antiferromagnetic Néel temperature is the same as the ferromagnetic Curie temperature.

Original work in this dissertation is found in Chapters Three through Six as follows. Three: Examination of a widely used simulation procedure showing a previously unknown failure of the method. Four: Complete
thermodynamic analysis of the nearest neighbor triangular antiferromagnet in the presence of an external magnetic field. Five: Investigation of the triangular model with the inclusion of the next nearest neighbors. Six: New results for the ground states of a variety of Ising models in the critical magnetic field.

In Chapter Two we present the details of the Monte Carlo simulation used for the study in Chapter Four and in part of Chapter Five. We also discuss here the possibility of using a finite system and finite ensemble to obtain results in the thermodynamic limit. The decision making criterion used in Monte Carlo calculations on the Ising lattice is not unique. Metropolis et al.\textsuperscript{8} introduced a decision making scheme with the first attempt at the application of the Monte Carlo technique to statistical physics in 1953. Most researchers since then have adopted this scheme. Yang\textsuperscript{9,10}, in 1961, proposed an alternative criterion which is free of the high temperature nonergodicity encountered in the former method. In Chapter Three these two criteria are contrasted in the low temperature regime. Rigorous proof is given of the nonergodic behavior of the Metropolis criterion under certain conditions of interaction and magnetic field strengths, even at nonzero temperatures. It is also shown that the criterion of Yang overcomes this difficulty.

The two-dimensional nearest neighbor triangular
lattice has been exactly solved for zero magnetic field\textsuperscript{11-17}. A curious feature of this lattice is that the ferromagnetic model ($J>0$) possesses a Curie temperature $kT_C/J = 3.64\ldots$ whereas the antiferromagnetic model ($J<0$) has no Neél point. It has been suggested that the Neél temperature is zero\textsuperscript{17,18}. This feature is a result of the particular topology of the triangular lattice. The behavior of this lattice in a nonzero field will be studied in Chapter Four where the variation of the Neél temperature as a function of magnetic field strength is mapped out. The results are compared with those from the approximation method used by Burley\textsuperscript{19}, and conjectures on the shape of the phase diagram made by Domb\textsuperscript{20} and by Temperley\textsuperscript{21}. The thermomagnetic behavior of this lattice will be discussed in detail.

Recently experimental results have come forth dealing with the adsorption of certain gasses upon graphite\textsuperscript{22,23,24}. The hexagonal structure of the graphite substrate affords a dual triangular lattice for occupation by the adatoms. Low energy electron diffraction and neutron diffraction experiments have yielded ordered structures indicating a two-dimensional, lattice gas type of behavior. By renaming "spin up" and "spin down" with "site occupied" and "site empty" respectively, the Ising canonical partition function has the same mathematical form as the grand canonical partition function describing the lattice gas model\textsuperscript{25}. An extension of the nearest neighbor triangular model in-
cluding next-nearest neighbors constitutes the material in Chapter Five. The inclusion of second neighbor interactions will be shown to produce a multiplicity of differently ordered ground states depending on the relative sizes of the nearest and next-nearest neighbor interaction energies and the strength of the external magnetic field. The finite temperature behavior will be analysed for a particular ratio of interaction energies appropriate to the adsorption of helium monolayers. In Chapter Six the nearest neighbor model will be treated under conditions which yield extremely degenerate ground states, namely the behavior in the critical magnetic field. A transfer matrix formalism is developed in order to evaluate the zero point magnetization and entropy. This method is applied to a variety of lattice topologies. Low temperature antiferromagnetic critical field behavior is not amenable to series expansion analysis because of the high degeneracy of the ground state. The counting problem associated with this degeneracy is numerically solved in the thermodynamic limit. Such counting problems are frequently encountered in statistical physics. Highly accurate results are given.
CHAPTER II
SIMULATION OF THE MODEL

II. 1. Generation of the Ensemble

Relatively few exact solutions of Ising models exist to date. Those that do exist are cast into the form of a largest eigenvalue problem for a matrix of infinite dimension and thus are burdened with extreme mathematical complexity. Series expansion approximations involve the counting of configurations which become formidable after just a few terms. It is therefore beneficial to simulate the behavior of the model with a high speed computer.

Since we are dealing with a classical model, the process of its simulation involves the generation of a Boltzmann ensemble over which the statistical averaging is performed. In this ensemble the frequency of occurrence of a configuration \( C \) with energy \( E_C \) is dictated by the Boltzmann probability

\[
\rho_C = \frac{e^{-\beta E_C}}{\sum_{C'} e^{-\beta E_{C'}}}
\]

The ensemble must be ergodic, that is every configuration must have a nonzero probability of appearing in the
ensemble at finite temperature. Such an ensemble is
generated in the memory of a computer by forcing the
machine to make decisions probabilistically. The outcome
of a large number of these decisions should display the
characteristics of Boltzmann statistics.

Let us now look at one of these decisions made at the
\(i^{th}\) site of an Ising lattice. Suppose that the con-
figuration of the \(N\) site lattice at this time is specified
by the set \(\{\sigma_j\}_{j=1}^{N}\) of spin variables. We call this
particular configuration \(\alpha\). The configuration obtained
from \(\alpha\) by reversing only the \(i^{th}\) spin will be called \(\alpha'\),
or the \(i\)-mate of \(\alpha\). The machine now decides whether or
not to overturn the \(i^{th}\) spin, i.e. which of the configu-
rations \(\alpha'\) or \(\alpha\) will be the outcome of the decision. If
\(p_{\alpha}\) and \(p_{\alpha'}\) are the probabilities of the outcome being \(\alpha\)
or \(\alpha'\) respectively then

\[
p_{\alpha} + p_{\alpha'} = 1. \tag{3}
\]

To incorporate Boltzmann statistics into the program we
require that \(p_{\alpha} \propto e^{-\beta E_{\alpha}}\) and \(p_{\alpha'} \propto e^{-\beta E_{\alpha'}}\) so that the relative
probability ratio is given by

\[
\frac{p_{\alpha'}}{p_{\alpha}} = \frac{e^{-\beta E_{\alpha'}}}{e^{-\beta E_{\alpha}}}. \tag{4}
\]

Solving (3) and (4) simultaneously gives

\[
p_{\alpha} = \frac{e^{-\beta E_{\alpha}}}{e^{-\beta E_{\alpha}} + e^{-\beta E_{\alpha'}}},
\]
which holds for \( p_\alpha \) by interchanging \( \alpha \) with \( \alpha' \). The
interval \((0,1)\) is then divided into two sections, \( A = (0, p_\alpha) \)
of length \( p_\alpha \) and \( A' = (p_\alpha, 1) \) of length \( p_{\alpha'} \). The computer
chooses between the two configurations by generating a
random number \( R \). If \( R \in A' \) then the \( i \)th spin is overturned
resulting in the \( \alpha' \) configuration; otherwise the \( i \)th spin
is unchanged giving the \( \alpha \) configuration.

The elements of the ensemble are chosen in the fol­
lowing manner. First, the lattice is initialized with
some arbitrary configuration. Second, the decision making
process is carried out at every site in the lattice. The
resulting configuration is then taken as the first element
of the ensemble. We then return to the second step and
repeat the process. One entire pass through the lattice
is termed a cycle. The number of configurations in the
ensemble is then equal to the number of cycles executed.
This method of ensemble generation was examined by C. P.
Yang\(^9\) who gave rigorous proof that such an ensemble
converges to the Boltzmann ensemble as the number of
cycles increases.

To evaluate the first moment thermodynamic functions
such as internal energy or magnetization, a straight
arithmetic average is performed over the ensemble. A
weighted average is not used since the Boltzmann statis­
tical weighting occurs in the ensemble itself. Second
moment quantities such as susceptibilities or specific
heat are found from the fluctuations of the first moment variables. Generally the first few cycles of the chain are deleted from the averaging as they have not yet reached equilibrium.

II.2. Limitations of Finite Size and Finite Ensemble

The vantage ground of the Monte Carlo simulation lies in its rapid convergence to the desired ensemble. Usually not more than a few (less than ten) thousand cycles are required. In Fig. 1 the one thousand cycle Monte Carlo data are compared with the exact results for internal energy and specific heat for a 16x16 periodic square lattice. High precision agreement is seen for the internal energy. This is typical of the first moment quantities; agreement for first moments is usually to within 1%. The specific heat data is somewhat poorer in quality near the maximum, one of the data points being ~10% in error. One can nevertheless use the qualitative behavior of the specific heat data to get an estimate to the temperature where the maximum occurs.

Since for a finite system the partition function is a finite sum of exponentials, the finite-sized system is incapable of singular behavior. Computer hardware limitations force us to use a system of finite size. However, we are still able to make close approximations to the infinite system. This is illustrated in Fig. 2 where
Figure 1. Comparison of Monte Carlo Simulation With Exact Solution for a 16x16 Periodic Square Lattice.

(a) Internal Energy per Spin

(b) Specific Heat
Figure 2. Approach to the Thermodynamic Limit.

The specific heat vs. reduced temperature is plotted for a sequence of lattices of increasing size. The vertical line is at the Curie temperature where the infinite lattice specific heat diverges logarithmically.
the specific heat behavior is shown for a variety of finite square lattices of increasing size using the finite lattice analysis of Ferdinand and Fisher. It can be seen that for lattices of size 16x16 or greater, the maximum in the specific heat is very close to the infinite lattice Curie temperature. The lattice sizes used in the analyses of the following chapters are greater than 30x30 so that the infinite lattice behavior should be very closely simulated. Comparisons of Monte Carlo data with a transfer matrix approach to ground state critical field behavior can be found in Table 8 of Chapter Six. The close agreement found there indicates good reliability of the Monte Carlo approach.

II.3. Efficiency Considerations

The state of the lattice is stored in an array in the computer memory. If the lattice geometry is other than linear, square or simple cubic then a topological deformation to one of these structures is involved, keeping in mind the relative location of the neighbors of each site. To effect periodic boundary conditions an artificial layer completely enclosing the proper lattice is added. The sites on this artificial layer are not directly subject to the spin flipping decision. When those sites on the proper lattice which are represented on the artificial layer are altered, the corresponding artificial site is immediately
updated to the new state.

It is convenient to represent the "spin up" and "spin down" states of a site by a one and zero respectively. Furthermore, in order to reduce computer memory usage, each word of the above mentioned lattice array is packed with more than one spin variable. One word is composed of 32 bits, each bit being an elementary unit of information 1 or 0 (i.e. bit "on" or bit "off"). The maximum number of spin variables which can be packed in one word is determined by the lattice coordination number \( l \) (i.e. the number of nearest neighbors of each lattice site). For the triangular lattice \( l \) is equal to six. Three binary digits are needed to represent the decimal number six, 110. Neglecting the two highest order bits in a full word of memory we can then pack ten spin variables into one word. The lowest order bit of each three-bit group contains the state of the spin variable. For example the lattice site \( L(I,J) \) of ten two-dimensional lattices might be:

\[
L(\text{word}) = \begin{array}{cccccccccccc}
  X & x & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
\end{array}
\]

\[
l(\text{lattice number}) = 10 9 8 7 6 5 4 3 2 1 ,
\]

where the states of this particular site on lattices one through ten would be ++--+-++-++, respectively. The addition of the six neighbors of a particular site involves the addition of six such words. When packing is
performed in this fashion such addition will yield no
carryover from one three bit group into the next. The
packing and unpacking of lattice sites and neighbor sums
is accomplished by concatenating an assembly language
program to the main FORTRAN program. The random number
generation may also be performed in the assembler program
by a multiplicative congruential routine. It will be
noticed that such packing allows the same random number
sequence to be used in the processing of ten lattices
simultaneously which therefore saves computer time usage.
A detailed description of the assembler subroutine has
been given by Shirley\textsuperscript{28}.

The probability matrix used in the spin flipping
decisions depends on the state of the site in question and
the states of its $\mathcal{J}$ nearest neighbors. In fact, the
latter dependence is only on the sum of the nearest neigh-
bors. This sum can take on the $\mathcal{J} + 1$ values $0, 1, \ldots, \mathcal{J}$.
Thus the probability matrix can be doubly indexed,
$\text{PRB}(M, N)$, where $M$ takes on two values according to the
state of the site in question, and $N$ takes on $\mathcal{J} + 1$ values
accounting for the state of the neighbors. This matrix
need only be computed once and stored, then called when
needed thereby reducing the number of evaluations of
exponentials on the computer.

Integer arithmetic is used whenever possible.
Floating point arithmetic is performed in double precision
carrying twelve figures. Since round-off error for the addition of \( n \) number follows a normal distribution with zero mean and a variance of \( n \) times the variance of the addition of two rounded-off numbers \(^{29}\), we expect only a small round-off error in the results.
CHAPTER III

INVESTIGATION OF THE SPIN FLIPPING DECISION

III.1. The Two Criteria

The decision making method of Yang was discussed in section II.1. Reference to this method will use the Roman numeral I. We now outline a widely used alternative criterion II. For details the reader is referred to Fosdick. The decision making criterion II is executed as follows: 1) Find the energy $\Delta E$ required to overturn the spin in question; 2) calculate the Boltzmann factor $f = e^{-\beta \Delta E}$; 3) if $f \geq 1$ overturn the spin, but if $f < 1$ generate a random number $R \in (0,1)$, and overturn the spin if $R < f$. The machine then proceeds to the next site and the procedure is repeated.

In comparing the two methods it is convenient to introduce a transition matrix $S$ given by

$$S = \begin{pmatrix} p_{\alpha \alpha} & P_{\alpha \alpha'} \\ P_{\alpha' \alpha} & p_{\alpha' \alpha'} \end{pmatrix},$$

where $\alpha$ and $\alpha'$ are 1-mate configurations and the matrix elements give the probabilities for a transition from the configuration specified by the first index to the config-
uration of the second index. We will, without loss of generality, assume that $E_\alpha \geq E_{\alpha'}$. The two methods are then characterized by transition matrices

$$S_I = \frac{1}{e^{-\beta E_\alpha} + e^{-\beta E_{\alpha'}}} \begin{pmatrix} e^{-\beta E_\alpha} & e^{-\beta E_{\alpha'}} \\ e^{-\beta E_\alpha} & e^{-\beta E_{\alpha'}} \end{pmatrix}$$

and

$$S_\Pi = \begin{pmatrix} 0 & 1 \\ e^{-\beta (E_\alpha - E_{\alpha'})} & 1 - e^{-\beta (E_\alpha - E_{\alpha'})} \end{pmatrix}.$$

### III.2. The Zero Temperature Limit

In the limit of zero temperature ($\beta = 1/kT \to \infty$) the above two transition matrices become

\[
\lim_{T \to 0} S_I = \begin{cases} 
(0, 1) & \text{if } E_\alpha > E_{\alpha'} \\
(\frac{1}{2}, \frac{1}{2}) & \text{if } E_\alpha = E_{\alpha'}
\end{cases}
\]

and

\[
\lim_{T \to 0} S_\Pi = \begin{cases} 
(0, 1) & \text{if } E_\alpha > E_{\alpha'} \\
(\frac{1}{2}, \frac{1}{2}) & \text{if } E_\alpha = E_{\alpha'}
\end{cases}
\]

It can be seen that for $E_\alpha > E_{\alpha'}$ both $S_I$ and $S_\Pi$ select the state $\alpha'$ of lowest energy. This is in accordance with the minimization of the Helmholtz free energy, $F = \langle E \rangle$ at absolute zero, and thus gives the equilibrium state. However, if $E_\alpha = E_{\alpha'}$, the two methods select the subsequent configurations differently. $S_I$ chooses between the two
states with equal probability. \( S_{II} \) always overturns the spin in question. The subsequent configuration is then always the 1-mate of the previous configuration when a degeneracy is encountered with method II.

### III.3. Occurrence of 1-mate Degeneracy

In cases of degeneracy the two ensembles are, in general, not the same. We now give an example of such a case which may be treated analytically. With an exact solution at hand we may then test the accuracy of the two methods in simulating the model.

The ground state of the antiferromagnetic nearest neighbor Ising model in the critical magnetic field is very degenerate. The reader may find a detailed discussion of this degeneracy in Chapter Six. With this field any configuration is a ground state so long as each spin that is antiparallel to the field has all of its nearest neighbors aligned with the field. Overturning any spin which has all of its nearest neighbors aligned with the field does not change the energy of the system. This is because the change in configurational energy is exactly compensated by the change in magnetic energy associated with the spin flip. Thus occurs 1-mate degeneracy if the 1\(^{th} \) spin has field-aligned neighbors. We now focus attention on the periodic one-dimensional model in the critical field \( B_c = 2 |J| \). From the analytic solution\(^{31} \) the zero temperature critical magnetization per spin is exactly
It will be shown in Chapter Six that the number of degenerate ground states of a periodic, linear $N$-spin system in the critical field is exactly

$$\lim_{N \to \infty} \frac{\langle M_N \rangle}{N} = \frac{1}{\sqrt{5}} = 0.4472 \ldots$$  \hspace{1cm} (5)$$

III.4. The Nonergodicity of Method II at $B=B_0$ and $T = 0$

We now consider the application of the two spin flipping criteria to a finite one-dimensional system in the critical field. We carry out the decision making at sites 1,...,$N$, in that order, and retain the last configuration for the ensemble.

The ergodicity of method I is easily established through the following argument. First, starting with any arbitrary configuration, there is a finite probability of generating, in one cycle, that configuration in which all the spins are aligned with the magnetic field. This is because any spin with its neighbors aligned to the field has a probability $\frac{1}{2}$ of being aligned after the decision. Secondly, any configuration consistent with the critical field requirement may be generated in one cycle from the configuration with all spins aligned with the field.

Let us now use method II on a system with $N=6$. From equation (6) there are $\Omega_N = 18$ possible ground states. A
spin aligned with the field will be denoted by 1, anti-aligned spins by 0. Starting with the initial configuration \((1 1 1 1 1 1 1)\) we find that after eleven complete cycles we have once again generated the initial configuration. The ensemble thus far is composed of the eleven configurations

\[
\begin{align*}
(0 & 1 0 1 0 1) \\
(1 & 1 1 1 1 0) \\
(1 & 0 1 0 1 1) \\
(1 & 1 1 1 0 1) \\
(0 & 1 0 1 1 1) \\
(1 & 1 1 0 1 0) \\
(1 & 0 1 1 1 1) \\
(1 & 1 0 1 0 1) \\
(0 & 1 1 1 1 1) \\
(1 & 0 1 0 1 0) \\
(1 & 1 1 1 1 1).
\end{align*}
\]

Carrying the process further amounts to periodically passing through this eleven-element set of configurations. Since \(\mathcal{C}_6=18\), there are seven configurations which are unaccounted for. If we now take one of these missing configurations; for example \((1 1 0 1 1 1)\), as the initial configuration we find that after seven cycles we have generated the set of ensemble elements

\[
\begin{align*}
(0 & 1 1 0 1 1) \\
(1 & 0 1 1 0 1) \\
(1 & 1 0 1 1 0) \\
(1 & 1 1 0 1 1) \\
(0 & 1 1 1 0 1) \\
(1 & 0 1 1 1 0) \\
(1 & 1 0 1 1 1).
\end{align*}
\]

These are all the configurations missing from the first set and form a periodic seven-element set themselves. Therefore, the 18 critical field ground state configu-
rations of an \( N=6 \) spin periodic Ising model separate into two disjoint sets under the action of method II. If any six spin configuration whatsoever is used as the initial configuration, the machine will periodically cycle through one of these two sets. For example, initializing the system to \((1\ 0\ 0\ 1\ 1\ 0)\), which is not allowed under the critical field requirement, becomes \((1\ 1\ 1\ 0\ 1\ 1)\) after one cycle, which is a member of the seven-element set.

The application of method II to higher values of \( N \) leads to further disjoint grouping of configurations. For \( N=7, \ \omega_7=29 \), and it is found that there are three disjoint sets with periods 4, 12, and 13. Similarly the \( \omega_8=47 \) configurations for an eight spin model form three sets with periods 3, 15, and 29. We now prove that for \( N=3k, \ k \) is an integer greater than one, there are at least two disjoint sets, one of which is of period \( N+1 \). The proof will be by construction. Starting with the initial configuration \((1\ 1\ 0\ 1\ 1\ 0\ 1\ 1\ 0)\ldots\) we apply method II and write down the resulting configuration after each cycle. The period is obtained by noting the continual shift to the right of the underscored 1 in each configuration. The elements of this set are the following:
<table>
<thead>
<tr>
<th>Cycle</th>
<th>Element</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(1 1 0 1 1 0 1 1 0 ... 1 1 0 1 1 0)</td>
</tr>
<tr>
<td>1</td>
<td>(1 1 1 0 1 1 0 1 1 ... 0 1 1 0 1 1)</td>
</tr>
<tr>
<td>2</td>
<td>(0 1 1 1 0 1 1 0 1 ... 1 0 1 1 0 1)</td>
</tr>
<tr>
<td>3</td>
<td>(1 0 1 1 1 0 1 1 0 ... 1 1 0 1 1 0)</td>
</tr>
<tr>
<td>4</td>
<td>(1 1 0 1 1 0 1 1 0 ... 0 1 1 0 1 1)</td>
</tr>
<tr>
<td>5</td>
<td>(0 1 1 0 1 1 0 1 1 ... 1 0 1 1 0 1)</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
<tr>
<td>N-3</td>
<td>(1 0 1 1 0 1 1 0 1 ... 1 0 1 1 1 0)</td>
</tr>
<tr>
<td>N-2</td>
<td>(1 1 0 1 1 0 1 1 0 ... 1 1 0 1 1 1)</td>
</tr>
<tr>
<td>N-1</td>
<td>(0 1 1 0 1 1 0 1 1 ... 0 1 1 0 1 1)</td>
</tr>
<tr>
<td>N</td>
<td>(1 0 1 1 0 1 1 0 1 ... 1 0 1 1 0 1)</td>
</tr>
</tbody>
</table>

Similar construction proofs have been carried out for the cases \( N = 3k + 1 \) and \( N = 3k + 2 \). Generating configurations and set periods are displayed below.

<table>
<thead>
<tr>
<th>( N )</th>
<th>Generator</th>
<th>Period</th>
</tr>
</thead>
<tbody>
<tr>
<td>3k</td>
<td>(1 1 0 1 1 0 1 1 0 ... 1 1 0)</td>
<td>( N + 1 )</td>
</tr>
<tr>
<td>3k + 1</td>
<td>(0 1 1 1 0 1 1 0 1 1 ... 0 1 1)</td>
<td>( N + 1 )</td>
</tr>
<tr>
<td>3k + 2</td>
<td>(1 1 0 1 1 0 1 1 0 ... 1 1 0 1 1)</td>
<td>3</td>
</tr>
</tbody>
</table>

Further disjoint grouping has been found for the case \( N = 4k' + 3 \) with generator \((1 1 1 0 1 1 1 0 ... 1 1 1)\) and a period of 4. Thus, for example, the critical field ground states of an \( N=23 \) spin system form at least three disjoint groups, two of which have periods 3 and 4.

An example in two dimensions can be found. Consider a periodic \( N=4\times4 \) model. Using the antiferromagnetic configuration

\[
\begin{pmatrix}
0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0
\end{pmatrix}
\]

as the initial configuration, we proceed row or column-
wise using method II. One cycle takes us to the state with all spins aligned. The next cycle brings us back to the initial configuration, implying a disjoint set of period 2. The three-dimensional analogue for the simple cubic lattice is obvious.

These results show the nonergodicity of method II in a critical field ground state simulation. The ensemble generated is highly dependent on the initialization of the lattice. Such dependence is undesirable in a Monte Carlo calculation.

III.5. Comparison of the Two Methods

Many researchers have used the configuration generated after each individual spin flipping decision as a member of the ensemble rather than choosing configurations after completing each cycle. Since there are $N$ spins in the system there will now be $N$ elements in the ensemble after one cycle, $2N$ elements after the second cycle, etc. This has the effect of multiplying the above mentioned periods by $N$. For large $N$ the $3k$ and $3k+1$ generators would have associated periods of order $N^2$, and the period of the severe $3k+2$ trap would be $3N$. Now $\omega_N \sim (\frac{1 + \sqrt{5}}{2})^N$ for large $N$, and certainly $3N < N^2 < \omega_N$, which shows that this method of selection is also incapable of sampling from all possible states. We use this selection technique in the following comparison.

Using the same random number sequence, both methods
were applied to the $N=98$ one-dimensional nearest neighbor model in the critical field at $T=0$. Seven random initial configurations labelled A, B, ..., G were used. The severe $3k+2$ trap of period 3 was also tested. Two thousand cycles of computation were executed. The results are found in Table 1 for the magnetization per spin. The percentage discrepancy with the exact result from equation (5) is listed for each initial configuration. It is seen that method I gives an error of less than one per cent in all cases, whereas method II yields errors as large as 10% for initial configuration B and 25% when the severe $3k+2$ trap is used. With the exception of initial configuration C, method I is always superior in approximating the exact result. The approach to equilibrium with increasing number of cycles may be monitored by printing out the average value of the magnetization per spin after each cycle. The results of monitoring both methods starting with random initial configuration B is presented in Fig. 3, where the average magnetization per spin is plotted against the number of cycles on a logarithmic scale. It is seen that the fluctuation in the average is substantially reduced with each logarithmic decade. Method II converges quite rapidly; this convergence however is to an incorrect value. The reason for the larger fluctuations in method I is that this method is selecting from a larger sample space. The exact value is indicated by the horizontal line.
<table>
<thead>
<tr>
<th>Initial Random Configuration</th>
<th>Method I</th>
<th>Method II</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\langle M/N \rangle$</td>
<td>Discrepency</td>
</tr>
<tr>
<td>A</td>
<td>0.4486</td>
<td>0.31%</td>
</tr>
<tr>
<td>B</td>
<td>0.4464</td>
<td>0.18</td>
</tr>
<tr>
<td>C</td>
<td>0.4502</td>
<td>0.67</td>
</tr>
<tr>
<td>D</td>
<td>0.4457</td>
<td>0.34</td>
</tr>
<tr>
<td>E</td>
<td>0.4453</td>
<td>0.42</td>
</tr>
<tr>
<td>F</td>
<td>0.4469</td>
<td>0.07</td>
</tr>
<tr>
<td>G</td>
<td>0.4450</td>
<td>0.49</td>
</tr>
<tr>
<td>3k+2 trap</td>
<td>0.4470</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table 1. Monte Carlo results for magnetization per spin of the 98 spin one-dimensional Ising model in the critical field at absolute zero using the two methods of spin flipping. Two thousand cycles of computation were used. The exact result is $\langle M/N \rangle = 0.4472...$. 
Figure 3. Convergence of the two Monte Carlo methods -
The average magnetization per spin is plotted
against the number of cycles for a 98 spin
system in the critical magnetic field at
absolute zero. The abscissa is on a logarithmic
scale.
At zero temperature the disjoint sets are completely isolated from each other in configuration space. With method II there is no way for the computer, once started within a set, to escape from that set. At nonzero temperatures, thermal agitation is introduced and it becomes possible to make a transition to a state of higher energy. The probability of this event, using method II, is found from $S_{II}$. This probability is

$$P_{\alpha'\alpha} = e^{-\beta(E_{\alpha} - E_{\alpha'})}, \quad E_{\alpha} > E_{\alpha'}.$$  

For low temperatures ($\beta$ large) this is a very small probability which means that, on the average, a very large number of cycles is needed to escape the trap. This finite probability means that for nonzero temperatures there are corridors in configuration space which connect the disjoint sets. The higher the temperature, the wider the corridors become and escaping from a trap becomes more probable. It is interesting to examine the escape process from a given trap. To this end we present the magnetization per spin vs. reduced temperature $kT/|J|$ using method II in Fig. 4. Again two thousand cycles were executed for each input temperature. The severe $3k+2$ trap was initialized here in order to monitor the escape process as clearly as possible. From the graph we see that persistence of trapping holds up to $kT/|J| \sim 1$, after which the escape is realized and agreement with the exact result is achieved. The data
Figure 4. Magnetization per spin vs. $kT/|J|$ -

The exact result is shown with a solid line. The data points are the result of a simulation using method II. The results using method I coincide with the exact solution and are not plotted.
from method I are not plotted as they coincide with the exact solution for all temperatures.

III.6. Unreliable Areas of Study Using Method II

From the considerations of this chapter we conclude that a simulation, using method II, of the low temperature critical field behavior of the nearest neighbor Ising model cannot be trusted. It is precisely in this region where Shirley\textsuperscript{28,32}, using method I, observed the double transition phenomenon in the body centered cubic lattice. The Bethe-Peierls approximation indicates that such a double transition will occur for loose-packed lattices of coordination number greater than five\textsuperscript{33}. Monte Carlo simulations developed to check this should then incorporate method I.

It has been shown that a one-dimensional chain with both nearest and next-nearest neighbor interactions in zero field will exhibit a thermodynamic behavior identical with the nearest neighbor chain in a magnetic field\textsuperscript{34}. We would expect that an i-mate degeneracy similar to that of the critical field nearest neighbor model would occur for the zero field model with nearest and next nearest neighbor interactions $J$ and $J'$ in the ratio

$$\frac{J'}{J} = \frac{1}{2}.$$ 

In general, the nonergodic behavior of method II will occur under conditions which yield a high proliferation of
degenerate states. This is characteristic of order-order transitions, the low temperature behavior of which could not accurately be examined using method II. A very large degeneracy of equilibrium states is also encountered in the infinite temperature limit (β → 0). The number of available states is 2ᴺ, that is, every state is equally probable. It has been pointed out by Yang⁹ that using method II with any initial configuration will generate a two element set, namely, the initial configuration and the configuration obtained from it by reversing all spins. Again, method I is not burdened with this difficulty.
CHAPTER IV
THE NEAREST NEIGHBOR TRIANGULAR ANTIFERROMAGNET

IV.1. The Triangular Lattice

The two dimensional triangular lattice possesses a close-packed topology. This is in distinction to the loose-packed topology (e.g. square, honeycomb, simple cubic, body centered cubic) where the lattice can be decomposed into two equivalent sublattices, $\alpha$ and $\beta$, such that each lattice site on the $\alpha$ sublattice has its nearest neighbors on the $\beta$ sublattice and vice versa. Other close-packed topologies are found in the face centered cubic and hexagonal close-packed lattices. The triangular lattice can be decomposed into three equivalent triangular sublattices, labelled 1, 2 and 3, as seen in Fig. 5(a). It will be noticed that in this decomposition the $d = 6$ nearest neighbors of a site on one of the sublattices are located symmetrically on the other two sublattices. Furthermore, the six next nearest neighbors of a site on a sublattice are found to be on the same sublattice as the site itself. The triangular lattice may be topologically deformed to a square lattice with one diagonal bond as seen in Fig. 5(b). Two diagonal bonds would result in the
Figure 5. Topology of the Triangular Lattice

(a) Decomposition of the triangular lattice into three equivalent triangular sublattices; 1, 2, and 3.

(b) Topological equivalence of the triangular lattice to the square lattice with a diagonal bond.
so-called "union jack" lattice. Application of such diagonal bonding to the square lattice changes the topology from loose to close-packed.

Due to the close-packed topology, a perfectly regular antiferromagnetic spin arrangement cannot be fitted onto the triangular lattice. To obtain the ground state energy we argue as follows. For an N spin system there are 2N triangles in the deformed lattice of Fig. 5(b). With $J<0$ the best we can achieve energetically within any triangle is to have two spins of the same sign and one spin with the opposite sign. The energy of such a triangle is then equal to $-J(S_i S_j + S_j S_k + S_k S_i) = J$. Summing over all triangles gives a value of $2NJ$. This however must be divided by 2 since each spin-spin bond is a common side of two triangles. Thus the antiferromagnetic ground state energy is bounded below by

$$E(0) = NJ.$$ 

This energy is one-third of the ferromagnetic ground state energy. The realization of this antiferromagnetic ground state energy is not unique. In fact, there are so many configurations with this energy that the antiferromagnetic triangular lattice has a nonzero ground state entropy. The value of this entropy is given in the next section. This high degeneracy prohibits the occurrence of any long-range order at low temperatures and is responsible for the absence of the Neél point in zero magnetic field.
IV.2. Exact Solution in Zero Field

The antiferromagnetic partition function is exactly the same as the ferromagnetic partition function for Ising models with loose packed topology. Thus, the thermodynamic behavior of the loose-packed Ising lattice is invariant under a change in sign of $J$. A close-packed topology completely destroys this equivalence. Indeed, the ferromagnetic Curie temperature of the triangular lattice is given by

$$\frac{kT_c}{J} = 3.6406...,$$

at which temperature the specific heat blows up logarithmically, but the antiferromagnetic specific heat displays no singularity for any temperature. Conjectures have been made that the antiferromagnetic Néel temperature is zero\textsuperscript{17,18}. These conjectures are based on the possibility that the zero-field magnetic susceptibility is infinite at zero temperature.

Due to numerous mathematical errors and misprints in the literature on the triangular lattice\textsuperscript{*} we present here the correct expressions for the internal energy and specific heat. Using the notation of Domb we define

\footnote{There is a misprint in Houtappel's expression for $\xi_1$ for the antiferromagnetic case. Wannier's elliptic integral transformation is in error. Domb's expression of the internal energy has a sign error in the second term and an elliptic integral derivative is incorrect in the specific heat.}
\[ Z = e^{\frac{2|J|}{kT}} \]
\[ \varepsilon_1 = \frac{2(3z^2 - 1)^2}{(z^2 + 1)^2(z^2 - 1)} \]
\[ \kappa = \frac{(1 + 3z^2)^{\frac{3}{2}}(1 - z^2)^{\frac{3}{2}}}{(1 - 3z^2)^{\frac{3}{2}}(1 + z^2)^{\frac{3}{2}}}. \]

The internal energy per spin is then given by
\[ \frac{E}{N} = - J \left[ \coth \left( \frac{2J}{kT} \right) + \frac{2}{\pi} \varepsilon_1 \mathcal{K}(\kappa) \right], \tag{7} \]
where \( \mathcal{K}(\kappa) \) is the complete elliptic integral of the first kind,
\[ \mathcal{K}(\kappa) = \int_0^{\frac{\pi}{2}} \frac{d\psi}{\sqrt{1 - \kappa^2 \sin^2 \psi}}. \]

Taking the temperature derivative of equation (7) and using the identity
\[ \int_0^{\frac{\pi}{2}} \frac{d\psi}{(1 - \kappa^2 \sin^2 \psi)^{\frac{3}{2}}} = \frac{\mathcal{E}(\kappa)}{(1 - \kappa^2)^{\frac{3}{2}}}, \]
where \( \mathcal{E}(\kappa) \) is the complete elliptic integral of the second kind,
\[ \mathcal{E}(\kappa) = \int_0^{\frac{\pi}{2}} \sqrt{1 - \kappa^2 \sin^2 \psi} \, d\psi, \]
we arrive at the expression for the antiferromagnetic specific heat
\[ \frac{C}{Nk} = -2 \left( \frac{J}{kT} \right)^2 \left[ \csc^2 \left( \frac{2J}{kT} \right) + \frac{2z}{\pi} \left( \frac{d\varepsilon_4}{dz} - \frac{\varepsilon_4}{\kappa} \frac{d\kappa}{dz} \right) \mathcal{K}(\kappa) \right. \]
\[ \left. + \frac{2z \varepsilon_4}{\pi \kappa (1 - k^2)} \frac{d\kappa}{dz} \mathcal{E}(\kappa) \right]. \tag{8} \]
The derivatives appearing here are correctly given by
\[
\frac{d\varepsilon_i}{dz} = -\frac{8z}{\varepsilon_i} \frac{(3z^4+1)}{(z^2+1)^2(z^2-1)^3},
\]
and
\[
\frac{d\kappa}{dz} = 48z^5 \left(1-z^2\right)^2 \left(1-3z^2\right)^2 \left(1+z^2\right)^4.
\]
The function in equation (8) is nonsingular in $T$ and approaches zero as $T$ tends to zero. The entropy in this limit is, however, nonzero and has been derived by Wannier\textsuperscript{17}. Its value is given by
\[
\frac{S(0)}{Nk} = \frac{3}{\pi} \int_0^\pi \frac{1}{\pi} (2\cos \psi) d\psi = 0.32306 \ldots \tag{9}
\]

IV.3. Approximation Methods in Nonzero Field

From the results of the previous sections we see that the triangular system, in zero field, is disordered at all temperatures. The application of a nonzero magnetic field can, and in fact does, allow a regular spin ordering. The close-packed topology of the lattice makes antiferromagnetic series expansion approximations very difficult. It has been pointed out by Burley\textsuperscript{35,36} that to differentiate between loose-packed and close-packed lattices (e.g. for $\gamma = 6$ we have the simple cubic and triangular lattices respectively) an approximation better than that of Bethe and Peierls must be used. The method of Kikuchi\textsuperscript{37} gives us an approximation which will accomplish this distinction. Burley has applied this method to the triangular Ising lattice\textsuperscript{19} and to the planar lattice gas with rigid
The Kikuchi method assigns unknown probabilities to the occurrence of single spin states on each of the three sublattices, to pairs of spin states occurring between two spins on different sublattices, and to triplets of spin states with one spin on each sublattice. Consistency conditions among these probabilities are then written down. Then the internal energy, whereby enters the magnetic field parameter, and entropy are expressed in terms of these probabilities. The temperature parameter enters the calculation through the Helmholtz free energy \( F = \langle E \rangle - TS \). Minimization of the free energy is carried out using a Lagrange multiplier with the independent consistency conditions. These manipulations then lead to the immense problem of the simultaneous solution of twenty-seven nonlinear equations! In order to make progress, Burley forces the distribution of spins on two of the sublattices to be equal. This is done by equating appropriate probabilities and the resulting solution is called the partially ordered solution. The disordered solution is computed by making the spin distribution on all three sublattices equal. Where the partially ordered solution equals the disordered solution defines the phase boundary and gives the temperature and magnetic field coordinates of the critical curve. The thermodynamic functions can be evaluated using the appropriate partial derivatives and using the stable solutions which give the
minimum in the free energy. Burley's results will be compared with the Monte Carlo calculation in section IV.5.

**IV.4. Application of the Monte Carlo Method to the Problem**

A Monte Carlo program was developed for the triangular lattice with periodic boundary conditions using method I for the spin flipping decision. Two lattices of different size were used in the calculation. The smaller lattice had \( N = 2601 \) sites and required \( 1.08 \times 10^{-2} \) sec/cycle of computer time. This size was used away from the transition region. The larger lattice had \( N = 9801 \) requiring \( 3.9 \times 10^{-2} \) sec/cycle and was used at and near the phase transition in order to improve the results. 2050 cycles were used to generate the ensemble, the first 50 being deleted from the averaging. The Monte Carlo results for internal energy and specific heat were compared with the exact zero field results of section IV.2. and are displayed in Fig. 6. Good agreement is seen for the case of zero field.

The lattice was initialized to a random configuration and a nonzero magnetic field parameter was used as input. The program scanned a low temperature range and the last few configurations of the ensemble generated for each temperature were printed out in order to observe the presence of any spin ordering. These configurations should be typical of equilibrium at the input temperature. Ordering was observed at low temperatures. The pattern of
Figure 6. Comparison of Monte Carlo Data with Exact Result for Zero Magnetic Field -

(a) Internal Energy

(b) Specific Heat

The solid curve is the exact solution, data points are Monte Carlo results.
order is described by all of the spins on two of the sub-lattices being aligned with the magnetic field, while all of the spins of the remaining sublattice are antiparallel to the field. Precisely this magnetic spin arrangement was suggested by Domb\textsuperscript{20} to be the type of order, if any ordering occurred, for the triangular lattice in a field. This order persisted for low temperatures in the range of magnetic fields \(0 < B < B_c = 6|J|\). We refer to this as an antiferromagnetically ordered state. For \(B > B_c\) all spins are aligned with the field in the ground state.

In order to detect the phase transition we use three order parameters which were introduced by Campbell and Schick\textsuperscript{23}. Letting \(\langle \sigma_i \rangle\) denote the spin expectation value for sublattice \(i, i = 1, 2, 3\), the order parameters are defined as

\[
\xi_i = \frac{1}{2} (\langle \sigma_2 \rangle - \langle \sigma_3 \rangle)
\]

with \(\xi_2\) and \(\xi_3\) given by cyclic permutation of the indices. In the perfectly ordered antiferromagnetic state two of these order parameters are opposite in sign and have unit magnitude and the remaining order parameter vanishes. We define \(\xi^*\) to be equal to the magnitude of the nonvanishing order parameters. In general, as the ordering weakens, two of the order parameters remain opposite in sign and equal in magnitude which decreases with decreasing degree of order. The third order parameter remains zero. In a state of disorder we have
\[ \langle \sigma_1 \rangle = \langle \sigma_2 \rangle = \langle \sigma_3 \rangle \]

so that all order parameters vanish. Note that the vanishing of all three order parameters could also indicate a state with all spins aligned. This is checked by examining configuration print outs.

The order-disorder phase transition is also signaled by a spike in the specific heat at constant field. This is quite a pronounced peak in the intermediate and strong magnetic fields, but is rather poor in quality for the weak fields. Another method of locating the transition temperature is by the use of the "staggered" susceptibility. Previously this function was used in conjunction with the Padé approximants for loose-packed lattices only\(^3^9\). We now modify the definition for use on the close-packed triangular lattice. In a partially ordered state two of the triangular sublattices possess a majority of field aligned spins. Let the union of these two sublattices be called the \(\alpha\) sublattice and let the remaining sublattice, with a majority of spins oriented antiparallel to the field, be called the \(\beta\) sublattice. If now the magnetic field is "staggered" with \(B_\alpha\) and \(B_\beta\) being the fields on the \(\alpha\) and \(\beta\) sublattices respectively, we define

\[ h = \frac{1}{2}(B_\alpha - B_\beta), \]

and

\[ B = \frac{1}{2}(B_\alpha + B_\beta). \]

The "staggered" susceptibility is defined as
Writing the Hamiltonian of equation (1) as
\[ E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - m B_\alpha \sum_{\lambda \in \alpha} \sigma_\lambda - m B_\beta \sum_{\lambda \in \beta} \sigma_\lambda, \]
and using equation (2) for the free energy it is trivial to show that \( \mathcal{X}_s \) satisfies the relation
\[ \frac{kT \mathcal{X}_s}{Nm^2} = \frac{1}{N} \text{variance} \left( \sum_{\lambda \in \beta} \sigma_\lambda - \sum_{\lambda \in \alpha} \sigma_\lambda \right). \]

This expression is adaptable to the Monte Carlo calculation. The computer searches to find, for each microstate, the two sublattices with the largest magnetizations and thereby defines the \( \alpha \) sublattice. If there is ambiguity in the choice (e.g., two sublattices are equally magnetized) a predetermined definition is made.

The results of the Monte Carlo calculation are presented graphically in the following figures. In Figs. (7-10) are displayed respectively the behavior with reduced temperature \( kT/|J| \) of the antiferromagnetic order parameter \( \mathcal{F} \), the specific heat at constant magnetic field, the reduced "staggered" susceptibility, and the ordinary magnetic susceptibility. Each curve is at a constant magnetic field specified by the dimensionless reduced parameter \( B^* = B/B_c(T=0) \). In each figure the open circles represent data taken from the \( N=2601 \) lattice size and the closed circles are with \( N=9801 \). In Fig. 11 is shown the
Figure 7. Antiferromagnetic Order Parameter $\xi$ vs. $kT/|J|$ for Various Reduced Magnetic Fields $B^\ast$. 
Figure 8. Specific Heat at Constant Field $B^*$ vs. $kT/|J|$
Figure 9. Reduced "Staggered" Susceptibility vs. $kT/|J|$ for Various Values of $B^*$
Figure 10. Ordinary Magnetic Susceptibility per Spin vs. $kT/|J|$ for Various Values of $B^*$
Figure 11. Specific Heat Isotherm at $kT/|J| = 1.075$. The peak separation widens with decreasing temperature.
\frac{kT}{1|J|} = 1.075
isothermal behavior of the specific heat at $kT/|J| = 1.075$. The double peaks indicate disorder-antiferromagnetic order and antiferromagnetic-paramagnetic order transitions with increasing field. The peak separation widens with decreasing temperature. Fig. 12 shows the isotherms of (a) the magnetization per spin and (b) the antiferromagnetic order parameter. Both of these attain a plateau in the antiferromagnetically ordered region. The plateau width increases with decreasing temperature. The plateau level of the magnetization is at one-third which corresponds to the antiferromagnetically ordered state. The plateau level of the order parameter increases with decreasing $T$.

It is customary in the presentation of phase diagrams to normalize the temperature and magnetic field variables to dimensionless parameters. The temperature is usually normalized to the critical temperature at zero field. Since there is no zero field critical temperature for the triangular antiferromagnet and since we wish to compare with the Kikuchi approximation, we therefore normalize to $T_0(B^*=0) = 0.9858$, which is the critical temperature found by Burley. The Kikuchi and Bethe approximations both give an incorrect nonzero critical temperature in the absence of a field. The resulting dimensionless temperature parameter is called $T^*$. The uncertainty in the data points is taken to be the temperature increment used in the $N=9801$ computation; this was $\Delta(kT/|J|) = 0.05$. The phase
Figure 12. Isothermal Ordering

(a) Isothermal Magnetization per Spin at $kT/|J| = 1.075$.

(b) Antiferromagnetic Order Parameter Isotherm at $kT/|J| = 1.075$.

The plateau region widens with decreasing temperature in both (a) and (b).
\[ \frac{kT}{|J|} = 1.075 \]

(a) \[ \langle M \rangle N \]

(b) \[ \mu_0 \]

\[ B^* \]
diagram of the triangular antiferromagnet is presented in Fig. 13. The dashed curve is the result of Burley's calculation.

**IV.5. Discussion of Results**

The results of the previous section clearly show that the antiferromagnetic triangular system orders at low temperature in the presence of an external magnetic field. For a given field strength, the order parameter $F$ of Fig. 7 is unity at very low temperatures indicating perfect antiferromagnetic ordering. As the temperature is increased $F$ decreases continuously to zero. This continuous behavior of $F$ is not surprising since we are dealing with a finite system. For an infinite system a continuous variation of $F$ means that the phase transition is of second order. The reader may now ask whether one can infer the order of the transition for the infinite lattice from the data of the finite lattice. We suggest that this is possible and that the transition is of second order. Our reasoning for this is that for small lattices ($N=441, 900$ and $2025$) the steepness of the drop in $F$ was found to increase with increasing $N$. This steepness increase stabilized and terminated at $N=2601$ where it was found that no appreciable change in the $F$ data occurred when $N$ was further increased up to a maximum of $9801$ sites. Since $F$ is a first moment quantity the data should be quite accu-
Figure 13. Phase Diagram of the Nearest Neighbor Triangular Ising Antiferromagnet

Data points are Monte Carlo results. A solid curve is freely drawn through these points. Broken line is from Burley's Kikuchi approximation.
rate in representing the infinite system. We conclude that $\mathcal{F}$ vanishes continuously across the transition for the infinite system. The transition is apparently more diffuse in the weaker magnetic fields because the drop in $\mathcal{F}$ is spread out over a larger temperature range in this case as compared to the stronger field.

The phase transition is accompanied by a strong peak in the specific heat at constant field at the critical temperature $T_c$. This is indicative of a singularity at $T_c$ for the infinite system, probably of a logarithmic nature. In Burley's calculation the specific heat monotonically increases as the temperature approaches $T_c$ from below and displays a discontinuity (i.e. a vertical drop) at $T_c$. This discontinuity is even present in zero field which is at variance with the exact result and the Monte Carlo data (see Fig. 6(b)). The Kikuchi method clearly fails here.

The location of the maximum in the specific heat in weak fields was difficult owing to the poor quality of the data. For these weak fields we relied upon the behavior of the "staggered" susceptibility.

The modification of the definition of the "staggered" susceptibility to the triangular lattice worked very well in locating $T_c$ for all field strengths. From Fig. 9 we see that it is quite singular at $T_c$. At $T_c$ it must be true that the difference in $\alpha$ and $\beta$ sublattice magnetizations fluctuates wildly as indicated by equation (10). The
definition could easily be modified for the investigation of the close-packed face centered cubic lattice in which there occurs a four-sublattice decomposition.

The area enclosed by the critical curve and $B^*$ axis of Fig. 13 is the antiferromagnetically ordered region. The magnetization per spin in this region remains close to one-third in agreement with Burley's calculation. The derivative of the magnetization with respect to the field gives the magnetic susceptibility. The behavior of this susceptibility along the singular line of Fig. 13 depends on the strength of the field (see Fig. 10). For strong fields, $B^* \lesssim 1$, $\chi/N$ appears to be singular at the phase boundary. This means that a small variation in $B^*$ at $T_0$ produces a large change in $\langle M \rangle/N$. This change is essentially between the antiferromagnetic state ($\langle M \rangle/N \sim 1/3$) and the state with most spins aligned ($\langle M \rangle/N \sim 1$). We would then expect the system to be highly susceptible to magnetization for these values of $B^*$. For intermediate fields, $B^* \sim 0.5$, the critical temperatures are the highest. The antiferromagnetic ordering near the phase boundary is rather weak in this case. Consequently changing $B^*$ slightly varies the magnetization between a weakly ordered state and a state of disorder. $\langle M \rangle/N$ therefore does not change appreciably with $B^*$ giving a nonsingular $\chi/N$. For weak fields, a variation of $B^*$ at $T_0$ changes $\langle M \rangle/N$ between states of strong antiferromagnetic order and disorder.
Fig. 10 shows that the maximum value of $\chi/N$ increases with decreasing field. Recently, Sykes and co-workers have examined the behavior of $\chi/N$ by taking the zero temperature limit of high-temperature series expansions for $\chi$. Their expansion parameter is the usual $v = \tanh J/kT$. Such limiting requires an infinite radius of convergence of the series and many terms. They conclude that the zero field susceptibility is infinite as did Wannier by heuristic argument. Sykes et al. give the following bounds for the reduced susceptibility in zero field

$$0.141 < \frac{kT\chi}{Nm^2} < 0.150$$

They state that the upper limit is very uncertain and that many more terms in the expansion would be required to improve it. From the Monte Carlo results we have obtained

$$\frac{kT\chi}{Nm^2} = 0.1670$$

which is beyond their upper bound. This points to a $1/T$ dependence in the low temperature zero field susceptibility. The nonzero magnetic field data are quite consistent with the infinite $\chi(T=0,B^*=0)$ conjectures if it is assumed that the low temperature side of the maximum in $\chi/N$ becomes vertical as $B^* \to 0$. Burley's result gives a discontinuity in $\chi/N$ at $T_c$ for nonzero fields and an incorrect discontinuity in the gradient of $\chi/N$ at $T^*=1$ for $B^*=0$. The latter result again shows the failure of the Kikuchi method.

Exactly at the critical field, $B^*=1$, the average mag-
netization per spin approaches the value $<M>/N = 0.6751$ as $T \to 0$. Its graph is very similar to that of the one-dimensional model shown in Fig. 4. The critical field behavior of the triangular antiferromagnet along with many other lattices will be analysed in Chapter Six.

The phase diagram of Fig. 13 is in good agreement with Burley's calculation in the upper portion of the $B^* - T^*$ plane. The Monte Carlo result turns back to the origin for low $B^*$ in agreement with the conjectures of Domb$^{20}$ and Temperley$^{21}$. Burley's curve terminates at a nonzero temperature for $B^* = 0$. This indicates a failure of the Kikuohi approximation in nonzero weak fields as well as for zero field.

A summary of the Monte Carlo analysis of the triangular antiferromagnet is presented in Table 2.
Table 2. Summary of Thermodynamic Behavior of Nearest Neighbor Triangular Antiferromagnet in a Magnetic Field.

<table>
<thead>
<tr>
<th>Aspect</th>
<th>Magnetic Field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ground State</td>
<td>( B^* = 0 )</td>
<td>Highly degenerate and disordered</td>
</tr>
<tr>
<td></td>
<td>( 0 &lt; B^* &lt; 1 )</td>
<td>Nondegenerate. Ordered with the spins of two sublattices aligned with the field, one sublattice with spins antiparallel to field.</td>
</tr>
<tr>
<td></td>
<td>( B^* = 1 )</td>
<td>Degenerate with restriction. (See Chapter Six)</td>
</tr>
<tr>
<td></td>
<td>( B^* &gt; 1 )</td>
<td>Nondegenerate. All spins aligned with field.</td>
</tr>
<tr>
<td>Ordering at Nonzero Temperatures</td>
<td>( B^* = 0 )</td>
<td>None</td>
</tr>
<tr>
<td></td>
<td>( 0 &lt; B^* &lt; 1 )</td>
<td>Antiferromagnetic ordering below ( T_c(B) )</td>
</tr>
<tr>
<td>( \mathcal{F} )</td>
<td>( 0 &lt; B^* &lt; 1 )</td>
<td>Vanishes continuously at ( T_c(B) ) implying second-order phase transition. Isothermal plateau widens and increases in level with decreasing ( T ).</td>
</tr>
<tr>
<td>( C/Nk )</td>
<td>( B^* = 0 )</td>
<td>Nonsingular</td>
</tr>
<tr>
<td></td>
<td>( 0 &lt; B^* &lt; 1 )</td>
<td>Singular at ( T_c(B) )</td>
</tr>
<tr>
<td></td>
<td>( B^* &gt; 1 )</td>
<td>Nonsingular</td>
</tr>
<tr>
<td>( \langle M \rangle/N )</td>
<td>( B^* = 0 )</td>
<td>Zero</td>
</tr>
<tr>
<td></td>
<td>( 0 &lt; B^* &lt; 1 )</td>
<td>~1/3 below ( T_c(B) ). Isothermal plateau level ~1/3. Level widens with decreasing ( T ).</td>
</tr>
<tr>
<td></td>
<td>( B^* = 1 )</td>
<td>( = 0.6751 ) as ( T \to 0 )</td>
</tr>
<tr>
<td>( \chi_{\text{staggered}} )</td>
<td>( 0 &lt; B^* &lt; 1 )</td>
<td>Very singular at ( T_c(B) )</td>
</tr>
</tbody>
</table>
Table 2 continued

<table>
<thead>
<tr>
<th>Aspect</th>
<th>Magnetic Field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi = \frac{\partial \langle m \rangle}{\partial B}$</td>
<td>$B^* = 0$</td>
<td>Probably singular at $T = 0$.</td>
</tr>
<tr>
<td></td>
<td>$B^* \geq 0$</td>
<td>Maximum increases and shifts to lower temperatures with decreasing $B^*$.</td>
</tr>
<tr>
<td></td>
<td>$B^* \sim \frac{1}{2}$</td>
<td>Nonsingular</td>
</tr>
<tr>
<td></td>
<td>$B^* \approx 1$</td>
<td>Singular</td>
</tr>
<tr>
<td>$T_c(B^*)$ (Phase Diagram)</td>
<td>$B^* = 0$</td>
<td>$= 0$</td>
</tr>
<tr>
<td></td>
<td>$0 &lt; B^* &lt; \frac{1}{2}$</td>
<td>Increases monotonically with increasing $B^*$.</td>
</tr>
<tr>
<td></td>
<td>$\frac{1}{2} &lt; B^* &lt; 1$</td>
<td>Decreases monotonically with increasing $B^*$.</td>
</tr>
</tbody>
</table>
CHAPTER V

TRIANGULAR ISING MODEL WITH THE NEAREST AND NEXT NEAREST NEIGHBOR INTERACTIONS

V.1. The Ground State

With both the nearest neighbors (nn) and next nearest neighbors (nnn) interacting with energies $J$ and $J'$ respectively, we write the Ising Hamiltonian as

$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J' \sum_{\langle k,l \rangle} \sigma_k \sigma_l - B \sum_{k=1}^{N} \sigma_k,$$ (11)

the first sum is over all nn pairs and the second is over all nnn pairs. We define the dimensionless nnn to nn interaction energy ratio as

$$\alpha = \frac{J'}{J}.$$

The B=0 ground state of the square lattice was analytically investigated by Fan and Wu\textsuperscript{40} and by Domb and Potts\textsuperscript{41}. Their findings show three possible ground states depending on the size and sign of $\alpha$. Horiguchi and Morita\textsuperscript{42} looked at the square lattice spin orderings in the presence of a magnetic field. They suggest that there are four possible ordered ground states occurring for various $\alpha$ and $B$. These four states are called ferromagnetic, antiferromagnetic, superantiferromagnetic and field dependent and are displayed below.
The superantiferromagnetic state bears this name because in this arrangement there occurs two "super" lattices (i.e. the two sublattices) which individually take on the antiferromagnetic configuration. The field dependent ground state can exist only in the presence of a magnetic field.

A Monte Carlo program for the nn and nnn square lattice was run at low temperatures and the final configuration print outs were examined. We found that the B=0 spin arrangements generated by the machine were exactly those predicted by Fan and Wu for various $\alpha$. The machine-generated $B\neq0$ spin arrangements were in excellent agreement with the ground states suggested by Horiguchi and Morita. These calculations were performed with spin flipping method I of Chapter Three and there was no trapping effect observed. Landau, using method II, found the same. However, a similar study of the one-dimensional chain yielded all of the four ground states found analytically by Morita and Horiguchi plus one spurious state resulting from a low temperature trap. This shows that the Monte
The Carlo method is certainly capable of finding the true ground states but that the possibility of trapping must seriously be kept in mind.

Motivation for the study of the triangular lattice is found in adsorption experiments of gases upon surfaces of graphite \(^{22-24,47}\). Assuming that the gas atoms reside at the centers of graphite hexagons, we have a triangular lattice for occupancy of the adatoms. The appropriate theoretical model is then a two-dimensional triangular lattice gas. Ordered structures have been observed by low energy electron diffraction and neutron scattering experiments. As the grand canonical lattice gas partition function has the same form as the canonical Ising partition function, the two models are mathematically related. This relation is presently only formal because the chemical potential of the lattice gas depends on the temperature. A density regulation is impossible without the knowledge of the form of the chemical potential. A study of the triangular Ising ground states represents a starting point for an investigation of the corresponding lattice gas model.

V.2. Detecting the Ground State Configuration

A Monte Carlo program with a lattice size of \(N=2916\) was developed for the study of the nn and nnn triangular model. The interaction ratio \(\alpha\) was fixed to a certain value and the field parameter \(B\) was varied over a wide range of values. Then \(\alpha\) was adjusted to a new value and
the procedure repeated. It was seen from the configuration print outs that the low temperature spin arrangements were periodic and that the repeating unit was no larger than 3x3. These repeating units can be visualized as rectangular by using the deformed topology of Fig. 5(b) to represent the triangular lattice. Various initial configurations were used to see if trapping could be provoked. The final configurations were invariant when several random initial configurations were chosen. Trapping however did take place when an ordered nonequilibrium state was initialized. This happened because the initial state was such that any single spin flip would raise the energy of the system. In this case the true ground state could only be reached via intermediate states of higher energy than the initial state. To overcome this difficulty a method of multiple spin flips would have to be used.

The Monte Carlo results indicate a relatively small repeating unit. To further test against the possibility of trapping, an energy minimization with respect to repeating unit configurations was performed. For this purpose it is convenient to rewrite the energy of equation (11). For a particular configuration we define

\[ N_+ = \text{number of upspins} \]
\[ N_- = \text{number of downspins} \]
The $i^{th}$ nearest neighbor coordination number, $i=1,2$.

$N_{++}^{(1)}$ = number of $(++)$ interactions between $i^{th}$ nearest neighbors.

$N_{--}^{(1)}$ = number of $(-,-)$ interactions between $i^{th}$ nearest neighbors.

$N_{+-}^{(1)}$ = number of $(+-)$ or $(-+)$ interactions between $i^{th}$ nearest neighbors.

For the triangular lattice is equal to 6 for $i=1,2$. The first two sums appearing in the energy expression may then be written as

$$\sum_{\langle k,\ell \rangle} \sigma_k \sigma_{\ell} = N_{++}^{(i)} + N_{--}^{(i)} - N_{+-}^{(i)} \quad i=1,2$$

and the third sum as

$$\sum_{k=1}^{N} \sigma_k = N_+ - N_- .$$

For any configuration the following relations hold,

$$N = N_+ + N_-$$

$$\partial_i N_+ = 2N_{++}^{(i)} + N_{+-}^{(i)} \quad i=1,2$$

$$\partial_i N_- = 2N_{--}^{(i)} + N_{+-}^{(i)} .$$

Combining these equations we then have

$$\sum_{\langle k,\ell \rangle} \sigma_k \sigma_{\ell} = \frac{1}{2} \partial_i N - 2N_{+-}^{(i)} \quad i=1,2$$

and

$$\sum_{k=1}^{N} \sigma_k = 2N_+ - N .$$

Thus the energy of any configuration may be written in terms of only $N_+$, $N_{++}^{(1)}$, and $N_{+-}^{(1)}$ as follows

$$E = -J\left(\frac{1}{2} \partial_i N - 2N_{+-}^{(1)}\right) - J'\left(\frac{1}{2} \partial_i N - 2N_{++}^{(1)}\right) - B(2N_+ - N) \quad (13)$$
Using a 2x3 repeating unit as an example we now show how to express the energy per spin (E/N) of the infinite lattice in a periodic state. The 2x3 repeating unit is shown in the sketch on the right.

There are N/6 such units in an N site lattice. We let L(j) = 1 or 0 according to the jth spin of the unit being "up" or "down", j = 1, ... 6. The desired ratios are given by

\[
\left( \frac{N^+}{N} \right)_{N \to \infty} = \frac{1}{6} \sum_{j=1}^{6} L(j)
\]

\[
\left( \frac{N^{(j)}}{N} \right)_{N \to \infty} = \frac{1}{6} \sum_{j=1}^{6} (1 - L(j)) \sum' (i^{th} \text{ neighbors of } L(j))_{i=1,2}
\]

The summation \( \sum' \) is consistent with the arrangement of the unit on the lattice (e.g. for j=4, \( \sum' \) sums \( L(1) + L(2) + 2L(3) + L(5) + L(6) \)).

The repeating units examined were of sizes 1x1, 2x1, 2x2, 3x1, 3x2, 3x3, 4x1, 4x2, and 4x3. For a unit of size \( m \times n \) there are \( 2^{mn} \) possible spin states. The first step in the energy minimization process is to generate all the states. This is easily done on the computer using a sequence of nested DO loops. Following this a series of logical comparisons is performed in order to sort the states into groups, each group containing states which have the same values of \( (N_+ / N) \), \( (N^{(1)}_+ / N) \) and \( (N^{(2)}_+ / N) \). A reference index number is assigned to each such group. After this classification we are ready to scan the para-
meters $J$, $J'$ and $B$ to find the associated ground states. We can reduce this to a two parameter problem by dividing out the magnetic field parameter. The remaining problem is then to search over the $(J/B, J'/B)$ plane. Without loss of generality we assume that $B>0$. Plane polar coordinates were chosen for the scan of the plane. These coordinates $(r, \Theta)$ are shown in the sketch on the right and we have

$$\tan \Theta = \alpha,$$

$$\gamma = \sqrt{1 + \alpha^2} |\frac{J}{B}|.$$ 

With $\Theta$ fixed, $r$ was varied from 0 to 2 by increments of 0.01. When $\alpha \to \pm \infty$ (i.e. $J/B = 0$) modification was easy. The state reference index number was printed out for those values of $r$ just before, exactly at and immediately after a change in the ground state configuration. $\Theta$ was varied from $0^\circ$ to $355^\circ$ by increments of $5^\circ$.

**V.3. Results of the Polar $J/B - J'/B$ Plane Scan**

It was found that the $J/B - J'/B$ plane was sectioned into five regions. Each region represents a different ground state phase characterized by the values of $N_+ / N$, $N_+^{(1)} / N$ and $N_+^{(2)} / N$. The values of these ratios for the five phases, I through V, are given in Table 3. Using equation (13) and Table 3 we may write down the energy per spin $E = (E/N)$ for each phase. These are

$$E_I = -3J - 3J' - B$$

$$E_{II} = J - 3J' - 1/3 B$$
Table 3. Characteristic Ratios of the Five Ground State Phases

<table>
<thead>
<tr>
<th>Phase</th>
<th>$N_+/N$</th>
<th>$N_{+-}^{(1)}/N$</th>
<th>$N_{+-}^{(2)}/N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>II</td>
<td>2/3</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>III</td>
<td>3/4</td>
<td>3/2</td>
<td>3/2</td>
</tr>
<tr>
<td>IV</td>
<td>1/2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>V</td>
<td>2/3</td>
<td>4/3</td>
<td>2</td>
</tr>
</tbody>
</table>
\[ \begin{align*}
E_{\text{III}} &= -\frac{1}{2} B \\
E_{\text{IV}} &= J + J' \\
E_{\text{V}} &= -\frac{1}{3} J + J' - \frac{1}{3} B
\end{align*} \]

Using these energies we may now carry out analytic equalities to find the equations of the boundary lines between phases. The ground state partitioning of \((J/B, J'/B)\) space is shown in Fig. 14. The spin arrangements of the ground state phases are presented in Fig. 15. The spin arrangements for \(B < 0\) are obtained by interchanging open circles with closed circles. The two phases \(V-A\) and \(V-B\) both have the same values for \(N_+^1/N\), \(N_+^{(1)}/N\) and \(N_+^{(2)}/N\) and co-exist as the ground state for those values of \(J/B\) and \(J'/B\) in region \(V\) of Fig. 14.

**V.4. Discussion of the Ground State**

We interpret Fig. 14 as follows. Fixing the values of \(J\) and \(J'\), and hence \(\alpha\), constrains the phase point to move along a straight line of slope \(\alpha\), passing through the origin. \(B = 0\) puts this point infinitely far away from the origin along this line. As \(B\) increases in value the phase point moves inward and approaches the origin as \(B \to \infty\). When the phase point crosses a boundary line there occurs a change in the ground state phase. The magnetic field where this change takes place is found by inserting the values for \(J\) and \(J'\) in the boundary line equation. Thus, given the values of \(J\), \(J'\) and \(B\), we may predict the configuration
Figure 14. Partition of \((J/B, J'/B)\) Space for the Ground State of the Triangular Ising Model with \(nn\) and \(nnn\) Interactions
Figure 15. Ground State Spin Arrangements on the Triangular Lattice

Open circles represent spins aligned with the applied field. Closed circles indicate spins antiparallel to the field.
of the ground state.

Phase I is the ferromagnetic state with all spins aligned with the field. Both the spin-spin interactions and the magnetic field energetically favor the arrangement of complete alignment. We refer to phase II as antiferromagnetic in analogy with the square lattice since it exists with $J < 0$, $J' = 0$ and $0 < B < B_c = \gamma \mid J \mid$. Phase III we call "field dependent" due to its finite region of extent. For $B=0$ (i.e. infinitely far from the origin) the phase point may never reside in region III and hence phase III will not exist in the absence of a field. In this state each spin which is antialigned to the field is surrounded completely by field aligned nearest and next nearest neighbors. Phase IV is the "anisotropic antiferromagnetic" phase. We choose this name because the phase IV configuration was found to be the ground state of the zero field anisotropic nn triangular model with all interaction strengths less than zero. There is no counterpart to this phase in the ground state of the loose packed square lattice. Phase V admits two statistically equivalent ordered structures. Both of these may be termed "super-antiferromagnetic" due to the formation of three antiferromagnetic "super" lattices. That is, for both phases V-A and V-B, each of the three triangular sublattices possess the same order as phase II. To our knowledge, this is the first discussion of a close packed superantiferromagnetic
ground state.

For the case of $B=0$, $(J,J')$ space is partitioned into four regions as phase III is now nonexistent. All of the boundary lines pass through the origin. The spin orderings are all of a repeating unit no greater than $3\times3$ and possess only a small degeneracy (e.g. lattice rotation or translation and interchange of up and down spins). This small degeneracy leads us to conjecture that with the introduction of an arbitrarily weak nnn interaction $J'$ of either sign the nonzero entropy of equation (9) derived by Wannier for the nn problem with $J<0$, will vanish.

V.5. Results for Finite Temperature Behavior

We now study the finite temperature behavior of the nn and nnn triangular lattice starting with the case of zero magnetic field. Dalton and Wood have developed high temperature series expansions for $\Sigma_N$, and for the zero field susceptibility $\chi_0(T)$ for the interaction parameter values $J$, $J'>0$ and $B=0$. Using these series they looked at the dependence of the critical temperature $T_c$ on the interaction strength ratio $\alpha = J'/J$. Their findings indicate that the variation of the critical point is well represented by

$$T_c(\alpha) = T_c(0) \left( 1 + 1.35\alpha \right),$$

for $\alpha$ in the range $0 \leq \alpha \leq 1$. $T_c(0)$ is the critical temperature of the $J>0$ nn model. Our Monte Carlo calculations, with this set of interaction parameters, supports
such a linear dependence of $T_c$ on $\alpha$.

The series expansion analysis does not carry over to the case where $J < 0$. Recall, from section IV.2, that there is either no critical temperature or the critical temperature is zero for $J < 0$ and $\alpha = 0$ and that the ground state is very degenerate. We found however in section V.3-4 that phase II is the zero field ground state in the second quadrant of $J-J'$ space. This suggests that for $J < 0$, $J' > 0$ and $B=0$ there will be a transition to antiferromagnetic ordering at some finite temperature. To find the dependence of $T_c$ on $\alpha$ we examined the Monte Carlo data for various values of $\alpha$. Since there is no preferred direction when $B=0$, the ground state will be that of phase II shown in Fig. 15 or the state with all spins reversed. The spontaneous magnetization is therefore taken as $\langle \sum_{i=1}^{N} S_i^z \rangle$, and the zero field susceptibility is proportional to the fluctuation in the majority species of spins. For $\alpha < 0$ spontaneous magnetization was observed at finite temperatures. The zero field susceptibility per spin and spontaneous magnetization per spin for $\alpha = -0.2$ are shown in Fig. 16. The peak in the susceptibility identifies the critical temperature. Increasing $\alpha$ was found to shift the critical point to higher temperatures. The critical temperatures for various $\alpha$ are shown in Table 4. Assuming a linear dependence of the form $kT_c(\alpha)/|J| = m\alpha + b$, a standard linear regression data fit was performed. This
Figure 16. Zero Field Magnetic Susceptibility per Spin and Spontaneous Magnetization per Spin for $\alpha = -0.2 \ (J < 0, J' > 0)$
\[ \frac{\chi}{Nm^2} \]

\[ \frac{kT}{|J|} \]

\[ \frac{\langle M \rangle}{N} \]

\[ \frac{kT}{|J|} \]
Table 4. Zero Field Variation of the Critical Temperature with $\alpha < 0$ (i.e. $J < 0$, $J' > 0$)

| $\alpha$ | $kT_c(\alpha)/|J|$ |
|----------|-------------------|
| 0        | 0                 |
| -0.2     | 0.95              |
| -0.4     | 1.80              |
| -0.6     | 2.50              |
| -0.8     | 3.20              |
gave

\[ m = -3.975, \]

and

\[ b = 0.100. \]

The correlation coefficient \( r \), which is a measure of the goodness of the linear fit (i.e. \( r = 0 \) implies no correlation, \( r = 1 \) implies perfect correlation), came out to \( r = 0.9975 \) which strongly indicates linearity. The nonzero value of \( b \) implies a nonzero critical temperature for \( \alpha = 0 \) which therefore must be erroneous. This is probably a result of the inaccuracy in locating \( kT_\alpha /|J| \) when finite temperature increments are used on the computer. The increments were in steps of \( \Delta(kT_\alpha /|J|) = 0.05 \). Taking this inaccuracy into account we could safely say that if the dependence is of the form

\[ \frac{kT_\alpha(\alpha)}{|J|} = m\alpha, \quad m_i < 0 \]

then

\[ 3.93 \leq |m_i| \leq 5.00. \]

We now look at the effect of a nonzero magnetic field on the critical temperature. We specialize to the case \( \alpha = -0.2 \) which was chosen by Campbell and Schick\textsuperscript{26} in their study of this model. They state that this interaction strength ratio is appropriate (in the lattice gas model) to the interactions between helium atoms adsorbed on graphite. Using the same methods of detecting the transition temperature as we used for the nn model (see section
IV.4) the phase diagram was mapped out. This curve is shown in Fig. 17. The temperature axis is normalized to $T_c(B^*=0) = 0.95$. The zero temperature critical field is the same as for the nn model. The reason for this is that in phase II of Fig. 15 the configurational energy associated with the nnn pairs (i.e. the second term in equation (11)) is not changed when all of the field-antialigned spins are flipped. Thus only the nn antiferromagnetic interactions compete with the field giving $B_c(T=0) = 6|J|$, and $B^* = B/6|J|$. The error bars again denote the temperature increment used on the computer.

V.6. Discussion of Finite Temperature Behavior

Phase II is the antiferromagnetic ground state and exists for the nn model when $J < 0$ in the presence of a field. We now see that there is a transition to phase II at a finite temperature when $J < 0$ and $J' > 0$ whether or not there is an applied field. The presence of the ferromagnetic nnn interaction $J'$ enhances this antiferromagnetically ordered state. That this is true can be seen in Fig. 15 where we note that in phase II every nnn pair of spins is aligned. Thus $J' > 0$ fortifies this spin configuration. As $J'$ increases (i.e. $|\alpha|$ increases) this fortification becomes stronger and hence we would anticipate that the destruction of this order would occur at higher temperatures. This is consistent with the observed increase in $T_c$ with increasing $|\alpha|$ for zero field. For a given $\alpha < 0$
Figure 17. Phase Diagram of Nearest and Next Nearest Neighbor Triangular Ising Model with $\alpha = -0.2 \ (J < 0, J' > 0)$
and $B^*>0$ we would also expect that the critical temperature $T_c(B^*)$ would be larger than when $\alpha=0$. This is certainly the case for in Fig. 17 we find that the maximum value of $T_c(B^*)/T_c(0)$ is around 2.47 and if the phase diagram of the nn model (Fig. 13) were plotted on the same axes, the maximum would occur around 1.47. In both cases the maximum temperature of transition occurs for fields around $B^*\sim 0.5$. Our result $(T_c(B^*)/T_c(0))_{\text{max}} \approx 2.47$ is quite close to the value obtained by Campbell and Schick, which was 2.45. The Monte Carlo data showed that for fields $B^*\sim 0.5$ the magnetization per spin remained close to 1/3 even for temperatures slightly above $T_c$. In the language of the lattice gas this would mean that the chemical potential is rather insensitive to a change in temperature. At $T_c$ there appeared a spike in the Ising specific heat. Relabelling "spin down" with "site occupied" would result in the simulation of the lattice gas at density 1/3. Campbell and Schick observed a vertical drop discontinuity in the 1/3 density lattice gas specific heat. Experiments on the adsorption of helium on graphite do show a large peak in the specific heat at this density. However, as Campbell and Schick point out, the classical lattice gas model does not take into account the inherent quantum mechanical nature of the helium system which remains to be investigated.
CHAPTER VI

ANALYSIS OF THE CRITICAL FIELD GROUND STATE FOR THE ANTIFERROMAGNETIC NEAREST NEIGHBOR ISING MODEL

VI.1. Statement of the Problem

The methods of Bethe-Peierls, Kikuchi, constant coupling, Monte Carlo, and series expansions with Padé approximants have given us approximations to the antiferromagnetic phase diagram \(19, 20, 32, 36, 39, 50, 51\). This diagram represents the curve of thermodynamic singularities in the \(B-T\) plane enclosing the region of antiferromagnetic ordering. Where this curve intersects the magnetic field axis at zero temperature yields an extremely degenerate, highly singular behavior of the model. Away from these intersections the zero point entropy vanishes. We found in Chapter Four that the phase diagram of the triangular antiferromagnet displays two such singularities (see Fig. 13). The zero field intersection has been examined by Wannier\(^{17}\) who computed the ground state entropy of equation (9). In the case of \(B=0\), Danielian\(^{52, 53, 54}\) has shown that despite the degeneracy of the antiferromagnetic face-centered cubic (f.c.c.) model, there is no zero point entropy. His results show that the number of allowed ground states for an \(N\) spin f.c.c. lattice is \(\mathcal{E}^\text{DN}_N\),

96
where $D$ is a constant. It follows that in the limit $N \to \infty$ the entropy per spin tends to zero.

In this chapter we will investigate the ground state degeneracy at the nonzero critical magnetic field for several lattices. The associated configuration counting problem will be numerically solved in the limit $N \to \infty$ and the thermodynamic functions evaluated.

**VI.2. Ground State Degeneracy in the Critical Field - General**

Recalling the definitions from equations (12) we set $J'=0$ in equation (13) and write the energy of the nn model as

$$E = -\left(\frac{1}{2}J + B\right)N + 2(JN_+ + BN_-).$$

This is completely general and gives the Ising energy for any topology or dimension with coordination number $\mathcal{Z}$. We will consider the antiferromagnetic case so that $J < 0$.

Now the state in which the magnetic field $B > 0$ completely dominates is that state in which all spins are aligned with $B$ (the ferromagnetic state) and so $N_-=N_+=0$. The energy of this state is

$$E_F = -\left(\frac{1}{2}J + B\right)N.$$

In the antiferromagnetic ground state $J$ dominates so that any spin that is antialigned to $B$ is surrounded by nn spins which are aligned with $B$. Hence,

$$N_+ = \mathcal{Z} N_-.$$  \hspace{1cm} (14)
We remark here that this relation is certainly true for the antiferromagnetic state with $N_- = N/2$ for all loose packed lattices. In Chapter Four we found this to be the case for the close packed triangular lattice with $N_- = N/3$. However, the antiferromagnetic spin configurations of the close packed f.c.c. and h.c.p. lattices in the presence of a non-zero field are currently unknown. At this juncture we may then be departing from complete generality. The energy of the antiferromagnetic state is

$$E_A = -(\frac{3}{2}J + B)N + 2(\frac{3}{4}J + B)N_- .$$

Equating $E_F$ and $E_A$ gives the ground state critical field at which these two states become degenerate,

$$B_0 = \gamma |J| .$$

Notice that the perfect ferro- and antiferromagnetic states are not the only states which share this energy. For $B = B_0$ any configuration subject to the constraint of equation (14) has an energy which is independent of $N_-$ and is degenerate in this energy. The critical field ground state configurations may have any number of field-antialigned spins so long as each such spin has all of its neighbors aligned with the field. Herein lies a large degeneracy. The problem of counting the number of these states may be stated as follows: How many ways can one distribute downspins among $N$ sites such that each downspin is surrounded completely by upspins? The number of ways to accomplish
such a distribution for the periodic, two-dimensional square ($\mathcal{J}=4$) or triangular ($\mathcal{J}=6$) lattices with $N_- = 0, 1, 2, 3$ are listed below.

<table>
<thead>
<tr>
<th>$N_-$</th>
<th>Number of ways</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>$N$</td>
</tr>
<tr>
<td>2</td>
<td>$\frac{1}{2}N^2 - \frac{1}{2}(\mathcal{J}+1)N$</td>
</tr>
<tr>
<td>3</td>
<td>$\frac{1}{6}N^3 - \frac{1}{2}(\mathcal{J}+1)N^2 + \frac{1}{6}(2\mathcal{J}^2 + 7\mathcal{J} + 2)N$</td>
</tr>
</tbody>
</table>

The number of ways for $N_- = 3$ is evaluated as follows: there are $N$ ways to insert the first downspin. The placing of the second downspin gives us three cases: (1) $\mathcal{J}$ ways to place the second spin as a nnn of the first spin and thus $N-2\mathcal{J}$ ways to place the third spin; (2) $\mathcal{J}$ ways of placing the second spin as a third nearest neighbor of the first spin and thus $N-2\mathcal{J}-1$ ways to place the third spin; and (3) $N-3\mathcal{J}-1$ ways to place the second spin such that the first and second spin have no nearest neighbors in common and thus $N-2\mathcal{J}-2$ ways to place the third spin. The result is divided by $3!$ to account for the spin permutation.

Hence, for $N_- = 3$ the number of ways is

$$\frac{1}{3!}N \left[ \mathcal{J}(N-2\mathcal{J}) + \mathcal{J}(N-2\mathcal{J}-1) + (N-3\mathcal{J}-1)(N-2\mathcal{J}-2) \right] = \frac{1}{6}N^3 - \frac{1}{2}(\mathcal{J}+1)N^2 + \frac{1}{6}(2\mathcal{J}^2 + 7\mathcal{J} + 2)N$$

This method of counting becomes progressively more difficult with higher $N_-$, as the number of cases in which two or more of the downspins share common neighbors gets very
large. The final goal is to get the sum of the number of ways for \( N_\ell = 0, 1, \ldots, (N_\ell)_{\max} \) which is the degeneracy factor. The entropy is proportional to the log of the degeneracy factor. We now look at the one-dimensional model.

**VI.3. The One-dimensional Model**

Consider a one dimensional (\( \gamma = 2 \)) system of spins. In order to see what effect periodic boundary conditions have on the number of accessible states we present the following inductive arguments. We first relax the requirement of periodic boundary conditions and show that the number of critical field ground state configurations for a non-periodic linear system of \( m \) spins, \( m = 2, 3, \ldots \), is the \( m \)th element of the Fibonacci sequence generated by \( \{2, 3\} \). In this sequence each element is equal to the sum of the preceding two elements, \( \{2, 3, 5, 8, 13, 21, \ldots\} \). Let \( \omega'_m \) be the number of allowed \( m \)-spin configurations without periodic boundary conditions. For \( m = 2 \) and \( 3 \) we find \( \omega'_m \) by constructing the allowed states, these are

\[
\begin{align*}
\omega'_2 &= 3 \\
\omega'_3 &= 5
\end{align*}
\]

\[
\begin{align*}
\uparrow \uparrow & \quad \uparrow \downarrow & \quad \downarrow \uparrow \\
\uparrow \uparrow \uparrow & \quad \downarrow \uparrow \uparrow & \quad \uparrow \uparrow \downarrow & \quad \downarrow \uparrow \downarrow
\end{align*}
\]

By the induction hypothesis we suppose that \( \omega'_{m-2} \) and \( \omega'_{m-1} \) are the \( (m-2) \) and \( (m-1) \) elements respectively of the Fibonacci sequence described above. For an \( m \) spin system we decompose \( \omega'_m \) as

\[
\omega'_m = (\text{number of states with the last spin, } \sigma_m, \text{ aligned to field}) + (\text{number of states with } \sigma_m \text{ antialigned}).
\]
If $\sigma_m$ is aligned then there are no further restrictions imposed on the remaining $m-1$ spins, hence with $\sigma_m$ aligned there are $\omega^1_{m-1}$ allowed states. Now if $\sigma_m$ is antialigned to the field then $\sigma_{m-1}$ must be aligned leaving $m-2$ spins with no further restrictions giving $\omega^1_{m-2}$ states. Therefore

$$\omega^1_m = \omega^1_{m-1} + \omega^1_{m-2}.$$  

We now prove that the number of states forbidden by periodic boundary conditions for a $k$ spin system is equal to the number of states without periodic boundary conditions for a $k-4$ spin system. To prove this we note that the configurations forbidden exclusively by imposing periodicity are all of those with both $\sigma_1$ and $\sigma_k$ antialigned to the field. All of these states must have $\sigma_2$ and $\sigma_{k-1}$ aligned with the field. Deleting $\sigma_1, \sigma_2, \sigma_{k-1}$ and $\sigma_k$ leaves $k-4$ spins with no further restriction and thus $\omega^1_{k-4}$ possible configurations. Letting $\omega^1_m$ be the number of allowed configurations with periodic boundary conditions we then can write

$$\omega^1_m = \omega^1_m - \omega^1_{m-4}, \quad m > 4$$

$$= (\omega^1_{m-1} + \omega^1_{m-2}) - (\omega^1_{m-5} + \omega^1_{m-6})$$

$$= (\omega^1_{m-1} - \omega^1_{m-5}) + (\omega^1_{m-2} - \omega^1_{m-6})$$

$$= \omega^1_{m-1} + \omega^1_{m-2}.$$  

Thus with periodic boundary conditions, the number of allowed $m$-spin configurations in the critical field ground
state is found to be

\[ \omega_m = m^{th} \text{ element of } \{1,3,4,7,11,18,\ldots\} \]

We now formulate the problem with periodic boundary conditions in terms of a transfer matrix which will allow us to evaluate the entropy and magnetization. The formalism will then be extended to two and three dimensions. Realizing that for any allowed critical field ground state each upspin (direction of field) may have its right side neighbor in either state, and that each downspin must have its right side neighbor in a "spin up" state, we define the elements of a transfer matrix \( A \) as follows:

\[
\langle \sigma_i^- | A | \sigma_j^+ \rangle = \begin{cases} 
1 & \text{if } \sigma_i^- \text{ and } \sigma_j^+ \text{ are allowed in succession} \\
0 & \text{otherwise.}
\end{cases}
\]

The total number of allowed states for an \( m \) spin system is given by

\[
\omega_m = \sum_{\sigma_i = \pm 1} \cdots \sum_{\sigma_m = \pm 1} \langle \sigma_1^- | A | \sigma_2^+ \rangle \langle \sigma_2^- | A | \sigma_3^+ \rangle \cdots \langle \sigma_m^- | A | \sigma_1^+ \rangle.
\]

That this gives the correct number of states is seen from the fact that an unallowed set of spin values will have at least one zero matrix element occurring in the corresponding product, thus contributing nothing to the sum. After summing out \( \sigma_2, \ldots, \sigma_m \) we are left with

\[
\omega_m = \text{Trace } A^m = \lambda_1^m + \lambda_2^m,
\]
where $\lambda_1$ and $\lambda_2$ are the eigenvalues of $A$. This matrix has the form

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix},$$

with characteristic equation

$$\lambda^2 - \lambda - 1 = 0,$$

so

$$\lambda_1 = \frac{1 + \sqrt{5}}{2}, \quad \lambda_2 = \frac{1 - \sqrt{5}}{2}.$$

Using the Hamilton Cayley theorem we see that $A$ satisfies

$$A^2 = A + I,$$

hence

$$A^m = A^{m-1} + A^{m-2}, \quad m=3,4,\ldots$$

Taking the trace we get

$$\omega_m = \omega_{m-1} + \omega_{m-2}, \quad m=3,4,\ldots$$

$$\omega_1 = 1, \quad \omega_2 = 3,$$

retrieving our previous result. We now have a closed form expression

$$\omega_m = \left(\frac{1 + \sqrt{5}}{2}\right)^m + \left(\frac{1 - \sqrt{5}}{2}\right)^m, \quad m=1,2,\ldots$$

to generate any element of the desired Fibonacci sequence.

The entropy per spin is found from

$$\frac{S_m}{mk} = \ln \omega_m.$$

In the thermodynamic limit its value is

$$\lim_{m \to \infty} \frac{S_m}{mk} = \ln \left(\frac{1 + \sqrt{5}}{2}\right).$$

The average magnetization per spin is calculated from
\[ \langle M \rangle_m = \frac{1}{\omega_m} \sum_{\sigma_i} \cdots \sum_{\sigma_m} \left( \sum_{k=1}^{m} \sigma_k \right) \langle \sigma_1 | A | \sigma_2 \rangle \langle \sigma_2 | A | \sigma_3 \rangle \cdots \langle \sigma_m | A | \sigma_i \rangle \]

\[ = \frac{1}{\omega_m} \sum_{k=1}^{m} \sum_{\sigma_i} \cdots \sum_{\sigma_m} \langle \sigma_1 | A | \sigma_2 \rangle \cdots \langle \sigma_m | A | \sigma_i \rangle \]

\[ = \frac{m}{\omega_m} \sum_{\sigma_i} \cdots \sum_{\sigma_m} \langle \sigma_1 | A | \sigma_2 \rangle \cdots \langle \sigma_m | A | \sigma_i \rangle \]

\[ = \frac{m}{\omega_m} \sum_{\sigma_i} \langle \sigma_1 | A^m | \sigma_i \rangle \]

\[ \frac{\langle M \rangle_m}{m} = \frac{1}{\omega_m} \text{Trace} \, \sigma A^m , \]

where \( \sigma \) is the Pauli z spin matrix \( \sigma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \). To evaluate this it is convenient to note that

\[ A^m = \begin{pmatrix} a_{m+2} & a_{m+1} \\ a_{m+1} & a_m \end{pmatrix} \quad m=1,2,... \]

where \( a_k = k^{th} \) element of the Fibonacci sequence \( \{0,1,1,2,3,5,8,\ldots\} \).

This is easily proved by induction. Comparing the sequences \( \{a_m\}_{m=1}^{\infty} \) and \( \{\omega_m\}_{m=1}^{\infty} \) we find the relation

\[ \omega_m = a_{m+1} + 2a_m , \]

hence,

\[ \lim_{m \to \infty} \frac{\langle M \rangle_m}{m} = \lim_{m \to \infty} \frac{a_{m+1}}{\omega_m} = \frac{1}{1 + 2 \lim_{m \to \infty} \left( \frac{a_m}{a_{m+1}} \right)} . \]

The limit \( L = \lim_{m \to \infty} \left( \frac{a_m}{a_{m+1}} \right) \) is easily found from
\[
L = \lim_{m \to \infty} \left( \frac{a_m}{a_{m+1}} \right) = \frac{1}{1 + \lim_{m \to \infty} \left( \frac{a_{m-1}}{a_m} \right)} = \frac{1}{1 + L}
\]

\[
L = \frac{\sqrt{5} - 1}{2}.
\]

So the average magnetization per spin has the value

\[
\lim_{m \to \infty} \frac{\langle M \rangle_m}{m} = \frac{1}{\sqrt{5}},
\]

for the critical field ground state.

VI.4. Extension to Two and Three Dimensions

The above formalism can be extended to various topologies in two and three dimensions. As an example we carry out the details for the triangular lattice. Using the deformed lattice of Fig. 5(b) we consider a periodic array consisting of \(m \times n\) lattice as in the sketch on the right. The indexing of states is done columnwise by letting the states of the \(k^{th}\) column be indexed by \(\mu_k, \ k = 1, \ldots, n\). Each \(\mu_k\) can take on \(\omega_m\) values since an allowed column state is itself a periodic one-dimensional chain. The transfer matrix element \(\langle \mu_1 | A | \mu_{1+1} \rangle\) is unity if column state \(\mu_1\) can be directly followed by column state \(\mu_{1+1}\) without violating the critical field requirement, and is zero otherwise. This implies that the dimension of the transfer matrix describing an \(m \times n\) lattice is \(\omega_m\). We label this matrix \(A_m\). For the triangular lattice \(A_m\) is an asymmetric matrix.
reflecting the nonsymmetric diagonal bonding. For the square lattice $A_m$ would be symmetric. The total number of allowed states is

$$\Omega_{N=mn} = \sum \sum \langle \mu_1 | A | \mu_2 \rangle \langle \mu_2 | A | \mu_3 \rangle \cdots \langle \mu_n | A | \mu_\text{h} \rangle = \text{Trace} A_m^n.$$ 

The expression for the average magnetization per spin straightforwardly carries over to

$$\langle M \rangle_{N=mn} = \frac{1}{m \Omega_{N=mn}} \text{Trace} \Gamma A_m^n,$$

(15)

where the matrix $\Gamma$ is given by

$$\Gamma = \text{diag}(\vartheta_1, \vartheta_2, \ldots, \vartheta_{\omega_m})$$

and $\vartheta_k$ is the magnetization of a column in the state $k$, $k=1,2,\ldots,\omega_m$. The $\vartheta_k$'s take on values $m, m-2, m-4, \ldots$ down to 1 or 0 depending on whether $m$ is odd or even.

Since the dimension of the transfer matrix $A_m$ increases as $\omega_m$ analytic solution soon becomes unfeasible. In fact, for a lattice of $N=9\times n$ spins there are $5,776$ matrix elements to be found. Thus the generation of the matrix elements was computerized by constructing all $2^m$ possible column states in the computer memory and then selecting only those $\omega_m$ allowed states satisfying the critical field requirement. After this $\omega_m^2$ logical comparisons were performed between the allowed column states to obtain the matrix elements.

The approach to the thermodynamic limit is a double
limiting process, viz.

\[ \lim_{N \to \infty} \frac{\langle m \rangle_N}{N} = \lim_{m \to \infty} \lim_{n \to \infty} \frac{\text{Trace} \int A^n_m}{m \ \text{Trace} A^n_m} \]

To carry this out we fixed \( m \) to a certain value, the ratio of equation (15) was evaluated for \( n=2,3,\ldots,15 \). After this, \( m \) was increased and the procedure repeated. Values for \( m=2,3,\ldots,9 \) were examined. For fixed \( m \) the process converged nicely. The results for the particular case of \( m=6 \) are shown in Table 5. It is seen that stabilization to four place accuracy is achieved for \( n \geq 10 \), after which the values oscillated about the true value with decreasing amplitude. The convergence in \( m \) is displayed in Table 6. From this table we see that the value (to four decimal places) in the thermodynamic limit is attained for \( m \geq 8 \), and that the critical magnetization per spin of the triangular lattice is

\[ \lim_{N \to \infty} \frac{\langle m \rangle_N}{N} = 0.6751 \]

Before discussing the evaluation of the critical entropy we first establish upper and lower bounds. An upper bound is easily found since there are \( 2^N \) possible states, ignoring the critical field requirement, for an \( N \) spin system. Thus the entropy per spin must be less than \( k \ln 2 \). To find a lower bound we use the decomposition of the triangular lattice into three triangular sublattices shown in Fig. 5(a). Pick one sublattice \( \beta \) and distribute
Table 5. Average magnetization per spin for the triangular lattice critical field ground state with lattice width $m=6$ and length $n$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\langle M \rangle_N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.661539</td>
</tr>
<tr>
<td>3</td>
<td>0.665072</td>
</tr>
<tr>
<td>4</td>
<td>0.678192</td>
</tr>
<tr>
<td>5</td>
<td>0.675231</td>
</tr>
<tr>
<td>6</td>
<td>0.674754</td>
</tr>
<tr>
<td>7</td>
<td>0.675052</td>
</tr>
<tr>
<td>8</td>
<td>0.675100</td>
</tr>
<tr>
<td>9</td>
<td>0.675029</td>
</tr>
<tr>
<td>10</td>
<td>0.675041</td>
</tr>
<tr>
<td>11</td>
<td>0.675054</td>
</tr>
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<td>12</td>
<td>0.675043</td>
</tr>
<tr>
<td>13</td>
<td>0.675048</td>
</tr>
<tr>
<td>14</td>
<td>0.675046</td>
</tr>
<tr>
<td>15</td>
<td>0.675047</td>
</tr>
</tbody>
</table>

Table 6. Average magnetization per spin for increasing width $m$.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\langle M \rangle_N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.6115</td>
</tr>
<tr>
<td>3</td>
<td>0.6667</td>
</tr>
<tr>
<td>4</td>
<td>0.6788</td>
</tr>
<tr>
<td>5</td>
<td>0.6745</td>
</tr>
<tr>
<td>6</td>
<td>0.6751</td>
</tr>
<tr>
<td>7</td>
<td>0.6752</td>
</tr>
<tr>
<td>8</td>
<td>0.6751</td>
</tr>
<tr>
<td>9</td>
<td>0.6751</td>
</tr>
</tbody>
</table>
spins antialigned to the field over this sublattice, keeping the spins on the remaining two sublattices aligned with the field. There are $2^{N/3}$ ways to accomplish this. Clearly there are more critical field ground state configurations than can be found in this manner so that

$$\Omega_N > 3 \cdot 2^{N/3} - 2,$$

where the factor of 3 is due to the 3 choices of $\beta$, and the 2 is subtracted to keep from overcounting the case where there are no antialigned spins distributed. The entropy is therefore bounded by

$$\frac{1}{N} \ln(3 \cdot 2^{N/3} - 2) < \frac{S_N}{Nk} < \ln 2.$$

Passing to the thermodynamic limit gives

$$\frac{1}{3} \ln 2 = 0.2310 < \lim_{N \to \infty} \frac{S_N}{Nk} < 0.6931 = \ln 2.$$

We digress temporarily from discussing the triangular lattice to establish some results for the loose packed lattices. Since the loose packed lattices decompose into two sublattices the corresponding bounds are

$$2^{N/2} + 1 - 1 < \Omega_N < 2^N,$$

and in the $N \to \infty$ limit

$$\frac{1}{2} \ln 2 = 0.347 < \frac{S_N}{Nk} < 0.693 = \ln 2.$$

Furthermore, the degeneracy factors of the loose packed lattice may be ordered. Viewing the square $m \times n$ lattice as $n$ successive columns of $m$ spins it is clear that

$$\left[\Omega_m^{(1-D)}\right]^n > \Omega_{N=mn}^{(\text{square})}.$$
Similarly viewing the three dimensional simple cubic (s.c.) lattice as \( p \) successive planes of \( mn \) spins we have

\[
\left[ \bigcup_{mn}^{(\text{square})} \right] ^{p} > \bigcup_{N=pmn}^{(s.c.)}.
\]

Thus, for the loose packed lattices we see that the larger the coordination number, the smaller the entropy

\[
0.693 > \frac{S(1-D)}{Nk} > \frac{S^{(\text{square})}}{Nk} > \frac{S^{(s.c.)}}{Nk} > 0.347,
\] (16)

This ordering is reasonable since a larger coordination number imposes more restrictions on the state of an individual spin subject to the critical field requirement.

The transfer matrix evaluation of the entropy utilizes its extensive property. For sufficiently large \( N \) the total entropy should depend linearly on \( N \). We therefore plotted \( \ln \text{Trace} A_{m}^{n} \) as a function of \( n \) for \( n=8,9,\ldots,15 \). This was carried out for \( m=2,3,\ldots,9 \), and we found in each case that the data points fell on a straight line. The straight line of best fit was computed for each value of \( m \) using linear regression. This gave, for each \( m \), the slope \( s_{m} \), intercept \( b_{m} \) and the correlation coefficient \( r_{m} \). These fitted lines are shown in Fig. 18 and are meaningful only for \( n \geq 8 \). We found that \( r_{m}=1 \) for all \( m \) indicating perfect linear correlation. The results of this data fit are found in Table 7. Inspection of these values highly suggests that in general,

\[
s_{m} = \frac{m}{3}, \quad b_{m} = 0 .
\]

The entropy can now be obtained through the following steps...
Figure 18. In Trace $A_m^n$ vs. $n$ for $m=2,3,\ldots,9$. 
Table 7. Results of linear data fit for ln Trace $A_n^m$ vs. $n$ for $m=2,3,...,9$, slope $s_m$ and intercept $b_m$.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$s_m$</th>
<th>$s_m/m$</th>
<th>$b_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.7645</td>
<td>0.3823</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>1.005</td>
<td>0.3350</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>1.329</td>
<td>0.3323</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>1.667</td>
<td>0.3334</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>2.000</td>
<td>0.3333</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>2.333</td>
<td>0.3333</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>2.667</td>
<td>0.3333</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>3.000</td>
<td>0.3333</td>
<td>0</td>
</tr>
</tbody>
</table>
\[ \ln \Omega_{N=mn} = s_{mn} + b_m = \frac{mn}{3} = \frac{N}{3} \quad \text{N large} \]

\[ \lim_{N \to \infty} \frac{S_N}{Nk} = \frac{1}{3} \quad \text{(17)} \]

This result is quite close in value to Wannier's zero field result of equation (9) which gives 0.32306. The restriction in the case \( B=0 \) is that each triangle on the lattice must not have its three vertex spins all in the same state. We can find no equivalence between the counting problem at \( B=0 \) with that at \( B=0 \), and feel that the entropy is not the same in the two cases. The zero point entropy vanishes for any value of \( B \) other than 0 or \( B_c \).

For sufficiently large \( N \) the critical field counting problem is solved with \( e^{N/3} \) ways to accomplish the distribution. The relative increase in the number of configurations is

\[ \frac{\Omega_{N+1}}{\Omega_N} = e^{1/3} - 1 \]

The above calculations were carried out for the square and simple cubic lattices also. With these topologies, however, a relation as simple as equation (17) could not be found. The results of these calculations are presented in Table 8. The entropy values all fall within the bounds given previously and the ordering with respect to coordination number (inequality (16)) holds.

The values for the magnetization per spin can be cross
Table 8. Summarized results for various antiferromagnetic Ising models. Ground state in the critical magnetic field $B_c = \sqrt{J} |J|$

| Lattice                  | $E_c/N|J|$ | $\langle M \rangle/N$ | Monte Carlo | $S/Nk$   |
|--------------------------|------------|------------------------|-------------|---------|
| 1-Dimensional ($\mathcal{g} = 2$) | 1          | 0.4472                 | 0.4475      | 0.4812  |
| Square ($\mathcal{g} = 4$)   | 2          | 0.5470                 | 0.5472      | 0.4075  |
| Triangular ($\mathcal{g} = 6$) | 3          | 0.6751                 | 0.6753      | 0.3333  |
| Simple Cubic ($\mathcal{g} = 6$) | 3          | 0.6208*                | 0.5902      | 0.3563* |
| Body Centered Cubic ($\mathcal{g} = 8$) | 4          | ?                      | 0.5228      | ?       |

*Results have only been carried as far as $3 \times 4 \times (n \rightarrow \infty)$
checked with results obtained by Monte Carlo calculations. It is interesting to note the precision of the Monte Carlo calculations which gives the result to three figures. Previous attempts at entropy evaluation by the Monte Carlo method have resulted in failure and so were not executed. When applied to three dimensional lattices, the transfer matrix technique presented here should give accurate results. The indexing of states is plane-wise. Consequently, the number of planar states, and therefore the dimension of the transfer matrix, increases so rapidly that even present day computer facilities present an obstacle. Because of this limitation the computations for the simple cubic lattice were only carried as far as $3 \times 4 (n \to \infty)$, and the body centered cubic information is limited to the Monte Carlo data only$^{32}$.

We have presented, in this chapter, high precision results for the ground state of Ising models in the presence of a magnetic field, and have given an algorithm for the solution of a certain class of restricted counting problems. With the advance of computer hardware these results can be extended and applied to other problems in statistical physics.


BIBLIOGRAPHY (CONTINUED)


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